UvA DL Notebooks

Release v1.2

Phillip Lippe

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GUIDES

Course website: https://uvadlc.github.io/
Course edition: DL1 - Fall 2023, DL2 - Spring 2023, Being kept up to date
Repository: https://github.com/phlippe/uvadlc_notebooks
Recordings: YouTube Playlist
Author: Phillip Lippe

Note: Interested in learning JAX? We have recently started translating the notebooks from PyTorch to JAX+Flax. Check out our new notebooks in the tab *Deep Learning 1 (JAX+Flax)* to learn how you can speedup the model training with JAX!

For this year's course edition, we created a series of Jupyter notebooks that are designed to help you understanding the "theory" from the lectures by seeing corresponding implementations. We will visit various topics such as optimization techniques, transformers, graph neural networks, and more (for a full list, see below). The notebooks are there to help you understand the material and teach you details of the PyTorch framework, including PyTorch Lightning. Further, we provide one-to-one translations of the notebooks to JAX+Flax as alternative framework.

The notebooks are presented in the first hour of every group tutorial session. During the tutorial sessions, we will present the content and explain the implementation of the notebooks. You can decide yourself whether you just want to look at the filled notebook, want to try it yourself, or code along during the practical session. The notebooks are not directly part of any mandatory assignments on which you would be graded or similarly. However, we encourage you to get familiar with the notebooks and experiment or extend them yourself. Further, the content presented will be relevant for the graded assignment and exam.

The tutorials have been integrated as official tutorials of PyTorch Lightning. Thus, you can also view them in their documentation.

CHAPTER

ONE

SCHEDULE (DEEP LEARNING 1, EDITION 2023)

Date	Notebook
Tuesday, 31. October 2023, 15:00-16:00	Tutorial 2: Introduction to PyTorch
Tuesday, 7. November 2023, 15:00-16:00	Tutorial 3: Activation functions
Tuesday, 14. November 2023, 15:00-16:00	Tutorial 4: Optimization and Initialization
Tuesday, 21. November 2023, 15:00-16:00	Tutorial 5: Inception, ResNet and DenseNet
Tuesday, 28. November 2023, 15:00-16:00	Tutorial 6: Transformers and Multi-Head Attention
Tuesday, 5. December 2023, 15:00-16:00	Tutorial 7: Graph Neural Networks
Tuesday, 12. December 2023, 15:00-16:00	Tutorial 17: Self-Supervised Contrastive Learning with SimCLR

CHAPTER

TWO

HOW TO RUN THE NOTEBOOKS

On this website, you will find the notebooks exported into a HTML format so that you can read them from whatever device you prefer. However, we suggest that you also give them a try and run them yourself. There are three main ways of running the notebooks we recommend:

- **Locally on CPU**: All notebooks are stored on the github repository that also builds this website. You can find them here: https://github.com/phlippe/uvadlc_notebooks/tree/master/docs/tutorial_notebooks. The notebooks are designed so that you can execute them on common laptops without the necessity of a GPU. We provide pretrained models that are automatically downloaded when running the notebooks, or can manually be downloaded from this Google Drive. The required disk space for the pretrained models and datasets is less than 1GB. To ensure that you have all the right python packages installed, we provide a conda environment in the same repository (choose the CPU or GPU version depending on your system).
- **Google Colab**: If you prefer to run the notebooks on a different platform than your own computer, or want to experiment with GPU support, we recommend using Google Colab. Each notebook on this documentation website has a badge with a link to open it on Google Colab. Remember to enable GPU support before running the notebook (`Runtime -> Change runtime type`). Each notebook can be executed independently, and doesn't require you to connect your Google Drive or similar. However, when closing the session, changes might be lost if you don't save it to your local computer or have copied the notebook to your Google Drive beforehand.
- **Snellius cluster**: If you want to train your own (larger) neural networks based on the notebooks, you can make use of the Snellius cluster. However, this is only suggested if you really want to train a new model, and use the other two options to go through the discussion and analysis of the models. Snellius might not allow you with your student account to run Jupyter notebooks directly on the gpu partition. Instead, you can first convert the notebooks to a script using `jupyter nbconvert --to script ...ipynb`, and then start a job on Snellius for running the script. A few advices when running on Snellius:
  - Disable the tqdm statements in the notebook. Otherwise your slurm output file might overflow and be several MB large. In PyTorch Lightning, you can do this by setting `enable_progress_bar=False` in the trainer.
  - Comment out the matplotlib plotting statements, or change `plt.show()` to `plt.savefig(...)`.

CHAPTER

THREE

TUTORIAL-LECTURE ALIGNMENT

We will discuss 7 of the tutorials in the course, spread across lectures to cover something from every area. You can align the tutorials with the lectures based on their topics. The list of tutorials in the Deep Learning 1 course is:

- Guide 1: Working with the Snellius cluster
- Tutorial 2: Introduction to PyTorch
- Tutorial 3: Activation functions
- Tutorial 4: Optimization and Initialization
- Tutorial 5: Inception, ResNet and DenseNet
- Tutorial 6: Transformers and Multi-Head Attention
- Tutorial 7: Graph Neural Networks
- Tutorial 8: Deep Energy Models
- Tutorial 9: Autoencoders
- Tutorial 10: Adversarial attacks
- Tutorial 11: Normalizing Flows on image modeling
- Tutorial 12: Autoregressive Image Modeling
- Tutorial 15: Vision Transformers
- Tutorial 16: Meta Learning - Learning to Learn
- Tutorial 17: Self-Supervised Contrastive Learning with SimCLR

CHAPTER

FOUR

FEEDBACK, QUESTIONS OR CONTRIBUTIONS

This is the first time we present these tutorials during the Deep Learning course. As with any other project, small bugs and issues are expected. We appreciate any feedback from students, whether it is about a spelling mistake, implementation bug, or suggestions for improvements/additions to the notebooks. Please use the following link to submit feedback, or feel free to reach out to me directly per mail (p dot lippe at uva dot nl), or grab me during any TA session.

If you find the tutorials helpful and would like to cite them, you can use the following bibtex:

```
@misc{lippe2024uvadlc,
   title        = {{UvA Deep Learning Tutorials}},
   author       = {Phillip Lippe},
   year         = 2024,
   howpublished = {\url{https://uvadlc-notebooks.readthedocs.io/en/latest/}}
}
```

4.1 Guide 1: Working with the Snellius cluster

Authors: Phillip Lippe, Danilo de Goede

This tutorial explains how to work with the Snellius cluster for the Deep Learning course at the University of Amsterdam. Every student will receive an account to have resources for training deep neural networks and get familiar with working on a cluster. It is recommended to have listened to the presentation by the SURFsara team or the TA team before going through this tutorial. Further, this tutorial assumes that you are familiar with using the terminal in Linux. If not, a crash course can be found here.

4.1.1 The Snellius cluster

The following section gives a quick introduction to the Snellius cluster, and how it is build up. A detailed description of the system can be found in the SURFsara user guide.

What is a cluster computer?

(Disclaimer: the following paragraph is an adapted version of the HPC user guide. Credits: SURFsara team)

You can imagine a cluster computer as a collection of regular computers (known as nodes), tied together with network cables that are similar to the network cables in your home or office (see the figure below - credit: SURFsara team). Each node has its own CPU, memory and disk space, in addition to which they generally have access to a shared file system. On a cluster computer, you can run hundreds of computational tasks simultaneously.

Interacting with a cluster computer is different from a normal computer. Normal computers are mostly used interactively, i.e. you type a command or click with your mouse, and your computer instantly responds by e.g. running a program. Cluster computers are mostly used non-interactively.

A cluster computer such as Snellius mainly has two types of nodes: login nodes and batch nodes. You connect to Snellius through the login node (see next section). This is an interactive node: similar to your own PC, it immediately responds to the commands you type. There are only a few login nodes on a cluster computer, and you only use them for light tasks: adjusting your code, preparing your input data, writing job scripts, etc. Since the login nodes are only meant for light tasks, many users can be on the same login node at the same time. To prevent users from over-using the login node, any command that takes longer than 15 minutes will be killed.

Your 'big' calculations such a neural network training will be done on the batch nodes. These perform what is known as batch jobs. A batch job is essentially a recipe of commands (put together in a job script) that you want the computer to execute. Calculations on the batch nodes are not performed right away. Instead, you submit your job script to the job queue. As soon as sufficient resources (i.e. batch nodes) are available for your job, the system will take your job from the queue, and send it to the batch nodes for execution.

Architecture of Snellius

A visual description of the Snellius architecture can be found below (figure credit - SURFsara team). You can connect to any login node of Snellius to interact with the system. Over the login nodes, you have access to the shared file system across nodes. The one you will mainly interact is `/home` where you can store your code, data, etc. You can access your files from any login node, as well as any compute node. You have a maximum disk space of 200GB which should be sufficient for the DL course.

You do not directly interact with any compute node. Instead, you can request computational resources with a job script, and Snellius will assign a compute node to this job using a SLURM job scheduler. If all computational resources are occupied, your job will be placed in a queue, and scheduled when resources are available.

Snellius has multiple sets of compute nodes with different computational resources, also called partitions. The one we will use for the Deep Learning course is called `gpu`, and provides us compute nodes with the following resources:

Processor	CPU Cores	RAM Memory	GPUs
Platinum 8360Y (2.4GHz)	72	480GB	4x NVIDIA A100, 40 GB HBM2

These computational resources are more than sufficient for the assignments in this course. For a job, we usually only use a single GPU from a compute node, meaning that we would also use 1/4th of the other resources (18 CPU cores, 120GB RAM). The scheduler of Snellius will assign multiple jobs to the same node if its computational resources are not exhausted yet, thus not wasting any if we only use a single GPU.

4.1.2 First steps

After discussing the general architecture of Snellius, we are ready to discuss the practical aspects of how to use the Snellius cluster.

REMINDER: When you first receive your login data for Snellius, make sure to go to the user portal and change the password.

How to connect to Snellius

You can login to Snellius's login nodes using a secure shell (SSH):

```
ssh -X scur____@snellius.surf.nl
```

Replace `scur___` by your username. You will be connected to one of its login nodes, and have the view of a standard Linux system in your home directory. Note that you should only use the login node as an interface, and not as compute unit. Do not run any trainings on this node, as it will be killed after 15 minutes, and slows down the communication with Snellius for everyone. Instead, Snellius uses a SLURM scheduler to handle computational expensive jobs (see below).

If you want to transfer files between Snellius and your local computer, you can use standard Unix commands such as `scp` or `rsync`, GitHub, or graphical interfaces such as FileZilla (use port 22 in FileZilla) or WinSCP (for Windows PC). Note that using GitHub on Snellius requires adding the SSH key from Snellius to your GitHub account.

A copy operation from Snellius to your local computer with `rsync`, started from your local computer, could look as follows:

```
rsync -av scur___@snellius.surf.nl:~/source destination
```

Replace `scur___` by your username, `source` by the directory/file on Snellius you want to copy on your local machine, and `destination` by the directory/file it should be copied to. Note that `source` is referenced from your home directory on Snellius. If you want to copy a file from your local computer to Snellius, use:

```
rsync -av source scur___@snellius.surf.nl:~/destination
```

Again, replace `source` with the directory/file on your local computer you want to copy to Snellius, and `destination` by the directory/file it should be copied to.

Modules

Snellius uses modules to provide you various pre-installed software. This includes simple Python, but also the NVIDIA libraries CUDA and cuDNN that can be necessary to access GPUs. However, for our course, we only need the Anaconda module:

```
module load 2022
module load Anaconda3/2022.05
```

Note: Loading `Anaconda3/2022.05` may result in a warning about the potential for corruption in the user environment due to mixing Conda and module environments. Since we are only loading the `2022` and `Anaconda3/2022.05` modules, you can safely ignore this message. However, be aware that loading additional modules could cause issues.

Install the environment

To run the Deep Learning assignments and other code like the notebooks on Snellius, you need to install the provided environment for Snellius (`dl2023_gpu.yml`). You can either download it locally and copy it to your Snellius account via rsync or scp as described before, or simply clone the practicals github on Snellius:

```
git clone https://github.com/uvadlc/uvadlc_practicals_2023.git
```

Snellius provides an Anaconda module, which you can load via `module load Anaconda3/2022.05` as mentioned before (remember to load the `2022` module beforehand). We recommend installing the package via a job file since the installation can take 20-30 minutes, and any command on the login node will be killed without warning after 15 minutes.

To do that, save the following content into a file called `install_environment.job` in your home directory:

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gpus=1
#SBATCH --job-name=InstallEnvironment
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=18
#SBATCH --time=04:00:00
#SBATCH --output=slurm_output_%A.out

module purge
module load 2022
module load Anaconda3/2022.05

cd $HOME/uvadlc_practicals_2023/
conda env create -f dl2023_gpu.yml
```

You can use e.g. `nano` to do that. If the environment file is not in the cloned repository or you haven't cloned the repo, change the cd statement to the directory where it is stored. Once the file is saved, start the job with the command `sbatch install_environment.job`. The installation process is started on a compute node with a time limit of 4 hours, which should be sufficiently long. Let's look at the next section to understand what we have actually done here with respect to 'job files'.

Trouble shooting

If the installation via job file does not work, try to install the environment with the following command from the login node after navigating to the directory the environment file is in:

```
conda env create -f dl2023_gpu.yml
```

Note that the jobs on the login node on Snellius are limited to 15 minutes. This is often not enough to install the full environment. If the installation command is killed, you can simply restart it. If you get the error that a package is corrupted, go to `/home/scur___/.conda/pkgs/` under your home directory and remove the directory of the corrupted package. If you get the error that the environment dl2023 already exists, go to `/home/scur___/.conda/envs/`, and remove the folder 'dl2023'.

If you experience issues with the Anaconda module, you can also install Anaconda yourself (download link) or ask your TA for help.

Verifying the installation

When the installation process is completed, you can check if the process was successful by activating your environment on the login node via `source activate dl2023` (remember to have loaded the anaconda module beforehand), and starting a python console with executing `python`. It should say `Python 3.11.5 | packaged by conda-forge`. If you see a different python version, you might not have activated the environment correctly.

In the python console, try to import pytorch via `import torch` and check the version: `torch.__version__`. It should say `2.1.0`. Finally, check whether PyTorch can access the GPU: `torch.cuda.is_available()`. Note that in most cases, this will return `False` because the login nodes on Snellius do not have GPUs. However, when you run the same command on a compute node (i.e., when submitting a job with `sbatch`), it should return `True`. To do this, save the following content into a file called `check_environment.job`, and start the job using `sbatch check_environment.job`.

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gpus=1
#SBATCH --job-name=CheckEnvironment
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=18
#SBATCH --time=00:05:00
#SBATCH --output=slurm_output_%A.out

module purge
module load 2022
module load Anaconda3/2022.05

# Activate your environment
source activate dl2023
# Check whether the GPU is available
srun python -uc "import torch; print('GPU available?', torch.cuda.is_available())"
```

If the resulting slurm output contains the line `GPU available? True`, you should be all set.

4.1.3 The SLURM scheduler

Snellius relies on a SLURM scheduler to organize the jobs on the cluster. When logging into Snellius, you cannot just start a python script with your training, but instead submit a job to the scheduler. The scheduler will decide when and on which node to run your job, based on the number of nodes available and other jobs submitted.

Job files

We provide a template for a job file that you can use on Snellius. Create a file with any name you like, for example `template.job`, and start the job by executing the command `sbatch template.job`.

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gpus=1
#SBATCH --job-name=ExampleJob
#SBATCH --ntasks=1
```

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```
#SBATCH --cpus-per-task=18
#SBATCH --time=04:00:00
#SBATCH --output=slurm_output_%A.out

module purge
module load 2022
module load Anaconda3/2022.05

# Your job starts in the directory where you call sbatch
cd $HOME/...
# Activate your environment
source activate dl2023
# Run your code
srun python -u ...
```

Job arguments

You might have to change the `#SBATCH` arguments depending on your needs. We describe the arguments below:

- `partition`: The partition of Snellius on which you want to run your job. As a student, you only have access to the partition gpu, which provides you nodes with NVIDIA A100 GPUs (40GB).
- `gpus`: Number of GPUs you request from the nodes. You can select up to four GPUs with your account, but if you haven't designed your code to explicitly run on multiple GPUs, please use only one GPU (so no need to change what we have above).
- `job-name`: Name of the job to pop up when you list your jobs with squeue (see below).
- `ntasks`: Number of tasks to run with the job. In our case, we will always use 1 task.
- `cpus-per-task`: Number of CPUs you request from the nodes. The gpu partition restricts you to max. 18 CPUs per job/GPU.
- `time`: Estimated time your job needs to finish. It is no problem if your job finishes earlier than the specified time. However, if your job takes longer, it will be instantaneously killed after the specified time. Still, don't specify unnecessarily long times as this causes your job to be scheduled later (you need to wait longer in the queue if other people also want to use the cluster). A good rule of thumb is to specify ~20% more than what you would expect.
- `output`: Output file to which the slurm output should be written. The tag "%A" is automatically replaced by the job ID. Note that if you specify the output file to be in a directory that does not exist, no output file will be created.

SLURM allows you to specify many more arguments, but the ones above are the important ones for us. If you are interested in a full list, see here.

Scratch

If you work with a lot of data, or a larger dataset, it is advised to copy your data to the `/scratch-local/<username>` directory of the node. Otherwise, the read/write operation might become a bottleneck of your job. To do this, simply use your copy operation of choice (`cp`, `rsync`, ...), and copy the data to the directory `$TMPDIR` (which is set `/scratch-local/<username>` by default). You should add this command to your job file before calling `srun ...`. Remember to point to this data when you are running your code. If you have a dataset that can be downloaded, you can also directly download it to the scratch (can sometimes be faster than copying). In case you also write something on the scratch, you need to copy it back to your home directory before finishing the job.

Edit Dec. 6, 2021: Due to internal changes to the SURF filesystems, it is required to **use the scratch for any dataset** such as CIFAR10. In PyTorch, the CIFAR10 dataset is structured into multiple large batches (usually 5), and only that batch is loaded which is currently needed. This is why during training, it requires a lot of reading operations on the disk which can slow down your training and constitutes a challenge when hundreds of students share the same filesystem. Hence, you have to use the scratch for such datasets. For most parts in the assignment, you can do this by specifying `--data_dir $TMPDIR` on the python command in your job file (check if the argument parser has this argument, otherwise you can add it yourself). This will download the dataset to the scratch and only load it from there. We recommend using this approach also for future course editions.

Starting and organizing jobs

To start a job, you simply have to run `sbatch jobfile` where you replace `jobfile` by the filename of the job. Note that no specific file postfix like `.job` is necessary for the job (you can use `.txt` or any other you prefer). After your job has been submitted, it will be first placed into a waiting queue. The SLURM scheduler decides when to start your job based on the time of your job, all other jobs currently running or waiting, and available nodes.

Besides `sbatch`, you can interact with the SLURM scheduler via the following commands:

- `squeue`: Lists all jobs you have currently submitted to Snellius. See the slurm documentation for details.
- `scancel JOBID`: Cancels and stops a job, independent of whether it is running or pending. The job ID can be found using `squeue`, and is printed when submitting the job via `sbatch`.
- `scontrol show job JOBID`: Shows additional information of a specific job, like the estimated start time.

Interactive sessions

As alternative to running jobs via `sbatch`, you can request an interactive job session. In this format, you gain access to the node via the terminal/command line, and can interact with it as you would have connected via ssh directly to this compute node. Hence, you can debug your script much easier and have faster respond time. However, please keep in mind the following two disadvantages: 1. If you happen to disconnect from Snellius because of an instable connection or your computer going in stand-by mode, the job will be canceled. 2. Your job is not automatically terminated when your script has finished running, but you have to manually kill the job once you are done. If you forget it, you block the compute node for other students and waste credits that UvA payed for Hence, only use interactive sessions for short jobs/scripts, for example, if you want to debug whether your script starts running and train the model. Do not use interactive session to train a model for a long time.

In order to start an interactive session on Snellius, you can use `srun` with the same input parameters as for the job file. For example:

```
srun --partition=gpu --gpus=1 --ntasks=1 --cpus-per-task=18 --time=00:10:00 --pty bash -i
```

This will start an interactive session with a GPU for 10 minutes. Once resources have been allocated, you will see in your terminal that you are now on one of the compute nodes, for example, `r32n5`. As a first step, you need to load the modules (`module load 2022; module load Anaconda3/2022.05`) and activate your conda environment. Then, you are ready to run your script.

4.1.4 Troubleshooting

It can happen that you encounter some issues when interacting with Snellius. A short FAQ is provided on the SURFSara website, and here we provide a list of common questions/situations we have experienced from past students.

Snellius is refusing connection

It can occasionally happen that Snellius refuses the connection when you try to ssh into it. If this happens, you can try to use the Pulse Secure UvA VPN before connecting to Snellius. If this still does not work, then the connection issue is likely not on your side. The problem often resolves after 2-3 hours, and Snellius let's you login after it again. If the problem doesn't resolve after couple of hours, please contact your TA, and eventually the SURFSara helpdesk.

Slurm output file missing

If a job of yours is running, but no slurm output file is created, check whether the path to the output file specified in your job file actually exists. If the specified file points to a non-existing directory, no output file will be created. Note that this is not an issue by default, but you are running your job "blind" without seeing the stdout or stderr channels.

Slurm output file is empty for a long time

The slurm output file can lag behind in showing the outputs of your running job. If your job is running for couple of minutes and you would have expected a few print statements to have happened, try to flush your stdout stream (how to flush the output in python).

All my jobs are pending

With your student account, the SLURM scheduler restricts you to run only two jobs in parallel at a time. However, you can still queue more jobs that will run in sequence. This is done because with more than 200 students, Snellius could get crowded very fast if we don't guarantee a fair share of resources. If all of your jobs are pending, you can check the reason for pending in the last column of `squeue`. All reasons are listed in the squeue documentation under *JOB REASON CODES*. The following ones are common:

- `Priority`: There are other jobs on Snellius with a higher priority that are also waiting to be run. This means you just have to be patient.
- `QOSResourceLimit`: The job is requesting more resources than allowed. Check your job file as you are only allowed to have at max. 4 GPUs, 72 CPU cores and 480GB RAM.
- `Resources`: All nodes on Snellius are currently busy, yours will be scheduled soon.

You can also see the estimated start time of a job by running `scontrol show job JOBID`. However, note that this is the "worst case" scenario for the current number of submitted jobs, as in if all currently running jobs would need their maximum runtime. At the same time, if more people would submit their job with higher priority, yours can fall back in the queue and get a later start time.

PyTorch or other packages cannot be imported

If you run a job and see the python error message in the slurm output file that a package is missing although you have installed it in the environment, there are two things to check. Firstly, make sure to not have the environment activated on the login node when submitting the job. This can lead to an error in the anaconda module such that packages are not found on the compute node. Secondly, check that you activate the environment correctly. To verify that the correct python version is used, you can add the command `which python` before your training file. This prints out the path of the python that will be used, in which you should see the anaconda version in the dl2023 environment.

My job runs very slow

If your job executes your script much slower than you expect, check for two things: (1) have you requested a GPU and are you using it, and (2) are you using the scratch for your dataset? Not using the scratch for your dataset can create a significant communication bottleneck, especially if multiple students do it at the same time. Make sure to download or copy your dataset to the scratch and load it from there.

I am not able to use Snellius at all

If during the course, there will be major issues with Snellius (e.g. cluster goes into maintenance for a long time, issues with the filesystem, etc.), you can make use of GoogleColab, as we do already for all notebook tutorials here. All assignments do not necessarily require large amount of compute, and can often be comfortably trained on a GPU provided by GoogleColab. For an introduction to GoogleColab, see this tutorial.

4.1.5 Advanced topics

Password-less login

Typing your password every time you connect to Snellius can become annoying. To enable a safe, password-less connection, you can add your public ssh key to the SURFsara user portal. Next time you login from your machine to Snellius, it will only check the ssh key and not ask you for the password anymore.

Remote development with VSCode or PyCharm

The common workflow with clusters is that you first code locally and test your implementation on short runs on the CPU or evt. a local GPU, then sync your code to the cluster (e.g. via git), and finally run the full training/process on a compute node of the cluster. If you prefer to directly code on Snellius, you can do so via remote connections in tools like VSCode or PyCharm. Essentially, these IDEs can connect via SSH to Snellius, so that it looks to you like you code locally, but all code you are editing is directly saved on Snellius. Note though that to run your code, you still need to create a job script and submit it via SLURM. The login nodes, on which these IDEs connect you to, are not meant for debugging or running code. Any process that takes longer than 15 minutes will be killed (this can sometimes also include the SSH connection of VSCode/PyCharm). For more details on remote development and how to set it up, see the SURFsara documentation on VSCode and PyCharm.

Tracking GPU stats

If you are curious whether you use the GPU to its full capacity, you can monitor its utilization as follows. First, you submit your job and check its job ID via `squeue` or the ID that has been printed out after submitting the job via `sbatch`. Next, you can log into the node via `slurm_jobmonitor [jobid]` where you need your job ID. This gives you an interactive view on the node. Finally, you can run `nvtop` to track the GPU utilization. More details can be found here.

Job Arrays

You might come into the situation where you need to run a hyperparameter search over multiple values, and don't want to write an endless number of job scripts. A much more elegant solution is a job array. Job arrays are created with two files: a job file, and a hyperparameter file. The job file will start multiple sub-jobs that each use a different set of hyperparameters, as specified in the hyperparameter file. In the job file, you need to add the argument `#SBATCH --array=...`. The argument specifies how many sub-jobs you want to start, how many to run in parallel (at maximum), and which lines to use from the hyperparameter file. For example, if we specify `#SBATCH --array=1-16%8`, this means that we start 16 jobs using the lines 1 to 16 in the hyperparameter file, and running at maximum 8 jobs in parallel at the same time. Note that the number of parallel jobs is there to limit yourself from blocking the whole cluster. However, with your student accounts, you will not be able to run more than 1 job in parallel anyways. The template job file `array_job.job` looks slightly different than the one we had before. The slurm output file is specified using `%A` and `%a`. `%A` is being automatically replaced with the job ID, while `%a` is the index of the job within the array (so 1 to 16 in our example above). Below, we also added a block for creating a checkpoint folder for the job array, and copying the job file including hyperparameters to that folder. This is good practice for ensuring reproducibility. Finally, in the training call, we specify the path checkpoint path (make sure to have implemented this argument in your argparse) with the addition of `experiment_${SLURM_ARRAY_TASK_ID}` which is a sub-folder in the checkpoint directory with the sub-job ID (1 to 16 in the example). The next line, `$(head -$SLURM_ARRAY_TASK_ID $HPARAMS_FILE | tail -1)`, copies the N-th line of the hyperparameter file to this job file, and hence submits the hyperparameter arguments to the training file.

File `array_job.job`:

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gpus=1
#SBATCH --job-name=ExampleArrayJob
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=18
#SBATCH --time=04:00:00
#SBATCH --array=1-16%8
#SBATCH --output=slurm_array_testing_%A_%a.out

module purge
module load 2022
module load Anaconda3/2022.05

# Your job starts in the directory where you call sbatch
cd $HOME/...
# Activate your environment
source activate ...

# Good practice: define your directory where to save the models, and copy the job file␣
↪to it
```

(continues on next page)

(continued from previous page)

```
JOB_FILE=$HOME/.../array_job.job
HPARAMS_FILE=$HOME/.../array_job_hyperparameters.txt
CHECKPOINTDIR=$HOME/.../checkpoints/array_job_${SLURM_ARRAY_JOB_ID}

mkdir $CHECKPOINTDIR
rsync $HPARAMS_FILE $CHECKPOINTDIR/
rsync $JOB_FILE $CHECKPOINTDIR/

# Run your code
srun python -u train.py \
               --checkpoint_path $CHECKPOINTDIR/experiment_${SLURM_ARRAY_TASK_ID} \
               $(head -$SLURM_ARRAY_TASK_ID $HPARAMS_FILE | tail -1)
```

The hyperparameter file is nothing else than a text file in which each line denotes one set of hyperparameters for which you want to run an experiment. There is no specific order in which you need to put the lines, and you can extend the lines with as many hyperparameter arguments as you want.

File `array_job_hyperparameters.txt`:

```
--seed 42 --learning_rate 1e-3
--seed 43 --learning_rate 1e-3
--seed 44 --learning_rate 1e-3
--seed 45 --learning_rate 1e-3
--seed 42 --learning_rate 2e-3
--seed 43 --learning_rate 2e-3
--seed 44 --learning_rate 2e-3
--seed 45 --learning_rate 2e-3
--seed 42 --learning_rate 4e-3
--seed 43 --learning_rate 4e-3
--seed 44 --learning_rate 4e-3
--seed 45 --learning_rate 4e-3
--seed 42 --learning_rate 1e-2
--seed 43 --learning_rate 1e-2
--seed 44 --learning_rate 1e-2
--seed 45 --learning_rate 1e-2
```

Additional links

Many more details on Snellius, SLURM, etc. can be found on the SURFSara wiki, as well as a different perspective on the aspects we have discussed in this tutorial. A (non-exclusive) list of useful links:

- How to use SSH on Windows/Mac/Linux, authenticate with SSH keys instead of passwords, and transfer files with SCP or FTP
- How to write your own job script
- How to submit/cancel a job
- How to see a job's status in the queue
- How to do remote development with VSCode and PyCharm
- Snellius hardware and file systems
- Snellius usage and accounting

4.2 Guide 2: Research projects with PyTorch

- Based on some feedback I got, we will try to summarize tips and tricks on how to setup and structure large research projects in PyTorch, such as your Master Thesis
- Feel free to contribute yourself if you have good ideas

4.2.1 Setup

Framework

- Choosing the right framework can be essential. If you have standard optimization loops of a single forward pass and return a loss, consider going with PyTorch Lightning. It reduces the code overhead a lot and allows to easily scale your model to multiple GPUs and/or nodes if needed. Nonetheless, if you expect that you need to change the default training procedure quite a bit, consider going with plain PyTorch and write your own framework. It might take more time initially, but makes edits in the optimization procedure easier.
- For an own framework, the following can be used as an example setup:

```
general/
|    train.py
|    task.py
|    mutils.py
layers/
experiments/
|    task1/
|         train.py
|         task.py
|         eval.py
|         dataset.py
|    task2/
|         train.py
|         task.py
|         eval.py
|         dataset.py
```

- The `general/train.py` file summarizes the default operations every model needs (training loop, loading/saving model, setting up model, etc.). If you use PyTorch Lightning, this reduces to a train file per task, and only needs the specification of the trainer object.
- The `general/task.py` file summarizes a template for the specific parts you have to do for a task (training step, validation step, etc.). If you use PyTorch Lightning, this would be the definition of the Lightning Module.
- The `layers/models` folder contains the code for specifying the `nn.Modules` you use for setting up the model.
- The `experiments` folder contains the task-specific code. Each task has its own `train.py` for specifying the argument parser, setting up the model, etc., while the `task.py` overwrites the template in `general/task.py`. The `eval.py` file should has as input a checkpoint directory of a trained model, and should evaluate this model on the test dataset. Finally, the file `dataset.py` contains all parts you need for setting up the dataset.
- Note that this template assumes that you might have multiple different tasks and multiple different models. If you have a simpler setup, you can inherently shrink the template together.

Argument parser

- It is a good practice to use argument parsers for specifying hyperparameters. Argument parsers allow you to call a training like `python train.py --learning ... --seed ... --hidden_size ...` etc.
- If you have multiple models to choose from, you will have multiple set of hyperparameters. A good summary on that can be found in the PyTorch Lightning documentation without the need of using Lightning. In essence, you can define a static method for each model that returns a parser for its specific hyperparameters. This makes your code cleaner and easier to define new tasks without copying the whole argument parser.
- To ensure reproducibility (more details below), it is recommended to save the arguments as a json file or similar in your checkpoint folder.

4.2.2 Hyperparameter search

- In general, hyperparameter search is all about experience. Once you have trained a lot of models, it will become easier for you to pick reasonable first-guess hyperparameters.
- The first approach to take is to look at related work to your model, and see what others have used as hyperparameters for similar models. This will help you to get started with a reasonable choice.
- Hyperparameter search can be expensive. Thus, try to do the search on shallow models first before scaling them up.
- Although a large grid search is the best way to get the optimum out of your model, it is often not reasonable to run. Try to group hyperparameters, and optimize each group one by one.

Toolkits

- PyTorch Lightning provides a lot of useful tricks and toolkits on hyperparameter searching, such as:
  - Learning rate finder that plots the learning rate vs loss for a few initial batches, and helps you to choose a reasonable learning rate.
  - Autoscaling batch sizes which finds the largest possible batch size given your GPU (helpful if you have very deep, large models, and it is obvious you need the largest batch size possible).
- For comparing multiple hyperparameter configurations, you can add them to TensorBoard. This is a clean way of comparing multiple runs. If interested, a blog on this can be found here.
- There are multiple libraries that support you in automatic hyperparameter search. A good overview for those in PyTorch can be found here.

Reproducibility

- Everything is about reproducibility. Make sure you can reproduce any training you do with the same random values, batches, etc. You will come to a point where you have tried a lot of different approaches, but none were able to improve upon one of your previous runs. When you try to run the model again with the best hyperparameters, you don't want to have a bad surprise (believe me, enough people have this issue, and it might also happen to you). Hence, before starting any grid search, make sure you are able to reproduce runs. Run two jobs in parallel on Snellius with the same hyperparams, seeds, etc., and if you don't get the exact same results, stop and try to fix it before anything else.
- Another fact about reproducibility is that saving and loading a model works without any problems. Make sure before a long training that you are able to load a saved model from the disk, and achieve the exact same test score as you had during training.

- Snellius executes the job you intended to. Further, hyperparameters should be stored in a separate file in your checkpoint directory, whether saved by PyTorch Lightning or yourself.
- When running a job, copy the job file automatically to your checkpoint folder. This improves reproducibility by ensuring you have the exact running comment ready.
- Besides the slurm output file, create a output file in which you store the best training, validation and test score. This helps you when you want to quickly compare multiple models or create statistics of your results.
- If you want to be on the safe side and use git, you can even print/save the hash of the git commit you are currently on, and any changes you had made to the files. An example of how to do this can be found here.

Seeds

- DL models are inherently noisy, and no two runs are the same if you don't ensure a deterministic execution. Before running a grid search, try to get a feeling of how noisy your experiments might be. The more noise you expect compared to your result scale, the more versions of your model you need to run to get a statistically significant difference between settings.
- After finishing the grid search, run another model of the best configuration with a new seed. If the score is still the best, take the model. If not, consider running a few more seeds for the top k models in your grid search. Otherwise, you risk taking a suboptimal model, which was just lucky to be the best for a specific seed.

Learning rate

- The learning rate is an important parameter, which depends on the optimizer, the model, and many more other hyperparameters.
- A usual good starting point is 0.1 for SGD, and 1e-3 for Adam.
- The deeper the model is, the lower the learning rate usually should be. For instance, Transformer models usually apply learning rates of 1e-5 to 1e-4 for Adam.
- The lower your batch, the lower the learning rate should be. Consider using gradient accumulation if your batch size is getting too small (PyTorch Lightning supports this, see here).
- Consider using the PyTorch Lightning learning rate finder toolkit for an initial good guess.

LR scheduler

- Similarly to the learning rate, the scheduler to apply again depends on the classifier and model.
- For image classifiers and SGD as optimizer, the multi-step LR scheduler has shown to be good choice.
- Models trained with Adam commonly use a smooth exponential decay in the learning rate or a cosine-like scheduler.
- For Transformers: remember to use a learning rate warmup. The cosine scheduler is often used for decaying the learning rate afterwards, but can also be replaced by an exponential decay.

Regularization

- Regularization is important in networks if you see a significantly higher training performance than test performance.
- The regularization parameters all interact with each other, and hence must be tuned together. The most commonly used regularization techniques are:
  - Weight decay
  - Dropout
  - Augmentation
- Dropout is usually a good idea as it is applicable to most architectures and has shown to effectively reduce overfitting.
- If you want to use weight decay in Adam, remember to use `torch.optim.AdamW` instead of `torch.optim.Adam`.

Domain specific regularization

- There are couple of regularization techniques that depend on your input data/domain. The most common include:
  - Computer Vision: image augmentation like horizontal flip, rotation, scale-and-crop, color distortion, gaussian noise, etc.
  - NLP: input dropout of whole words.
  - Graphs: dropping edges, nodes, or part of the features of all nodes.

Grid search with SLURM

- SLURM supports you to do a grid search with job arrays. We have discussed job arrays in the Snellius guide.
- Job arrays allow you to start N jobs in parallel, each running with slightly different settings.
- It is effectively the same as creating N job files and calling N times `sbatch ...`, but this can become annoying and is messy at some point.

PyTorch Lightning

Writing the job arrays can be sometimes annoying, and hence it is advised to write a script that can automatically generate the hyperparameter files if you have to do this often enough (for instance, by adding the seed parameter 4 times to each other hyperparam config). However, if you are using PyTorch Lightning, you can directly create a job array file. The documentation for this can be found here.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.3 Guide 3: Debugging in PyTorch

When you start learning PyTorch, it is expected that you hit bugs and errors. To help you debug your code, we will summarize the most common mistakes in this guide, explain why they happen, and how you can solve them.

4.3.1 My model is underperforming

Situation: Your model is not reaching the performance that it should, but PyTorch is not telling you why that happens. These errors are the most annoying bugs since those can be hard to debug. Nonetheless, there are couple of things you can check. If none of these solve the problem for you, one of us TAs will help you debug your code more in detail.

Softmax, CrossEntropyLoss and NLLLoss

The most common mistake is the mismatch between loss function and output activation function. The loss module `nn.CrossEntropyLoss` in PyTorch performs two operations: `nn.LogSoftmax` and `nn.NLLLoss`. Hence, the input to this loss module should be the output of your last linear layer. **Do not apply a softmax before the Cross-Entropy loss**. Otherwise, PyTorch will apply a log-softmax on your softmax outputs, which will significantly worsen the performance, and give you headaches.

If you use the loss module `nn.NLLLoss`, you need to apply the log-softmax yourself. **NLLLoss requires log-probabilities, not plain probabilities.** Hence, make sure to apply `nn.LogSoftmax` or `nn.functional.log_softmax`, and **not** `nn.Softmax`.

Softmax over the right dimension

Pay attention to the dimension you apply your softmax over. Usually, this is the last dimension of your output tensor, which you can identify with e.g. `nn.Softmax(dim=-1)`. If you mix up the dimension, your model ends up with random predictions.

Categorical data and Embedding

Categorical data, as for example language characters or the datasets you are given in assignment 2, require special care. Data like language characters 'a', 'b', 'c' etc. are usually represented as integers 0, 1, 2, etc. **Do not use integers as input for categorical data.** If you would enter those integers as inputs to the model, two problems arise.

1. You bias the model to see relations where there are none. In the language example above, the model would think that 'a' is closer to 'b' than to 'o', although 'a' and 'o' are both vocals, and the closeness of 'a' and 'b' does not necessarily say anything about their usage.
2. If you have many categories, you will have input values between 0 and >50. The model will have a hard time separating all those >50 categories without blending over some. Hence, the model loses a lot of information although this is not necessary.

The much better option in the case of categorical data is to use one-hot vectors, or embeddings. A one-hot vector represents each category by a vector of 0s, with one index being 1. This makes the model's life much easier as it can distinguish between the categories in a very simple manner (if feature !=0, it is a specific category). Alternatively, you can learn an embedding with the help of `nn.Embedding`. The inputs to this module are:

- `num_embeddings` which is the number of different categories you have in your input data (in case of language characters, something like 26 as you have 'a' to 'z')

- `embedding_dim` which is the number of features you want to represent each category with. If you use the embedding directly as input to an LSTM or RNN, a good rule of thumb is to use 1/4 - 1/2 of your hidden size inside the LSTM.
- `padding_idx` which would allow you to assign a specific index for the padding symbol. Can be skipped if you do not use "-1" as padding index.

The embedding feature vectors are randomly initialized from $\mathcal{N}(0, 1)$. **Do not overwrite this init by Kaiming, Xavier or similar.** The used standard deviation is 1 because the initialization, activation functions etc. have been designed to have a input standard deviation of 1. Example usage of the embedding module:

[1]:
```
import torch
import torch.nn as nn
# Create 5 embedding vectors each with 32 features
embedding = nn.Embedding(num_embeddings=5,
                         embedding_dim=32)

# Example integer input
input_tensor = torch.LongTensor([[0, 4], [2, 3], [0, 1]])

# Get embeddings
embed_vectors = embedding(input_tensor)

print("Input shape:", input_tensor.shape)
print("Output shape:", embed_vectors.shape)
print("Example features:\n", embed_vectors[:,:,:2])
```

```
Input shape: torch.Size([3, 2])
Output shape: torch.Size([3, 2, 32])
Example features:
 tensor([[[ 0.0504, -0.2422],
         [ 0.0342,  0.2217]],

        [[ 2.7813, -0.3641],
         [-0.0981,  0.4069]],

        [[ 0.0504, -0.2422],
         [ 1.2092,  0.1760]]], grad_fn=<SliceBackward>)
```

The `nn.Embedding` object is a module like a linear layer or convolution. Thus, it needs to be defined in the `__init__` function of your higher-level module. **Do not create the Embedding module in the forward pass.** Otherwise, you will have different embeddings every time you run the model, and hence, your model is not able to learn.

Time dimension in nn.LSTM

By default, PyTorch's `nn.LSTM` module assumes the input to be sorted as `[seq_len, batch_size, input_size]`. Make sure that you do not confuse the sequence length and batch dimension. The LSTM would still run without an error, but will give you wrong results. If you want to change this behavior to accepting an input shape of `[batch_size, seq_len, input_size]`, you can specify the argument `batch_first=True` when creating the LSTM object. Have a closer look at the documentation for details.

Hidden shape mismatch

If you perform matrix multiplications and have a shape mismatch between two matrices, PyTorch will complain and throw an error. However, there are also situations where PyTorch does not throw an error because the misaligned dimensions have (unluckily) the same size. For instance, imagine you have a weight matrix of size $d_{in} \times d_{out}$. If you take the input x of size $B \times d_{in}$ (B being the batch dimension), and in your hyperparameter setting, $B = d_{in}$, you can end up performing the matrix multiplication over the wrong dimension while PyTorch is not detecting it. **Test your code with multiple, different batch sizes to prevent shape misalignments with the batch dimension.**

Training and Evaluation switch

In PyTorch, a module and/or neural network has two modes: training and evaluation. You switch between them using `model.eval()` and `model.train()`. The modes decide for instance whether to apply dropout or not, and how to handle the forward of Batch Normalization. However, a common mistake is to forget to set your model back into training mode after evaluation. **Make sure to set your model back to train mode after validation.** In case your model does not contain dropout, BatchNorm or similar modules, this might not affect your performance.

Parameter handling

As you might know from the PyTorch Tutorial, PyTorch supports hierarchical usage of `nn.Modules`. One module can contain another module, which can again contain a module, and so on. When you call `.parameters()` on a module, PyTorch looks for all modules inside the module to also add their parameters to the highest-level module's parameter. However, **PyTorch does not detect parameters of modules in lists, dicts or similar structures.** If you have a list of modules, make sure to put them into a `nn.ModuleList` or `nn.Sequential` object. Parameters of modules inside those containers are detected. Similarly, for dictionaries, you can use `nn.ModuleDict`.

Parameters and ".to(device)"

To push your model and/or data to GPU, you can use `.to(device)` where `device` is an device object or string ("cpu" for CPU-only machines, and "cuda"/"cuda:0" for GPUs). However, **do not call ``.to(device)`` during parameter init**. If you define a parameter like `self.W = nn.Parameter(torch.Tensor(64, 128)).to(device)`, your model will not register the parameter on GPU because the ".to" operator creates a new Tensor. Parameters, nonetheless, have to be leaf Tensors, hence your parameters will not be recognized (corresponding GitHub issue). It is much better practice to only call `.to(device)` once *after* finishing the init of the model, and not inside the model.

My model runs fine on CPU, but gets NaN loss on GPU

If this is the case, you likely have the bug of parameters and `.to(device)` as explained above.

Initialization

Initializing the parameters of your model correctly is very important (see Tutorial 4 for details on this). Initializing parameters with a standard normal distribution is not a good practice and often fails. It can occasionally work for very shallow networks, but don't risk it! **Think about your initialization, and use proper methods like Kaiming or Xavier.**

Zero-grad in optimizers

Remember to call optimizer.zero_grad() before doing loss.backward(). If you do not reset the gradients for all parameters before performing backpropagation, your gradients will be added to those from the previous batch. Hence, your gradients end up to be not the ones you intended them to be.

Weight decay and Adam

Adam is known to have a different implementation of weight decay in many frameworks than you would expect. Specifically, the weight decay is usually added as gradients **before** determining the adaptive learning rate, and hence scaling up the weight decay for parameters with low gradient norms. Details on this problem, which is actually shared across most common DL frameworks, can be found here. In PyTorch, you can use the desired version of weight decay in Adam using `torch.optim.AdamW` (identical to `torch.optim.Adam` besides the weight decay implementation).

Check your metric calculation

This might sound a bit stupid but check your metric calculation twice or more often before doubting yourself or your model. Metrics like accuracy are easy to calculate, but it is as easy to add a bug into the code. For instance, check that you are averaging over the batch dimension and not accidentally over the class dimension or any other.

My bits per dimension score is very low

If you obtain a very low bits per dimension score for likelihood-based generative models after already the first iteration, the calculation might not be fully correct. Specifically, the negative log likelihood input to the bpd-metric function is expected to be the **sum** of the individual pixel's log likelihood of an image, not the mean. The mean is taken inside the bpd function.

4.3.2 PyTorch throws an error

These errors are the easier bugs to correct because PyTorch actually talks to you about what is wrong. Until these are not solved, you probably cannot train your model.

Trying to backward through the graph a second time, specify retain_graph=True

This error occurs if you re-use a tensor from the computation graph of the previous batch. This should usually not happen. Make sure to not keep tensors across batches if not strictly necessary. Example where this issue can occur: when implementing your own LSTM, make sure that the initial hidden state is a constant zero tensor, and not the last hidden state of the previous batch.

Size mismatch

This usually occurs if your dimension of the input to a module does not match the specified input dimension of the weight tensor, like in a linear layer. Make sure to have specified the correct dimensions. Usually, a good way to debug this is to print the shape of the input tensor before every layer you call.

If this happens for a matrix multiplication you have implemented, print the shapes of both matrices, and try to figure out over which dimension the matrix multiplication should actually have been performed, and over which PyTorch currently does it.

Device mismatch

You might sometimes see a mistake such as: `Runtime Error: Input type (torch.FloatTensor) dand weigh type (torch.cuda.FloatTensor) should be on the same device`. This error indicates that the input data is on CPU, while your weights are on the GPU. Make sure that all data is on the same device. This is usually the GPU as it support acceleration for both training and testing.

4.3.3 Good practices

There are many good practices in PyTorch. We try to add a few below that might make your life easier. Another list of good practices can be found here.

Use nn.Sequential and nn.ModuleList

If you have a model with a lot of layers, you might want to summarize them into a `nn.Sequential` or `nn.ModuleList` object. In the forward pass, you only need to call the sequential, or iterate through the module list. A MLP can be implemented as follows:

[2]:
```
class MLP(nn.Module):

    def __init__(self, input_dims=64, hidden_dims=[128,256], output_dims=10):
        super().__init__()
        hidden_dims = [input_dims] + hidden_dims
        layers = []
        for idx in range(len(hidden_dims)-1):
            layers += [
                nn.Linear(hidden_dims[i], hidden_dims[i+1]),
                nn.ReLU(inplace=True)
            ]
        self.layers = nn.Sequential(*layers)

    def forward(self, x):
        return self.layers(x)
```

In-place activation functions

Some activation functions like `nn.ReLU` or `nn.LeakyReLU` have the argument `inplace`. By default it is `False`, but it is recommended to set it to `True` in neural networks. What it does is that the forward pass overwrites the original values of the input with the new output. This option is only available for activation functions where we do not need to know the original input for backpropagation. For instance, in ReLU, the values that are set to zero, have a gradient of zero independent of its specific input value. In-place operation can save a bit of memory, especially if you have large feature maps.

Create modules for repeating blocks

In deep neural networks, you usually have blocks that are repeatedly added to the model. If those blocks require a more complex forward function than just `x = layer(x)`, it is recommended to implement them in a separate module. For example, a ResNet consists of multiple ResNet blocks with a residual connection. The ResNet blocks apply a small neural network, and add the output back to the input. It is better to implement this dynamic in a separate `nn.Module` class to keep the main model class small and clear.

Stack layers/weights with same input

If you have multiple linear layers or convolutions that have the same input, you can stack them together to increase efficiency. Suppose we have two layers on x: $y_1 = W_1x + b_1$, $y_2 = W_2x + b_2$. While you could implement it by two linear layers, you can get the exact same neural network by stacking the two layers into one. The single layer is more efficient as this represents a single matrix operation instead of two for the GPU, and hence we can parallelize the computation. An example is shown below:

[3]:
```
x = torch.randn(2, 10)

# Implementation of separate layers:
y1_layer = nn.Linear(10, 20)
y2_layer = nn.Linear(10, 30)
y1 = y1_layer(x)
y2 = y2_layer(x)

# Implementation of a stacked layer:
y_layer = nn.Linear(10, 50)
y = y_layer(x)
y1, y2 = y[:,:20], y[:,20:50]
```

If you implement the linear layer manually, you need to stack the weight and bias tensor accordingly. Note that you should change your initialization for the stacked case if necessary. If your initialization depends on the output size of a layer (as for example in Xavier), you would get a different standard deviation for initialization in the two implementations. Still, if your initialization solely depends on the input dimension (e.g. Kaiming), no change is necessary. An example case where this stacking can be beneficial is LSTMs as all four gates use the exact same input.

Use loss functions on logits

Classification loss functions such as Binary Cross Entropy have two versions in PyTorch: with and without logits. It is recommended and good practice to use the loss functions on logits. This is because it is numerically more stable and prevents any instabilities when your model is very wrong in its prediction. If you do not use the logit loss functions, you might run into problems when the model predicts very high or low values that are not correct. In BCE, you will then encounter a log over a value very close to 0. If you are lucky, you just get a very high number (and your model might still diverge because of this), or actually end up with NaN values.

Make use of torch.nn.functional

You do not always need modules. Many methods that do not have parameters are implemented as both modules and functions (e.g. log-softmax/softmax, binary cross entropy, etc.). If you need a softmax but do not have a `nn.Sequential` where you could add it to, the function option `F.softmax(...,dim=...)` is cleaner than defining a separate module first.

Clip gradient norms

Another good training practice is to clip gradient norms. Even if you set a high threshold, it can stop your model from diverging, even when it gets very high losses. While in MLPs not strictly necessary, RNNs, Transformers, and likelihood models can often benefit from gradient norm clipping. In PyTorch, you can use it via `torch.nn.utils.clip_grad_norm_(...)` (remember to call it after `loss.backward()` but before `optimizer.step()`). In PyTorch Lightning, you can set the clipping norm via `gradient_clip_val=...` in the Trainer.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.4 Guide 4: Research Projects with JAX

Filled notebook:
Author: Phillip Lippe

This guide summarizes some tips, tricks and practices that are useful when working with JAX for a research project. In my opinion, one key aspect that JAX is missing compared to PyTorch is a framework like PyTorch Lightning that can massively reduce code overhead while still being flexible enough for supporting almost any model/task. Although there exist such libraries for certain common tasks, like trax or scenic (attention-based CV), I have not come across one so far which was sufficiently flexible for my research. Hence, in this guide, we build a simpler version of a PyTorch Lightning trainer, that summarizes all training, logging, etc. behavior that we need for almost any model, and allows training various models with much fewer lines than from scratch. Moreover, we implement some simple examples to showcase possible training structures, and underline its flexibility by performing automatic hyperparameter tuning with Optuna. Since this guide will be about code structures, it is more code-heavy than the other guides and can also be run in Google Colab if preferred.

First, let's import some standard libraries. For this guide, we will use the data loading functionalities of PyTorch, but one could also use the TensorFlow dataset API. Additionally, we integrate loggers from PyTorch Lightning since they support a flexible API and have most popular logging application implemented (e.g. TensorBoard, Weights and Biases).

[1]:
```
# Standard libraries
import os
import sys
from typing import Any, Sequence, Optional, Tuple, Iterator, Dict, Callable, Union
import json
import time
from tqdm.auto import tqdm
import numpy as np
from copy import copy
from glob import glob
from collections import defaultdict

# JAX/Flax
# If you run this code on Colab, remember to install flax and optax
# !pip install --quiet --upgrade flax optax
import jax
import jax.numpy as jnp
from jax import random
from flax import linen as nn
from flax.training import train_state, checkpoints
import optax

# PyTorch for data loading
import torch
import torch.utils.data as data

# Logging with Tensorboard or Weights and Biases
# If you run this code on Colab, remember to install pytorch_lightning
# !pip install --quiet --upgrade pytorch_lightning
from pytorch_lightning.loggers import TensorBoardLogger, WandbLogger
```

4.4.1 Trainer module for JAX with Flax

As seen in previous tutorials, Flax gives us already some basic functionalities for training models. One part of it is the `TrainState`, which holds the model parameters and optimizers, and allows updating it. However, there might be more model aspects that we would like to add to the `TrainState`. For instance, if a model uses Batch Normalization as in Tutorial 5, we need to keep the batch statistics in order to evaluate the models on a test dataset. Furthermore, many models contain stochastic elements such as dropout or sampling in generative models (e.g. Normalizing Flows). Thus, we extend the `TrainState` class from Flax to also include the batch statistics as `batch_stats` and a pseudo-random number generation `rng`. Note that if models do not require these elements, they can simply be `None` without breaking our code.

[2]:
```
class TrainState(train_state.TrainState):
    # A simple extension of TrainState to also include batch statistics
    # If a model has no batch statistics, it is None
    batch_stats : Any = None
    # You can further extend the TrainState by any additional part here
    # For example, rng to keep for init, dropout, etc.
    rng : Any = None
```

Now we already come to the main part of this guide: the Trainer module for JAX/Flax. The shown module here is not meant to be the 'one and only' way of doing it, and is more meant as showcasing one possible option of obtaining a Lightning-like API in JAX. The module can easily be extended by more functionalities, depending on what is needed/preferred by the individual users.

First let's make a list of functionalities that we would want the Trainer module to include:

- **Logging**: For basically all usecases and models, we want to log our hyperparameters, training/validation performance, and model checkpoints. For the second point, we can make use of PyTorch Lightning's logger classes like `TensorBoardLogger` and `WandbLogger`. For the model checkpoints, we use `flax.checkpoints`. In terms of flexibility, the trainer should support arbitrary sets of hyperparameters, since different models may require different hyperparameters. Similarly, it should be easy to add new metrics for logging, like accuracy for classification or intersection over union for segmentation.
  - Implemented in: `init_logger`, `save_model`, `load_model`, `save_metrics`
- **Model state initialization**: In contrast to PyTorch, JAX separates the model itself from the learnable parameters. Creating a set of parameters for a model requires some boiler-template code, like creating a PRNG for the parameter generation and creating an initial `TrainState`. At the same time, we need to allow overwriting the `model.init` code, since different architectures will have different input arguments for the forward pass (e.g. models with dropout require a dropout-PRNG).
  - Implemented in: `init_model`, `run_model_init`, `print_tabulate`
- **Optimizer initialization**: Following with the parameter initialization, we also need to create an optimizer and its eventual parameters (e.g. momentum and adaptive learning rate parameters in Adam). Since most models use a similar set of optimizers (SGD or Adam) and extra functionalities like gradient clipping and learning rate scheduling, we can write a template method that creates an optimizers based on some hyperparameters. However, it should be possible to overwrite this method if very specific optimizer settings/learning rate schedulers are needed. Since some schedulers require information about the overall number of training iterations, we create the optimizer right before starting the training.
  - Implemented in: `init_optimizer`
- **Training loop**: Most models follow a similar training procedure where we train a model for several epoch on the training dataset, and evaluate it in between on the validation dataset. If a model is better than all previous models, we want to save its weight for loading them potentially later. Importantly, however, each model will have a very different training and validation step. Thus, similarly to PyTorch Lightning, we expect that an inheriting Trainer module has to define a training step function and evaluation step function, that can be jitted and used in the training loop. This is implemented in the function `train_model`, `train_epoch`, `eval_model`, `create_functions`, `create_jitted_functions`. Additional aspects to consider include:
  - Whether a model is better than the previous ones or not depends on the task at hand. For example, classification models are usually compared by their accuracy, trying to achieve the maximum value, while regression models aim for the lowest loss. Hence, we need a flexible API to support different ways of comparing models and finding the best one. Implemented in: `is_new_model_better`
  - Within the training loop, we might want to perform additional operations, like logging reconstruction examples of an autoencoder after every few epochs. To do so, PyTorch Lightning provides functions that are called at different stages during training, which we can similarly integrate in our Trainer module. Implemented in: `on_training_start`, `on_training_epoch_end`, `on_validation_epoch_end`
  - Depending on whether we run the model on a cluster with no display or on our local machine, we might want to see progress bars that track the training progress. Hence, the Trainer module should have to switch to enable or disable these progress bars. Implemented in: `tracker`
- **Inference**: After we have finished training, we might want to load a model at a later time and perform inference experiments with it. For example, in Tutorial 9, we use a trained autoencoder for an image search engine. To support this, two functionalities are needed: (1) loading a model from disk, including its hyperparameters (i.e. the

function `load_from_checkpoint` in PyTorch Lightning), and (2) binding parameters to a model to reduce code overhead. Both parts can be implemented in our Trainer module.

- Implemented in: `load_from_checkpoint`, `bind_model`

With these requirements in mind, let's finally implement the module. Note that it is a considerably long code cell since we want to support many different settings. We recommend to take some time to go through the code and understand how all the elements are implemented, and how one can extend it depending on their own needs.

[3]:
```
class TrainerModule:

    def __init__(self,
                 model_class : nn.Module,
                 model_hparams : Dict[str, Any],
                 optimizer_hparams : Dict[str, Any],
                 exmp_input : Any,
                 seed : int = 42,
                 logger_params : Dict[str, Any] = None,
                 enable_progress_bar : bool = True,
                 debug : bool = False,
                 check_val_every_n_epoch : int = 1,
                 **kwargs):
        """
        A basic Trainer module summarizing most common training functionalities
        like logging, model initialization, training loop, etc.

        Atributes:
          model_class: The class of the model that should be trained.
          model_hparams: A dictionary of all hyperparameters of the model. Is
            used as input to the model when created.
          optimizer_hparams: A dictionary of all hyperparameters of the optimizer.
            Used during initialization of the optimizer.
          exmp_input: Input to the model for initialization and tabulate.
          seed: Seed to initialize PRNG.
          logger_params: A dictionary containing the specification of the logger.
          enable_progress_bar: If False, no progress bar is shown.
          debug: If True, no jitting is applied. Can be helpful for debugging.
          check_val_every_n_epoch: The frequency with which the model is evaluated
            on the validation set.
        """
        super().__init__()
        self.model_class = model_class
        self.model_hparams = model_hparams
        self.optimizer_hparams = optimizer_hparams
        self.enable_progress_bar = enable_progress_bar
        self.debug = debug
        self.seed = seed
        self.check_val_every_n_epoch = check_val_every_n_epoch
        self.exmp_input = exmp_input
        # Set of hyperparameters to save
        self.config = {
            'model_class': model_class.__name__,
            'model_hparams': model_hparams,
            'optimizer_hparams': optimizer_hparams,
```

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```
            'logger_params': logger_params,
            'enable_progress_bar': self.enable_progress_bar,
            'debug': self.debug,
            'check_val_every_n_epoch': check_val_every_n_epoch,
            'seed': self.seed
        }
        self.config.update(kwargs)
        # Create empty model. Note: no parameters yet
        self.model = self.model_class(**self.model_hparams)
        self.print_tabulate(exmp_input)
        # Init trainer parts
        self.init_logger(logger_params)
        self.create_jitted_functions()
        self.init_model(exmp_input)

    def init_logger(self,
                    logger_params : Optional[Dict] = None):
        """
        Initializes a logger and creates a logging directory.

        Args:
          logger_params: A dictionary containing the specification of the logger.
        """
        if logger_params is None:
            logger_params = dict()
        # Determine logging directory
        log_dir = logger_params.get('log_dir', None)
        if not log_dir:
            base_log_dir = logger_params.get('base_log_dir', 'checkpoints/')
            # Prepare logging
            log_dir = os.path.join(base_log_dir, self.config["model_class"])
            if 'logger_name' in logger_params:
                log_dir = os.path.join(log_dir, logger_params['logger_name'])
            version = None
        else:
            version = ''
        # Create logger object
        logger_type = logger_params.get('logger_type', 'TensorBoard').lower()
        if logger_type == 'tensorboard':
            self.logger = TensorBoardLogger(save_dir=log_dir,
                                            version=version,
                                            name='')
        elif logger_type == 'wandb':
            self.logger = WandbLogger(name=logger_params.get('project_name', None),
                                      save_dir=log_dir,
                                      version=version,
                                      config=self.config)
        else:
            assert False, f'Unknown logger type \"{logger_type}\"'
        # Save hyperparameters
        log_dir = self.logger.log_dir
        if not os.path.isfile(os.path.join(log_dir, 'hparams.json')):
```

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```
            os.makedirs(os.path.join(log_dir, 'metrics/'), exist_ok=True)
            with open(os.path.join(log_dir, 'hparams.json'), 'w') as f:
                json.dump(self.config, f, indent=4)
        self.log_dir = log_dir

    def init_model(self,
                   exmp_input : Any):
        """
        Creates an initial training state with newly generated network parameters.

        Args:
          exmp_input: An input to the model with which the shapes are inferred.
        """
        # Prepare PRNG and input
        model_rng = random.PRNGKey(self.seed)
        model_rng, init_rng = random.split(model_rng)
        exmp_input = [exmp_input] if not isinstance(exmp_input, (list, tuple)) else exmp_
↪input
        # Run model initialization
        variables = self.run_model_init(exmp_input, init_rng)
        # Create default state. Optimizer is initialized later
        self.state = TrainState(step=0,
                                apply_fn=self.model.apply,
                                params=variables['params'],
                                batch_stats=variables.get('batch_stats'),
                                rng=model_rng,
                                tx=None,
                                opt_state=None)

    def run_model_init(self,
                       exmp_input : Any,
                       init_rng : Any) -> Dict:
        """
        The model initialization call

        Args:
          exmp_input: An input to the model with which the shapes are inferred.
          init_rng: A jax.random.PRNGKey.

        Returns:
          The initialized variable dictionary.
        """
        return self.model.init(init_rng, *exmp_input, train=True)

    def print_tabulate(self,
                       exmp_input : Any):
        """
        Prints a summary of the Module represented as table.

        Args:
          exmp_input: An input to the model with which the shapes are inferred.
        """
```

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```
        print(self.model.tabulate(random.PRNGKey(0), *exmp_input, train=True))

    def init_optimizer(self,
                       num_epochs : int,
                       num_steps_per_epoch : int):
        """
        Initializes the optimizer and learning rate scheduler.

        Args:
          num_epochs: Number of epochs the model will be trained for.
          num_steps_per_epoch: Number of training steps per epoch.
        """
        hparams = copy(self.optimizer_hparams)

        # Initialize optimizer
        optimizer_name = hparams.pop('optimizer', 'adamw')
        if optimizer_name.lower() == 'adam':
            opt_class = optax.adam
        elif optimizer_name.lower() == 'adamw':
            opt_class = optax.adamw
        elif optimizer_name.lower() == 'sgd':
            opt_class = optax.sgd
        else:
            assert False, f'Unknown optimizer "{opt_class}"'
        # Initialize learning rate scheduler
        # A cosine decay scheduler is used, but others are also possible
        lr = hparams.pop('lr', 1e-3)
        warmup = hparams.pop('warmup', 0)
        lr_schedule = optax.warmup_cosine_decay_schedule(
            init_value=0.0,
            peak_value=lr,
            warmup_steps=warmup,
            decay_steps=int(num_epochs * num_steps_per_epoch),
            end_value=0.01 * lr
        )
        # Clip gradients at max value, and evt. apply weight decay
        transf = [optax.clip_by_global_norm(hparams.pop('gradient_clip', 1.0))]
        if opt_class == optax.sgd and 'weight_decay' in hparams:  # wd is integrated in␣
↪adamw
            transf.append(optax.add_decayed_weights(hparams.pop('weight_decay', 0.0)))
        optimizer = optax.chain(
            *transf,
            opt_class(lr_schedule, **hparams)
        )
        # Initialize training state
        self.state = TrainState.create(apply_fn=self.state.apply_fn,
                                       params=self.state.params,
                                       batch_stats=self.state.batch_stats,
                                       tx=optimizer,
                                       rng=self.state.rng)

    def create_jitted_functions(self):
```

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```
        """
        Creates jitted versions of the training and evaluation functions.
        If self.debug is True, not jitting is applied.
        """
        train_step, eval_step = self.create_functions()
        if self.debug:  # Skip jitting
            print('Skipping jitting due to debug=True')
            self.train_step = train_step
            self.eval_step = eval_step
        else:
            self.train_step = jax.jit(train_step)
            self.eval_step = jax.jit(eval_step)

    def create_functions(self) -> Tuple[Callable[[TrainState, Any], Tuple[TrainState,␣
↪Dict]],
                                        Callable[[TrainState, Any], Tuple[TrainState,␣
↪Dict]]]:
        """
        Creates and returns functions for the training and evaluation step. The
        functions take as input the training state and a batch from the train/
        val/test loader. Both functions are expected to return a dictionary of
        logging metrics, and the training function a new train state. This
        function needs to be overwritten by a subclass. The train_step and
        eval_step functions here are examples for the signature of the functions.
        """
        def train_step(state : TrainState,
                       batch : Any):
            metrics = {}
            return state, metrics
        def eval_step(state : TrainState,
                      batch : Any):
            metrics = {}
            return metrics
        raise NotImplementedError

    def train_model(self,
                    train_loader : Iterator,
                    val_loader : Iterator,
                    test_loader : Optional[Iterator] = None,
                    num_epochs : int = 500) -> Dict[str, Any]:
        """
        Starts a training loop for the given number of epochs.

        Args:
          train_loader: Data loader of the training set.
          val_loader: Data loader of the validation set.
          test_loader: If given, best model will be evaluated on the test set.
          num_epochs: Number of epochs for which to train the model.

        Returns:
          A dictionary of the train, validation and evt. test metrics for the
          best model on the validation set.
```

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```
        """
        # Create optimizer and the scheduler for the given number of epochs
        self.init_optimizer(num_epochs, len(train_loader))
        # Prepare training loop
        self.on_training_start()
        best_eval_metrics = None
        for epoch_idx in self.tracker(range(1, num_epochs+1), desc='Epochs'):
            train_metrics = self.train_epoch(train_loader)
            self.logger.log_metrics(train_metrics, step=epoch_idx)
            self.on_training_epoch_end(epoch_idx)
            # Validation every N epochs
            if epoch_idx % self.check_val_every_n_epoch == 0:
                eval_metrics = self.eval_model(val_loader, log_prefix='val/')
                self.on_validation_epoch_end(epoch_idx, eval_metrics, val_loader)
                self.logger.log_metrics(eval_metrics, step=epoch_idx)
                self.save_metrics(f'eval_epoch_{str(epoch_idx).zfill(3)}', eval_metrics)
                # Save best model
                if self.is_new_model_better(eval_metrics, best_eval_metrics):
                    best_eval_metrics = eval_metrics
                    best_eval_metrics.update(train_metrics)
                    self.save_model(step=epoch_idx)
                    self.save_metrics('best_eval', eval_metrics)
        # Test best model if possible
        if test_loader is not None:
            self.load_model()
            test_metrics = self.eval_model(test_loader, log_prefix='test/')
            self.logger.log_metrics(test_metrics, step=epoch_idx)
            self.save_metrics('test', test_metrics)
            best_eval_metrics.update(test_metrics)
        # Close logger
        self.logger.finalize('success')
        return best_eval_metrics

    def train_epoch(self,
                    train_loader : Iterator) -> Dict[str, Any]:
        """
        Trains a model for one epoch.

        Args:
          train_loader: Data loader of the training set.

        Returns:
          A dictionary of the average training metrics over all batches
          for logging.
        """
        # Train model for one epoch, and log avg loss and accuracy
        metrics = defaultdict(float)
        num_train_steps = len(train_loader)
        start_time = time.time()
        for batch in self.tracker(train_loader, desc='Training', leave=False):
            self.state, step_metrics = self.train_step(self.state, batch)
            for key in step_metrics:
```

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```
                metrics['train/' + key] += step_metrics[key] / num_train_steps
        metrics = {key: metrics[key].item() for key in metrics}
        metrics['epoch_time'] = time.time() - start_time
        return metrics

    def eval_model(self,
                   data_loader : Iterator,
                   log_prefix : Optional[str] = '') -> Dict[str, Any]:
        """
        Evaluates the model on a dataset.

        Args:
          data_loader: Data loader of the dataset to evaluate on.
          log_prefix: Prefix to add to all metrics (e.g. 'val/' or 'test/')

        Returns:
          A dictionary of the evaluation metrics, averaged over data points
          in the dataset.
        """
        # Test model on all images of a data loader and return avg loss
        metrics = defaultdict(float)
        num_elements = 0
        for batch in data_loader:
            step_metrics = self.eval_step(self.state, batch)
            batch_size = batch[0].shape[0] if isinstance(batch, (list, tuple)) else␣
↪batch.shape[0]
            for key in step_metrics:
                metrics[key] += step_metrics[key] * batch_size
            num_elements += batch_size
        metrics = {(log_prefix + key): (metrics[key] / num_elements).item() for key in␣
↪metrics}
        return metrics

    def is_new_model_better(self,
                            new_metrics : Dict[str, Any],
                            old_metrics : Dict[str, Any]) -> bool:
        """
        Compares two sets of evaluation metrics to decide whether the
        new model is better than the previous ones or not.

        Args:
          new_metrics: A dictionary of the evaluation metrics of the new model.
          old_metrics: A dictionary of the evaluation metrics of the previously
            best model, i.e. the one to compare to.

        Returns:
          True if the new model is better than the old one, and False otherwise.
        """
        if old_metrics is None:
            return True
        for key, is_larger in [('val/val_metric', False), ('val/acc', True), ('val/loss',
↪ False)]:
```

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```
            if key in new_metrics:
                if is_larger:
                    return new_metrics[key] > old_metrics[key]
                else:
                    return new_metrics[key] < old_metrics[key]
        assert False, f'No known metrics to log on: {new_metrics}'

    def tracker(self,
                iterator : Iterator,
                **kwargs) -> Iterator:
        """
        Wraps an iterator in a progress bar tracker (tqdm) if the progress bar
        is enabled.

        Args:
          iterator: Iterator to wrap in tqdm.
          kwargs: Additional arguments to tqdm.

        Returns:
          Wrapped iterator if progress bar is enabled, otherwise same iterator
          as input.
        """
        if self.enable_progress_bar:
            return tqdm(iterator, **kwargs)
        else:
            return iterator

    def save_metrics(self,
                     filename : str,
                     metrics : Dict[str, Any]):
        """
        Saves a dictionary of metrics to file. Can be used as a textual
        representation of the validation performance for checking in the terminal.

        Args:
          filename: Name of the metrics file without folders and postfix.
          metrics: A dictionary of metrics to save in the file.
        """
        with open(os.path.join(self.log_dir, f'metrics/{filename}.json'), 'w') as f:
            json.dump(metrics, f, indent=4)

    def on_training_start(self):
        """
        Method called before training is started. Can be used for additional
        initialization operations etc.
        """
        pass

    def on_training_epoch_end(self,
                              epoch_idx : int):
        """
        Method called at the end of each training epoch. Can be used for additional
```

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```
        logging or similar.

        Args:
          epoch_idx: Index of the training epoch that has finished.
        """
        pass

    def on_validation_epoch_end(self,
                                epoch_idx : int,
                                eval_metrics : Dict[str, Any],
                                val_loader : Iterator):
        """
        Method called at the end of each validation epoch. Can be used for additional
        logging and evaluation.

        Args:
          epoch_idx: Index of the training epoch at which validation was performed.
          eval_metrics: A dictionary of the validation metrics. New metrics added to
            this dictionary will be logged as well.
          val_loader: Data loader of the validation set, to support additional
            evaluation.
        """
        pass

    def save_model(self,
                   step : int = 0):
        """
        Saves current training state at certain training iteration. Only the model
        parameters and batch statistics are saved to reduce memory footprint. To
        support the training to be continued from a checkpoint, this method can be
        extended to include the optimizer state as well.

        Args:
          step: Index of the step to save the model at, e.g. epoch.
        """
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir,
                                    target={'params': self.state.params,
                                            'batch_stats': self.state.batch_stats},
                                    step=step,
                                    overwrite=True)

    def load_model(self):
        """
        Loads model parameters and batch statistics from the logging directory.
        """
        state_dict = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir, target=None)
        self.state = TrainState.create(apply_fn=self.model.apply,
                                       params=state_dict['params'],
                                       batch_stats=state_dict['batch_stats'],
                                       # Optimizer will be overwritten when training␣
↪starts
                                       tx=self.state.tx if self.state.tx else optax.
↪sgd(0.1),
```

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```
                                    rng=self.state.rng
                                   )

    def bind_model(self):
        """
        Returns a model with parameters bound to it. Enables an easier inference
        access.

        Returns:
          The model with parameters and evt. batch statistics bound to it.
        """
        params = {'params': self.state.params}
        if self.state.batch_stats:
            params['batch_stats'] = self.state.batch_stats
        return self.model.bind(params)

    @classmethod
    def load_from_checkpoint(cls,
                             checkpoint : str,
                             exmp_input : Any) -> Any:
        """
        Creates a Trainer object with same hyperparameters and loaded model from
        a checkpoint directory.

        Args:
          checkpoint: Folder in which the checkpoint and hyperparameter file is stored.
          exmp_input: An input to the model for shape inference.

        Returns:
          A Trainer object with model loaded from the checkpoint folder.
        """
        hparams_file = os.path.join(checkpoint, 'hparams.json')
        assert os.path.isfile(hparams_file), 'Could not find hparams file'
        with open(hparams_file, 'r') as f:
            hparams = json.load(f)
        hparams.pop('model_class')
        hparams.update(hparams.pop('model_hparams'))
        if not hparams['logger_params']:
            hparams['logger_params'] = dict()
        hparams['logger_params']['log_dir'] = checkpoint
        trainer = cls(exmp_input=exmp_input,
                      **hparams)
        trainer.load_model()
        return trainer
```

Utility functions

Besides the Trainer module, we have seen other functionalities re-occurring several times in the tutorials. One of them is `numpy_collate`, which is needed for PyTorch's data loader to purely work with NumPy arrays. Similarly, creating Data Loaders for our datasets often follows the same structure, which we can also summarize in a function called `create_data_loaders`.

[4]:
```
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

def create_data_loaders(*datasets : Sequence[data.Dataset],
                        train : Union[bool, Sequence[bool]] = True,
                        batch_size : int = 128,
                        num_workers : int = 4,
                        seed : int = 42):
    """
    Creates data loaders used in JAX for a set of datasets.

    Args:
      datasets: Datasets for which data loaders are created.
      train: Sequence indicating which datasets are used for
        training and which not. If single bool, the same value
        is used for all datasets.
      batch_size: Batch size to use in the data loaders.
      num_workers: Number of workers for each dataset.
      seed: Seed to initialize the workers and shuffling with.
    """
    loaders = []
    if not isinstance(train, (list, tuple)):
        train = [train for _ in datasets]
    for dataset, is_train in zip(datasets, train):
        loader = data.DataLoader(dataset,
                                 batch_size=batch_size,
                                 shuffle=is_train,
                                 drop_last=is_train,
                                 collate_fn=numpy_collate,
                                 num_workers=num_workers,
                                 persistent_workers=is_train,
                                 generator=torch.Generator().manual_seed(seed))
        loaders.append(loader)
    return loaders
```

4.4.2 Example 1: Function regression

Using the `TrainerModule` and our few utility functions, we can now write a full training scenario with logging etc. in a few lines. To showcase this, we first consider a very simple scenario: regressing a sine-wave with a neural network.

Dataset

The first step is to create a dataset. Since we can use PyTorch's data package, this is straightforward. First, let's import needed plotting libraries for visualization and set the data and checkpoint path, similarly as in any other tutorial.

[5]:
```
## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()
sns.set()

DATASET_PATH = '../data/'
CHECKPOINT_PATH = '../saved_models/guide4/'
```

The dataset is kept very simple and contains pairs of input-output of a sine function:

[6]:
```
def target_function(x):
    return np.sin(x * 3.0)

class RegressionDataset(data.Dataset):

    def __init__(self, num_points, seed):
        super().__init__()
        rng = np.random.default_rng(seed)
        self.x = rng.uniform(low=-2.0, high=2.0, size=num_points)
        self.y = target_function(self.x)

    def __len__(self):
        return self.x.shape[0]

    def __getitem__(self, idx):
        return self.x[idx:idx+1], self.y[idx:idx+1]
```

We can create our needed data loaders with the utility function `create_data_loaders` and visualize the dataset for debugging:

[7]:
```
train_set = RegressionDataset(num_points=1000, seed=42)
val_set = RegressionDataset(num_points=200, seed=43)
test_set = RegressionDataset(num_points=500, seed=44)
train_loader, val_loader, test_loader = create_data_loaders(train_set, val_set, test_set,
                                                            train=[True, False, False],
                                                            batch_size=64)
```

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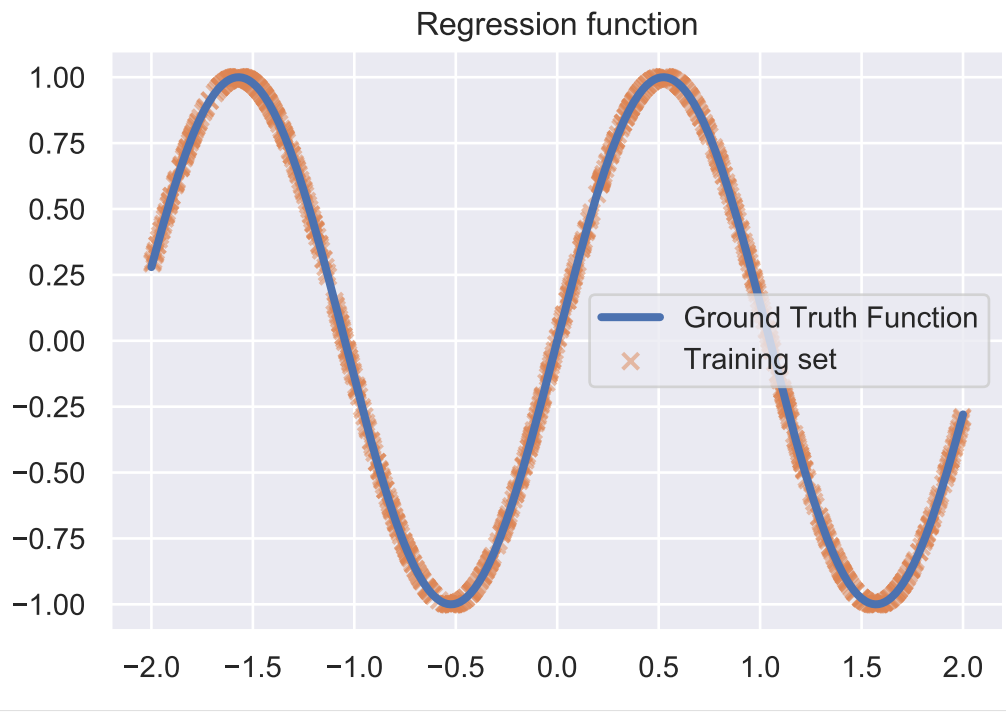
```
x = np.linspace(-2, 2, 1000)
plt.scatter(train_set.x, train_set.y, color='C1', marker='x', alpha=0.5, label='Training␣
↪set')
plt.plot(x, target_function(x), linewidth=3.0, label='Ground Truth Function')
plt.legend()
plt.title('Regression function')
plt.show()
```



Note that even with PyTorch Lightning, we would have needed the similar setup here.

Model

The Trainer module does not restrict us to any specific model, so let's implement our own MLP class for regression:

[8]:
```
class MLPRegressor(nn.Module):
    hidden_dims : Sequence[int]
    output_dim : int

    @nn.compact
    def __call__(self, x, **kwargs):
        for dims in self.hidden_dims:
            x = nn.Dense(dims)(x)
            x = nn.silu(x)
        x = nn.Dense(self.output_dim)(x)
        return x
```

Trainer

Now comes the interesting part. Using the `TrainerModule`, we only need to overwrite the aspects that are needed: the training and validation step. For the regression task and the small model, this reduces to writing the mean-squared error loss. Note that we still have some minor repetitive code here, such as creating the gradient function with `jax.value_and_grad` in the training step and applying the update with `state.apply_gradients`. One could reduce this further by restricting possible loss functions, but to keep flexibility high, we implement the whole training step here.

[9]:
```
class MLPRegressTrainer(TrainerModule):

    def __init__(self,
                 hidden_dims : Sequence[int],
                 output_dim : int,
                 **kwargs):
        super().__init__(model_class=MLPRegressor,
                         model_hparams={
                             'hidden_dims': hidden_dims,
                             'output_dim': output_dim
                         },
                         **kwargs)

    def create_functions(self):
        def mse_loss(params, batch):
            x, y = batch
            pred = self.model.apply({'params': params}, x)
            loss = ((pred - y) ** 2).mean()
            return loss

        def train_step(state, batch):
            loss_fn = lambda params: mse_loss(params, batch)
            loss, grads = jax.value_and_grad(loss_fn)(state.params)
            state = state.apply_gradients(grads=grads)
            metrics = {'loss': loss}
            return state, metrics

        def eval_step(state, batch):
            loss = mse_loss(state.params, batch)
            return {'loss': loss}

        return train_step, eval_step
```

And that's already it! This now looks much more like the minimal code of PyTorch Lightning and automatically logs our metrics as we want.

Training

To train the model, we simply specify our hyperparameters and create a Trainer module:

[10]:
```
trainer = MLPRegressTrainer(hidden_dims=[128, 128],
                            output_dim=1,
                            optimizer_hparams={'lr': 4e-3},
                            logger_params={'base_log_dir': CHECKPOINT_PATH},
                            exmp_input=next(iter(train_loader))[0:1],
                            check_val_every_n_epoch=5)
```

```
                  MLPRegressor Summary

 path          outputs          params

 Inputs        - float64[64,1]
               - train: True

 Dense_0       float32[64,128]  bias: float32[128]
                                kernel: float32[1,128]

                                256 (1.0 KB)

 Dense_1       float32[64,128]  bias: float32[128]
                                kernel: float32[128,128]

                                16,512 (66.0 KB)

 Dense_2       float32[64,1]    bias: float32[1]
                                kernel: float32[128,1]

                                129 (516 B)

 MLPRegressor  float32[64,1]

               Total            16,897 (67.6 KB)


             Total Parameters: 16,897 (67.6 KB)
```

As one can see, we also automatically print out all layers with their parameters and outputs with Flax's `nn.tabulate` function. This is quite helpful for debugging and gives an intuition about the size of the model. Since the task is not very difficult, we are fine with using less than 20k parameters.

Next, let's start the training:

[11]:
```
metrics = trainer.train_model(train_loader,
                              val_loader,
                              test_loader=test_loader,
                              num_epochs=50)
```

[12]:
```
print(f'Training loss: {metrics["train/loss"]}')
print(f'Validation loss: {metrics["val/loss"]}')
print(f'Test loss: {metrics["test/loss"]}')
```

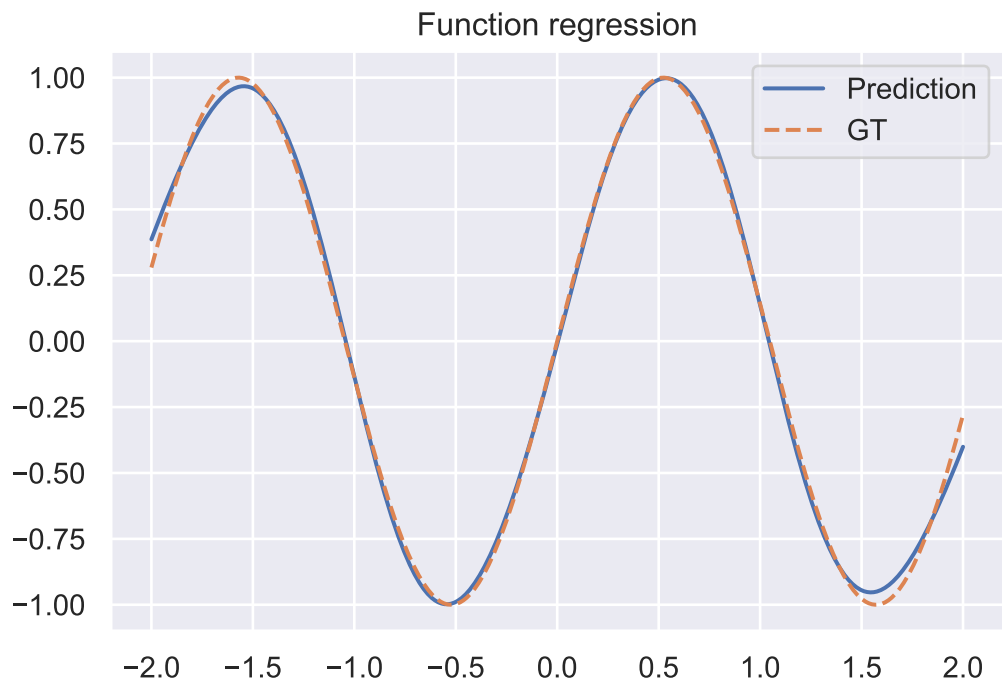
```
Training loss: 0.0008829445578157902
Validation loss: 0.0008724514045752585
Test loss: 0.0007670423365198076
```

With the speed of JAX, this takes only a few seconds. The logs can be found in `../saved_models/guide4/MLPRegressor/`, and we have a dictionary of the best results here as well. The training, validation and test loss suggest that our model learned the function quite well, but let's check it by predicting the whole function as inference task.

Inference

To perform inference, we first bind the model to the parameters. This enables us a simpler API, closer to PyTorch. Applying the model to a values between -2.0 and 2.0 shows that the model learned the sine wave indeed quite well and is only off at the corners.

[13]:
```
model_bd = trainer.bind_model()
x = np.linspace(-2, 2, 1000)[:,None]
y_pred = model_bd(x)
plt.plot(x, y_pred, label='Prediction')
plt.plot(x, target_function(x), '--', label='GT')
plt.title('Function regression')
plt.legend()
plt.show()
```



4.4.3 Example 2: CIFAR10 classification

As a second example, let's consider image classification on CIFAR10. We have done it before in Tutorial 5, but here, we want to showcase the flexibility of the Trainer module. For that, we will consider a more complicated setting in Flax: a model with both Batch Normalization and Dropout. However, with the Trainer module, this reduces to a simpler code again.

Dataset

First, let's load our dataset again. This is the same data loading as used in Tutorial 5 and Tutorial 15, but only considers flipping as regularization technique since we work with simple MLPs here.

[14]:
```
from torchvision.datasets import CIFAR10
from torchvision import transforms

# Transformations applied on each image => bring them into a numpy array
DATA_MEANS = np.array([0.49139968, 0.48215841, 0.44653091])
DATA_STD = np.array([0.24703223, 0.24348513, 0.26158784])
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    img = (img / 255. - DATA_MEANS) / DATA_STD
    return img


test_transform = image_to_numpy
# For training, we add some augmentation. Networks are too powerful and would overfit.
train_transform = transforms.Compose([transforms.RandomHorizontalFlip(),
                                      image_to_numpy])
# Loading the training dataset. We need to split it into a training and validation part
# We need to do a little trick because the validation set should not use the␣
↪augmentation.
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=train_transform,␣
↪download=True)
val_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=test_transform,␣
↪download=True)
train_set, _ = data.random_split(train_dataset, [45000, 5000], generator=torch.
↪Generator().manual_seed(42))
_, val_set = data.random_split(val_dataset, [45000, 5000], generator=torch.Generator().
↪manual_seed(42))

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=test_transform,␣
↪download=True)

train_loader, val_loader, test_loader = create_data_loaders(train_set, val_set, test_set,
                                                            train=[True, False, False],
                                                            batch_size=256)
```

```
Files already downloaded and verified
Files already downloaded and verified
Files already downloaded and verified
```

Model

The model definition is again relatively simple. We repeat a series of Dropout → Linear → BatchNorm → Swish blocks, with a final Dropout and Linear layer at the end.

[15]:
```
class MLPClassifier(nn.Module):
    hidden_dims : Sequence[int]
    num_classes : int
    dropout_prob : float = 0.0

    @nn.compact
    def __call__(self, x, train=True):
        x = x.reshape(x.shape[0], -1)
        for dims in self.hidden_dims:
            x = nn.Dropout(self.dropout_prob)(x, deterministic=not train)
            x = nn.Dense(dims)(x)
            x = nn.BatchNorm()(x, use_running_average=not train)
            x = nn.swish(x)
        x = nn.Dropout(self.dropout_prob)(x, deterministic=not train)
        x = nn.Dense(self.num_classes)(x)
        return x
```

Trainer

For the Trainer module, we again define our model hyperparameters in the init function, and write our own training and evaluation steps in `create_functions`. In these functions, we take care of the mutable batch statistics and the PRNG state for dropout. Note that since both parts are integrated in the `TrainState`, we do not need to alternate the training or validation step signature, and it is sufficient to pass the state and batch to the functions. Additionally, we overwrite the model call during initialization (`run_model_init`) and tabulate function (`print_tabulate`). And that's it! Overall, we didn't need to make many changes, showing that the trainer module is flexible enough to support a variety of layers. For now, we can ignore the `trial` object and come back to it later when discussing automated hyperparameter tuning.

[16]:
```
class MLPClassTrainer(TrainerModule):

    def __init__(self,
                 hidden_dims : Sequence[int],
                 num_classes : int,
                 dropout_prob : float,
                 trial : Any = None,
                 **kwargs):
        super().__init__(model_class=MLPClassifier,
                         model_hparams={
                             'hidden_dims': hidden_dims,
                             'num_classes': num_classes,
                             'dropout_prob': dropout_prob
                         },
                         **kwargs)
        self.trial = trial

    def create_functions(self):
        def loss_function(params, batch_stats, rng, batch, train):
```

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```
            imgs, labels = batch
            rng, dropout_rng = random.split(rng)
            output = self.model.apply({'params': params, 'batch_stats': batch_stats},
                                      imgs,
                                      train=train,
                                      rngs={'dropout': dropout_rng},
                                      mutable=['batch_stats'] if train else False)
            logits, new_model_state = output if train else (output, None)
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).mean()
            return loss, (rng, new_model_state, acc)

        def train_step(state, batch):
            loss_fn = lambda params: loss_function(params, state.batch_stats, state.rng,␣
↪batch, train=True)
            ret, grads = jax.value_and_grad(loss_fn, has_aux=True)(state.params)
            loss, rng, new_model_state, acc = ret[0], *ret[1]
            state = state.apply_gradients(grads=grads, batch_stats=new_model_state[
↪'batch_stats'], rng=rng)
            metrics = {'loss': loss, 'acc': acc}
            return state, metrics

        def eval_step(state, batch):
            _, (_, _, acc) = loss_function(state.params, state.batch_stats, state.rng,␣
↪batch, train=False)
            return {'acc': acc}

        return train_step, eval_step

    def run_model_init(self, exmp_input, init_rng):
        imgs, _ = exmp_input
        init_rng, dropout_rng = random.split(init_rng)
        return self.model.init({'params': init_rng, 'dropout': dropout_rng}, x=imgs,␣
↪train=True)

    def print_tabulate(self, exmp_input):
        imgs, _ = exmp_input
        print(self.model.tabulate(rngs={'params': random.PRNGKey(0), 'dropout': random.
↪PRNGKey(0)}, x=imgs, train=True))

    def on_validation_epoch_end(self, epoch_idx, eval_metrics, val_loader):
        if self.trial:
            self.trial.report(eval_metrics['val/acc'], step=epoch_idx)
            if self.trial.should_prune():
                raise optuna.exceptions.TrialPruned()
```

Training

With the Trainer fully defined, we can again start training. Let's pick some reasonable hyperparameters, and look at the layers created by the model:

[17]:
```
trainer = MLPClassTrainer(hidden_dims=[512, 512],
                          num_classes=10,
                          dropout_prob=0.4,
                          optimizer_hparams={
                              'weight_decay': 2e-4,
                              'lr': 1e-3
                          },
                          logger_params={
                              'base_log_dir': CHECKPOINT_PATH
                          },
                          exmp_input=next(iter(train_loader)),
                          check_val_every_n_epoch=5)
```

MLPClassifier Summary

path	outputs	batch_stats	params
Inputs	train: True		
	x: float64[256,32,32,3]		
BatchNorm_0	float32[256,512]	mean: float32[512]	bias: float32[512]
		var: float32[512]	scale: float32[512]
		1,024 (4.1 KB)	**1,024 (4.1 KB)**
BatchNorm_1	float32[256,512]	mean: float32[512]	bias: float32[512]
		var: float32[512]	scale: float32[512]
		1,024 (4.1 KB)	**1,024 (4.1 KB)**
Dense_0	float32[256,512]		bias: float32[512]
			kernel: float32[3072,512]
			1,573,376 (6.3 MB)

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```
┃ Dense_1        ┃ float32[256,512]        ┃                    ┃ bias: float32[512]      ┃
┃                ┃                         ┃                    ┃ kernel: float32[512,    ┃
↪512]  ┃
┃                ┃                         ┃                    ┃                         ┃
↪   ┃
┃                ┃                         ┃                    ┃ 262,656 (1.1 MB)        ┃
↪   ┃
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┃ Dense_2        ┃ float32[256,10]         ┃                    ┃ bias: float32[10]       ┃
↪   ┃
┃                ┃                         ┃                    ┃ kernel: float32[512,10]┃
↪   ┃
┃                ┃                         ┃                    ┃                         ┃
↪   ┃
┃                ┃                         ┃                    ┃ 5,130 (20.5 KB)         ┃
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┃ Dropout_0      ┃ float32[256,3072]       ┃                    ┃                         ┃
↪   ┃
┡━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━━━━━━┩
┃ Dropout_1      ┃ float32[256,512]        ┃                    ┃                         ┃
↪   ┃
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┃ Dropout_2      ┃ float32[256,512]        ┃                    ┃                         ┃
↪   ┃
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┃ MLPClassifier  ┃ float32[256,10]         ┃                    ┃                         ┃
↪   ┃
┡━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━━━━━━┩
┃                ┃                   Total ┃ 2,048 (8.2 KB)     ┃ 1,843,210 (7.4 MB)      ┃
↪   ┃
└────────────────┴─────────────────────────┴────────────────────┴─────────────────────────┘
↪

                          Total Parameters: 1,845,258 (7.4 MB)
↪
```

One interesting observation here is that the MLP has way more parameters than any of the CNNs in Tutorial 5, but yet significantly underperforms the models. Although to really see the performance, let's train the model again with the simple call from before:

[18]:
```
metrics = trainer.train_model(train_loader,
                              val_loader,
                              test_loader=test_loader,
                              num_epochs=50)
```

[19]:
```
print(f'Validation accuracy: {metrics["val/acc"]:4.2%}')
print(f'Test accuracy: {metrics["test/acc"]:4.2%}')
```

```
Validation accuracy: 60.22%
Test accuracy: 60.05%
```

The MLP achieves decent accuracy, but already for models like this, we have several hyperparameters to tune including learning rate, weight decay, dropout rate. Which should we choose? While we could use intuition to get a reasonable guess, it is unlikely that we hit the best hyperparameter set. In order to find a very strong hyperparameter set, a good practice is to use automatic hyperparameter tuning, which we shortly review next to showcase the flexibility of the Trainer module.

4.4.4 Automatic hyperparameter tuning with Optuna

Automatic hyperparameter tuner have the goal to efficiently identify sets of hyperparameters that achieve the best performance. Thereby, the key question is how can we search the hyperparameter space efficiently, since we don't have infinite compute. Optuna is a library that helps you setup this search with minimal code overhead and perform automatic hyperparameter tuning. Before getting started with Optuna, let's import the library and download a pre-executed hyperparameter search as an example.

[20]:
```
try:
    import optuna
except ModuleNotFoundError:
    !pip install --quiet --upgrade optuna pyplot
    import optuna
```

[21]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/guide4/"
# Files to download
pretrained_files = ["optuna_hparam_search.db", "MLPClassifier/version_16/checkpoint_150",
↪ "MLPClassifier/version_16/hparams.json"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please contact the author with the full output␣
↪including the following error:\n", e)
```

Defining objective and hyperparameters

The main part a user has to specify in Optuna is intuitively the the objective to optimize, and the hyperparameters over which we want to optimize. In our case, the objective is to optimize the validation accuracy of the MLP. Note that we do not use the test set here, since hyperparameter searches should only be done on the validation set, not the "unseen" test set! The function below, `objective(trial)`, creates a MLP with our trainer module and trains it for max. 200 epochs. The input argument, `trial`, is thereby an object which characterizes the current run. This includes, for example, the hyperparameters we want to optimize. In order to add a hyperparameter to our optimization set, we can simply call `trial.suggest_float` for continuous values and `trial.suggest_categorical` for categorical values (e.g. which optimizer to use). For the CIFAR10 classification, we consider the following three hyperparameters: dropout rate, weight decay, and the learning rate, which we define below. Finally, we return the best validation accuracy which will be used by Optuna to guide the next pick of hyperparameters.

[22]:
```
def objective(trial):
    my_train_loader, my_val_loader = create_data_loaders(train_set, val_set,
                                                         train=[True, False],
                                                         batch_size=256)
    trainer = MLPClassTrainer(hidden_dims=[512, 512],
                              num_classes=10,
                              dropout_prob=trial.suggest_float('dropout_prob', 0, 0.6),
                              optimizer_hparams={
                                  'weight_decay': trial.suggest_float('weight_decay', 1e-
↪6, 1e-2, log=True),
                                  'lr': trial.suggest_float('lr', 1e-4, 1e-2, log=True)
                              },
                              logger_params={
                                  'base_log_dir': CHECKPOINT_PATH
                              },
                              exmp_input=next(iter(my_train_loader)),
                              check_val_every_n_epoch=5,
                              trial=trial)
    metrics = trainer.train_model(my_train_loader,
                                  my_val_loader,
                                  num_epochs=200)
    del trainer
    del my_train_loader, my_val_loader
    return metrics['val/acc']
```

Running hyperparameter study

To run the hyperparameter search, we create a `Study` in Optuna. A study implements the search logic and summarizes the data/logs of all executed experiments. By default, Optuna uses the Tree-Structured Parzen Estimator algorithm, using Gaussian Mixture Models to estimate the performance surface of they hyperparameters. For more information, check out the documentation. The studies are usually stored in a database format, but can be easily accessed via the Python interface of Optuna. Let's run the hyperparameter search for up to 25 models:

[23]:
```
study = optuna.create_study(
    study_name='mlp_cifar10',
    storage=f'sqlite:///{CHECKPOINT_PATH}/optuna_hparam_search.db',
    direction='maximize',
    pruner=optuna.pruners.MedianPruner(n_startup_trials=5, n_warmup_steps=50),
    load_if_exists=True
```

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```
)
study.optimize(objective, n_trials=25-len(study.trials), n_jobs=1)
```

```
[I 2022-07-05 20:06:47,966] Using an existing study with name 'mlp_cifar10' instead of␣
↪creating a new one.
```

During the study creation, we used the input argument `pruner`. This specifies a strategy with which we want to stop experiments early if they don't look promising. For instance, a very low learning rate combined with high weight decay and dropout will likely achieve low performance, which we can already judge after 50 epochs and don't have to run the model for much longer. For this, we implemented the `on_validation_epoch_end` callback in our Trainer module before. After each epoch, it reports the current validation performance to Optuna. Depending on the previous performances and Optuna's pruning strategy, it may decide to stop the experiment early, which it does by throwing a `TrialPruned` error. This error is caught by Optuna, and the next trial is directly started.

Evaluate hyperparameter search

After finishing the hyperparameter search, we can analyze the results. First, let's print the best model found and its corresponding hyperparameters:

[24]:
```
trial = study.best_trial
print(f'Best Validation Accuracy: {trial.value:4.2%}')
print(f'Best Params:')
for key, value in trial.params.items():
    print(f'-> {key}: {value}')
```

```
Best Validation Accuracy: 63.44%
Best Params:
-> dropout_prob: 0.39573629692783413
-> lr: 0.002097404408052793
-> weight_decay: 0.0012107132860246818
```

The validation performance is quite a bit higher than the model we had manually designed before. Let's load the model and check its test performance. For this, we can make use of the `load_from_checkpoint` function of our Trainer module:

[25]:
```
trainer = MLPClassTrainer.load_from_checkpoint(os.path.join(CHECKPOINT_PATH,
↪'MLPClassifier/version_16/'),
                                               exmp_input=next(iter(train_loader)))
test_metrics = trainer.eval_model(test_loader)
print(f'Test accuracy: {test_metrics["acc"]:4.2%}')
```

```
                                MLPClassifier Summary

 path           outputs                  batch_stats         params

 Inputs         train: True                                                    ␣
↪   |
|               x: float64[256,32,32,3]                                        ␣
↪   |
|---------------|------------------------|-------------------|-------------------|
 BatchNorm_0    float32[256,512]         mean: float32[512]  bias: float32[512]  ␣
↪   |
|               |                        var: float32[512]   scale: float32[512]  ␣
↪   |
```

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```
│               │                         │                     │                          ␣
↪  │
│               │                         │ 1,024 (4.1 KB)      │ 1,024 (4.1 KB)           ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ BatchNorm_1   │ float32[256,512]        │ mean: float32[512]  │ bias: float32[512]       ␣
↪  │
│               │                         │ var: float32[512]   │ scale: float32[512]      ␣
↪  │
│               │                         │                     │                          ␣
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│               │                         │ 1,024 (4.1 KB)      │ 1,024 (4.1 KB)           ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ Dense_0       │ float32[256,512]        │                     │ bias: float32[512]       ␣
↪  │
│               │                         │                     │ kernel: float32[3072,
↪512] │
│               │                         │                     │                          ␣
↪  │
│               │                         │                     │ 1,573,376 (6.3 MB)       ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ Dense_1       │ float32[256,512]        │                     │ bias: float32[512]       ␣
↪  │
│               │                         │                     │ kernel: float32[512,
↪512]  │
│               │                         │                     │                          ␣
↪  │
│               │                         │                     │ 262,656 (1.1 MB)         ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ Dense_2       │ float32[256,10]         │                     │ bias: float32[10]        ␣
↪  │
│               │                         │                     │ kernel: float32[512,10]␣
↪  │
│               │                         │                     │                          ␣
↪  │
│               │                         │                     │ 5,130 (20.5 KB)          ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ Dropout_0     │ float32[256,3072]       │                     │                          ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ Dropout_1     │ float32[256,512]        │                     │                          ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ Dropout_2     │ float32[256,512]        │                     │                          ␣
↪  │
├──────────────────────────────────────────────────────────────────────────────────────────────
│ MLPClassifier │ float32[256,10]         │                     │                          ␣
↪  │
```

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```
├──────────────────────────────────────────────────────────────────────────────────
│                    │                       Total │ 2,048 (8.2 KB)       │ 1,843,210 (7.4 MB)     ␣
↪   │
└──────────────────────────────────────────────────────────────────────────────────
                                                                                   ␣
↪
                          Total Parameters: 1,845,258 (7.4 MB)                     ␣
↪
```

```
Test accuracy: 62.89%
```

The test performance is also quite strong, showing the benefit of the automatic hyperparameter search. However, often, we are not just interested in the best model. Optuna provides several ways of visualizing the results of the hyperparameter study, for instance by plotting all validation accuracy curves:

[26]:
```
fig = optuna.visualization.plot_intermediate_values(study)
fig.show()
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

As we can see, there is quite a big group of models that perform very similarly. At the same time, there were a few models with very poor results, which were lucky stopped early by Optuna to not waste compute.

Another question we might have is which hyperparameter was the most important for the performance? This can be directly visualized by `plot_param_importances`. By default, Optuna uses a random forest regression to estimate the importance of each hyperparameter (documentation), and shows it as values that sum up to 1 for all hyperparameters:

[27]:
```
fig = optuna.visualization.plot_param_importances(study)
fig.show()
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

Interestingly, the learning rate is the most important hyperparameter.

Finally, to get a good intuition of the interplay between hyperparameters, we can plot the estimated accuracy surface over hyperparameters:

[28]:
```
fig = optuna.visualization.plot_contour(study, params=['lr', 'dropout_prob'])
fig.show()
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

As the hyperparameter importance plot already suggested, the learning rate seems to be very important while we are more flexible in the dropout probability. However, there seems to be an optimal spot in the middle, overall maximizing the accuracy.

4.4.5 Conclusion

In this guide, we discussed tips and practices for doing research with JAX. We mainly focused on implementing a Trainer module that summarizes most common functionalities needed for training and testing models. To showcase the flexibility of the module, we implement a regression and classification model in a few lines. Moreover, we show how one can easily perform automatic hyperparameter optimization with Optuna in this setting. While this guide gives a possible template for a research code, it may not cover all parts that is needed for your specific usecase. Moreover, if you are specialized on a certain task, such as classification or generative models, you can further specialize the Trainer module to reduce your code for submodules.

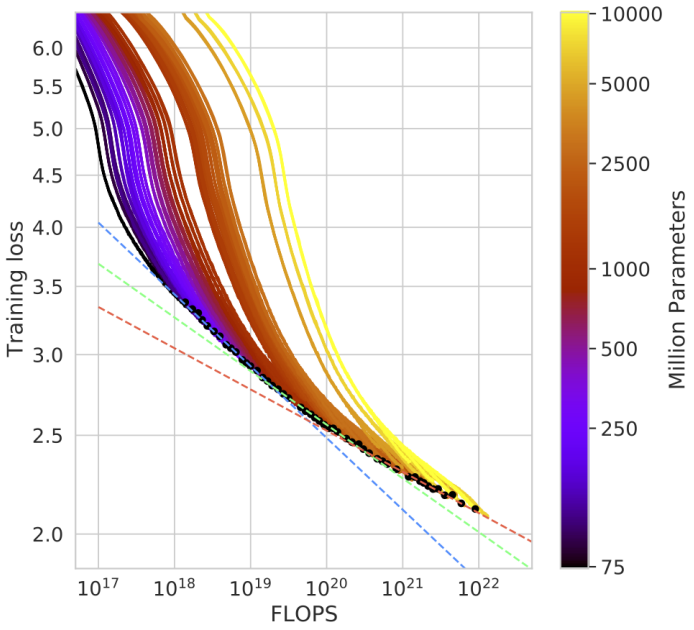
If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.5 Overview

Welcome to the UvA DL tutorial series on "**Training Models at Scale**", in which we explore parallelism strategies for training large deep learning models. The goal of this tutorial is to provide a comprehensive overview of techniques and strategies used for scaling deep learning models, and to provide a hands-on guide to implement these strategies from scratch in JAX with Flax using shard_map. If you are not familiar with JAX yet, we recommend to first check out our Intro to JAX+Flax tutorial.

4.5.1 Why scaling?

The field of deep learning has seen a rapid increase in model size over the past years, especially with models like GPT-4, Gemini, Llama, Mistral, and Claude. This trend is driven by the observation that larger models often lead to better performance, and the availability of more powerful hardware. For example, the Chincilla paper shows a scaling law for the performance of large language models, which states that the performance of a model scales with the number of parameters. This is illustrated in the figure below, which shows the loss of a model on the y-axis and the number of FLOPs used in training on the x-axis (the parameter count is shown in the legend). The figure shows that the loss decreases as the number of FLOPs and model size increases (figure credit: Hoffman et al., 2022).



Training large models is challenging, and requires careful consideration of the parallelism strategies to efficiently utilize the available hardware. Hence, understanding and implementing parallelism strategies is crucial for training large models. This is the focus of this tutorial series.

4.5.2 What to expect?

While we implement strategies for multi-GPU/-TPU training, the tutorial is designed to be accessible to everyone, regardless of the hardware you have available. All code can be executed on a single CPU, and applied to hardware with multiple GPUs or TPUs without changes. For reference, we provide profiles on a 8-GPU node for most implementations, and discuss the implications of scaling to larger setups.

All parallelization strategies are implemented from scratch in a modular way, so that you can easily reuse the code in your own projects. We provide Python scripts for each part, so that main functions can be reused across notebooks. We also combine all parallelization strategies in a final example, where we train a large model with 3D parallelism.

Generally, we will focus on the key concepts and ideas behind each parallelism strategy, and target with our implementation a one- or multi-node setup with tens or hundreds of GPUs. What we will not cover, since it is out of reach for most of us, is training on thousands of GPUs. In this realm, new challenges arise such as hardware failure, as for example mentioned in the Gemini report. Example resources on this topic are the OPT 175B logbook and Yi Tay's blog. We will also not cover data loading and preprocessing at scale, which is a topic on its own, and instead test our implementations on artificial data. If you are interested in this topic, you can check out TensorFlow Datasets, PyTorch DataLoader, or Grain.

Finally, the examples shown in these notebooks are focused on educational purposes, and may not always implement all optimizations or efficiency improvements that are possible. We put readability and understandability first, and aim to provide a solid foundation for you to build upon. Potential optimizations and improvements are discussed in the respective parts. If you are interested in code bases that provide highly optimized training setups to work out-of-the-box, you can check out MaxText and t5x (language models in JAX), BigVision and Scenic (vision models in JAX), and DeepSpeed (PyTorch).

4.5.3 Tutorial Structure

The tutorial is structured in 5 parts, each part focusing on a different parallelism strategy. We start with single-GPU optimizations, then move on to data parallelism, pipeline parallelism, tensor parallelism, and finally 3D parallelism. Each part is accompanied by a theoretical introduction, followed by a hands-on coding session. The coding sessions are designed to be self-contained, so that you can easily reuse the code in your own projects. A short overview of the parallelism strategies is given below.

The tutorials are structured as follows:

Single-GPU Optimizations: We start with covering techniques which can already be used for single-GPU trainings, such as *mixed precision*, *gradient accumulation*, and *gradient checkpointing*. We discuss the effect of these techniques on the memory and execution time during training, and show how to profile such models. In the second part, we take the Transformer model as an example and apply these techniques to train a larger model on a single GPU.

- Part 1.1: Training Larger Models on a Single GPU
- Part 1.2: Profiling and Scaling Single-GPU Transformer Models

Data Parallelism: The second part is dedicated to data parallelism, which is the simplest and most common parallelism strategy used for training large models. We start with an introduction to distributed computing in JAX, and then implement a data parallelism strategy. We then discuss fully-sharded data parallelism (FSDP) and ZeRO optimizer strategies to reduce the memory overhead of data parallelism, and scale to larger models.

- Part 2.1: Introduction to Distributed Computing in JAX
- Part 2.2: (Fully-Sharded) Data Parallelism

Pipeline Parallelism: We next turn to the first of two model parallelism strategies, pipeline parallelism. We start with an introduction to pipeline parallelism and how it distributes the layers of a model over multiple devices. We then implement a pipeline parallelism strategy with microbatching, and discuss the challenge of the pipeline bubble. As one example for mitigating the pipeline bubble, we discuss the concept of looping pipelines, in particular breadth-first pipeline parallelism, and implement it in JAX.

- Part 3.1: Pipeline Parallelism
- Part 3.2: Looping Pipelines

Tensor Parallelism: The fourth part deals with tensor parallelism, which is the second model parallelism strategy and splits the model over its feature dimension. We start with an introduction to tensor parallelism and how it distributes the parameters of a model over multiple devices. We then implement a tensor parallelism strategy, and discuss the challenge of communication-blocking operations. We then discuss the *asynchronous linear layers* of the 22b Vision Transformer (ViT-22b), and how to implement them in JAX. We use these layers in the third part, where we implement a transformer with tensor parallelism and scale it to a billion parameters. The profiling of the model shows compute-communcation overlap and remaining bottlenecks.

- Part 4.1: Tensor Parallelism
- Part 4.2: Asynchronous Linear Layers with Tensor Parallelism
- Part 4.3: Transformers with Tensor Parallelism

3D Parallelism: The final part combines all parallelism strategies in a final example, where we train a large Transformer model with 3D parallelism. We start with an introduction to 3D parallelism and how it combines data, pipeline, and tensor parallelism. We then implement a 3D parallelism strategy, and discuss the challenges of combining different parallelism strategies. We then profile different configurations of the model, and discuss the implications of scaling to larger setups.

- Part 5: Language Modeling with 3D Parallelism

4.5.4 Feedback, Questions or Contributions

We hope you enjoy the tutorial series and learn something new. If you have any questions, feedback, or suggestions, please feel free to reach out to us by creating an issue on the GitHub repository. Similarly, if you find a mistake or a bug, please let us know by creating an issue. We are also happy to accept contributions to the tutorial series, so if you have an addition or want to improve the existing code, feel free to create a pull request.

4.6 Part 1.1: Training Larger Models on a Single GPU

Filled notebook:

Author: Phillip Lippe

When thinking of "scaling" a model, we often think of training a model on multiple GPUs or even multiple machines. However, even on a single GPU, there are many ways to train larger models and make them more efficient. In this notebook, we'll explore some of these techniques, including mixed precision training, activation checkpointing, gradient accumulation, and more. Most of them aim at reducing the memory footprint of the training step, as memory is commonly the limited resource for single-device training. Moreover, these techniques will be also useful when training on multiple GPUs or TPUs. Hence, it's important to understand them before diving into distributed training.

We start with discussing each of these techniques separately on a toy example. This will help us understand the impact of each technique on the model's performance and memory consumption. Then, we'll combine these techniques to train a larger Transformer model on a single GPU in Part 1.2, and explore the benefits and trade-offs of each technique. Additionally, we will profile the model to get further insights into the efficiency of these techniques.

In this notebook, we will focus on JAX with Flax as the deep learning framework. However, the techniques discussed in this notebook are applicable to other deep learning frameworks like PyTorch as well, and are often implemented in training frameworks like PyTorch Lightning and DeepSpeed. If you are interested in learning more about these techniques in PyTorch, check out the additional resources at the end of this notebook. Further, if you want to closely follow the code in this notebook, it is recommended to have a basic understanding of JAX and Flax. If you are new to JAX and Flax, check out our introduction tutorial to get started.

This notebook is designed to run on CPU or an accelerator, such as a GPU or TPU. If you are running this notebook on Google Colab, you can enable the GPU runtime. You can do this by clicking on `Runtime` in the top menu, then `Change runtime type`, and selecting `GPU` from the `Hardware accelerator` dropdown. If the runtime fails, feel free to disable the GPU and run the notebook on the CPU.

JAX provides a high-performance backend with the XLA (Accelerated Linear Algebra) compiler to optimize our computations on the available hardware. As JAX continue to be developed, there are more and more features being implemented, that improve efficiency. We can enable some of these new features via XLA flags. At the moment of writing (JAX version 0.4.25, March 2024), the following flags are recommended in the JAX GPU performance tips tutorial and PAX:

[1]:
```
import os

os.environ["XLA_FLAGS"] = (
    "--xla_gpu_enable_triton_softmax_fusion=true "
    "--xla_gpu_triton_gemm_any=false "
    "--xla_gpu_enable_async_collectives=true "
    "--xla_gpu_enable_latency_hiding_scheduler=true "
    "--xla_gpu_enable_highest_priority_async_stream=true "
)
```

The last three flags focus on GPU communications, which are not relevant for this notebook, as we are focusing on single-GPU training. For later tutorials, these flags become more relevant.

With the flags set, we can start by importing the necessary libraries and setting up the notebook.

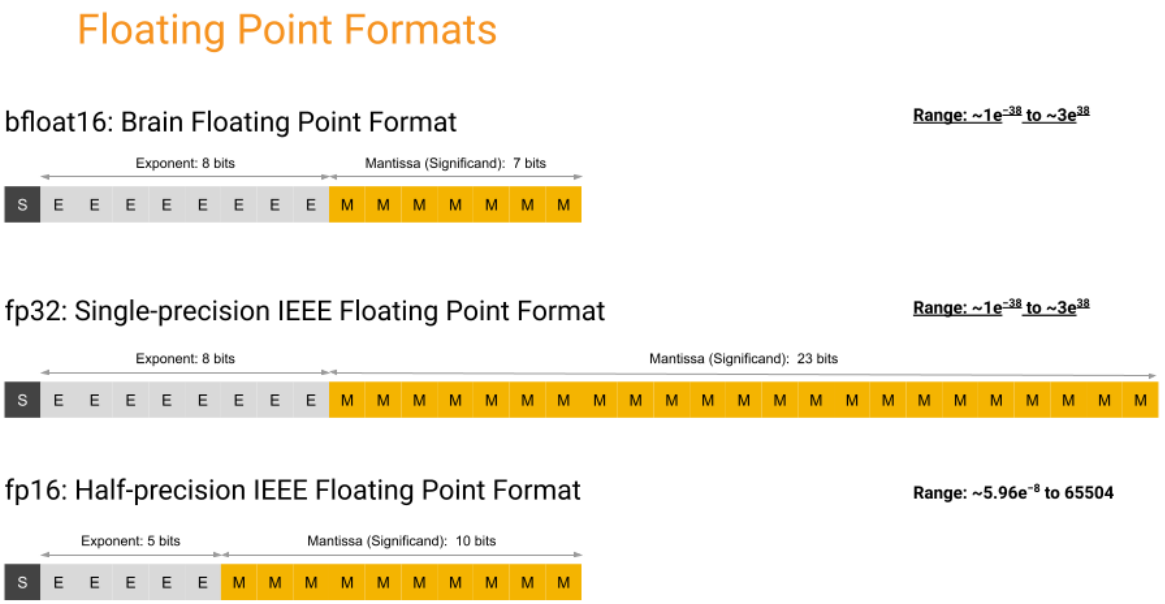
[2]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from flax.struct import dataclass
from flax.training import train_state

# Type aliases
PyTree = Any
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

4.6.1 Mixed Precision Training

As our first technique, we will explore mixed precision training. Mixed precision training is a technique that uses both 16-bit and 32-bit floating-point numbers to speed up training. The idea is to use 16-bit floating-point numbers for most of the computations, as they are faster and require less memory. However, 16-bit floating-point numbers have a smaller range and precision compared to 32-bit floating-point numbers. Therefore, we use 32-bit floating-point numbers for certain computations, such as the model's weight updates and the final loss computation, to avoid numerical instability.

A potential problem with `float16` is that we can encounter underflow and overflow issues during training. This means that the gradients or activations become too large or too small to be represented in the range of `float16`, and we lose information. Scaling the loss and gradients by a constant factor can help mitigate this issue to bring the values back into the representable range. This is known as loss scaling, and it is a common technique used in mixed precision training.

As an alternative, JAX and other deep learning frameworks like PyTorch also support the `bfloat16` format, which is a 16-bit floating-point format with 8 exponent bits and 7 mantissa bits. The `bfloat16` format has a larger range but lower precision compared to the IEEE half-precision type `float16`, and matches `float32` in terms of range. A closer comparison between the formats is shown in the figure below (figure credit: Google Cloud Documentation):



The main benefit of using `bfloat16` is that it can be used without loss scaling, as it has a larger range compared to `float16`. This allows `bfloat16` to be used as a drop-in replacement for `float32` in many cases to save memory and achieve performances close to `float32` (see e.g. JKalamkar et al., 2019). For situations where precision matters over range, `float16` may be the better option. Besides memory efficiency, many accelerators like TPUs and GPUs have native support for `bfloat16`, which can lead up to 2x speedup in training performance compared to `float32` on these devices. Hence, we will use `bfloat16` in this notebook.

We implement mixed precision training by lowering all features and activations within the model to `bfloat16`, while keeping the weights and optimizer states in `float32`. This is done to keep high precision for the weight updates and optimizer states, while reducing the memory footprint and increasing the training speed by using `bfloat16` for the forward and backward passes. While this does not reduce the memory footprint of the model parameters themselves, we often achieve a significant reduction in memory consumption due to the reduced memory footprint of the activations without influencing the model's performance. If the model itself is too large to fit into memory, one can also apply lower precision to the model parameters and/or optimizer (e.g. 1-bit Adam), but we will not cover this in this notebook.

Let's start by implementing mixed precision training on a toy example. We will use a simple MLP model for classification below. In Flax, we can control the data type of most modules in two ways: `param_dtype` is the data type in which the parameters are stored, and `dtype` is the data type in which the calculations are performed. We will set `param_dtype` to `float32` and `dtype` to `bfloat16` for the model's layers and activations. Other layers that do not require parameters, such as the activation functions or dropout layers, commonly use the data type of the input, which will be `bfloat16` in our case. To prevent numerical instabilities, it is commonly recommended to keep large reductions such as in softmax in `float32` (see e.g. here). Hence, we cast the final output to `float32` before computing the log softmax and the loss. With that, we can implement the mixed precision in Flax as follows:

[3]:
```
class MLPClassifier(nn.Module):
    dtype: Any
    hidden_size: int = 256
    num_classes: int = 100
    dropout_rate: float = 0.1

    @nn.compact
    def __call__(self, x: jax.Array, train: bool) -> jax.Array:
```

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```
        x = nn.Dense(
            features=self.hidden_size,
            dtype=self.dtype,  # Computation in specified dtype, params stay in float32
        )(x)
        x = nn.LayerNorm(dtype=self.dtype)(x)
        x = nn.silu(x)
        x = nn.Dropout(rate=self.dropout_rate, deterministic=not train)(x)
        x = nn.Dense(
            features=self.num_classes,
            dtype=self.dtype,
        )(x)
        x = x.astype(jnp.float32)
        x = nn.log_softmax(x, axis=-1)
        return x
```

We can investigate dtype usage in the model by using the `tabulate` function in Flax, listing all the parameters and module input/outputs with their dtype. This can be useful to ensure that the model is using the correct data types. Let's do this below for the original `float32` model:

[4]:
```
x = jnp.ones((512, 128), dtype=jnp.float32)
rngs = {"params": jax.random.PRNGKey(0), "dropout": jax.random.PRNGKey(1)}
model_float32 = MLPClassifier(dtype=jnp.float32)
model_float32.tabulate(rngs, x, train=True, console_kwargs={"force_jupyter": True})
```

MLPClassifier Summary

path	module	inputs	outputs	params
	MLPClassifier	- float32[512,128] - train: True	float32[512,100]	
Dense_0	Dense	float32[512,128]	float32[512,256]	bias: float32[256] kernel: float32[128,256] **33,024 (132.1 KB)**
LayerNorm_0	LayerNorm	float32[512,256]	float32[512,256]	bias: float32[256] scale: float32[256] **512 (2.0 KB)**
Dropout_0	Dropout	float32[512,256]	float32[512,256]	

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```
┃ Dense_1      ┃ Dense          ┃ float32[512,256]    ┃ float32[512,100] ┃ bias:␣
↪float32[100]        ┃
┃              ┃                ┃                     ┃                  ┃ kernel:␣
↪float32[256,100] ┃
┃              ┃                ┃                     ┃                  ┃                ␣
↪         ┃
┃              ┃                ┃                     ┃                  ┃ 25,700 (102.8␣
↪KB)         ┃
┡━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━
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```

[4]:
```
'\n\n'
```

As a comparison, we can now tabulate the same model with the `bfloat16` data type:

[5]:
```
model_bfloat16 = MLPClassifier(dtype=jnp.bfloat16)
model_bfloat16.tabulate(rngs, x, train=True, console_kwargs={"force_jupyter": True})
```

```
                                    MLPClassifier Summary
 path          module          inputs                outputs             params              ␣
↪
┃              ┃ MLPClassifier ┃ - float32[512,128] ┃ float32[512,100]  ┃                ␣
↪          ┃
┃              ┃               ┃ - train: True      ┃                   ┃                ␣
↪          ┃
┡━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━━━━╇━━━━━━━━━━━━━━━━
┃ Dense_0      ┃ Dense         ┃ float32[512,128]   ┃ bfloat16[512,256] ┃ bias:␣
↪float32[256]        ┃
┃              ┃               ┃                    ┃                   ┃ kernel:␣
↪float32[128,256] ┃
┃              ┃               ┃                    ┃                   ┃                ␣
↪          ┃
┃              ┃               ┃                    ┃                   ┃ 33,024 (132.1␣
↪KB)         ┃
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┃ LayerNorm_0  ┃ LayerNorm     ┃ bfloat16[512,256]  ┃ bfloat16[512,256] ┃ bias:␣
↪float32[256]        ┃
┃              ┃               ┃                    ┃                   ┃ scale:␣
↪float32[256]        ┃
┃              ┃               ┃                    ┃                   ┃                ␣
↪          ┃
┃              ┃               ┃                    ┃                   ┃ 512 (2.0 KB)   ␣
↪          ┃
```

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```
├──────────────────────────────────────────────────────────────────────────────────
│ Dropout_0    │ Dropout        │ bfloat16[512,256]  │ bfloat16[512,256]  │                    ␣
↪          │
├──────────────────────────────────────────────────────────────────────────────────
│ Dense_1      │ Dense          │ bfloat16[512,256]  │ bfloat16[512,100]  │ bias:␣
↪float32[100]        │
│              │                │                    │                    │ kernel:␣
↪float32[256,100] │
│              │                │                    │                    │                    ␣
↪          │
│              │                │                    │                    │ 25,700 (102.8␣
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└──────────────────────────────────────────────────────────────────────────────────
                                                                                   ␣
↪
                              Total Parameters: 59,236 (236.9 KB)                  ␣
↪
```

[5]: '\n\n'

As one can see, the model's parameters are still stored in `float32`, while the activations and inputs within the model are now in `bfloat16`. The initial input to the model is in `float32`, but the result of the first dense layer is casted down to `bfloat16` to enable the mixed precision training. The final output of the model is casted back to `float32` before computing the log softmax and the loss. In models like the Transformer, where we have a large activation memory footprint (batch size $\times$ sequence length $\times$ hidden size), this can lead to a significant reduction in memory consumption.

The rest of the training setup (loss function, gradient calculation, etc.) remains unchanged from the typical `float32` training. That's why we do not implement the full training loop here, but we will do so for the full transformer model later in this notebook.

4.6.2 Gradient Checkpointing / Activation Recomputation

Another technique to reduce the memory footprint of the activations is gradient checkpointing (this technique is known under several names, including activation checkpointing, activation recomputation, or rematerialization). Gradient checkpointing is a technique that trades compute for memory by recomputing some activations during the backward pass. The idea is to store only a subset of the activations during the forward pass, and recompute the rest of the activations during the backward pass. This can be useful when the memory consumption of the activations is the limiting factor for the model's size, and the recomputation of the activations is cheaper than storing them. This is often the case for models with a large memory footprint, such as the Transformer, where the activations can be a significant portion of the memory consumption.

As an example, consider a Transformer with only the MLP blocks (for simplicity). Each MLP block consists of two dense layers with a GELU activation in between, and uses a `bfloat16` activation (i.e. 2 bytes per activation). We refer to the batch size with B, sequence length with S, and hidden size H. The memory consumption of the activations in the forward pass is its input $2BSH$ bytes, the input to the GELU activations $8BSH$ bytes, the input to the output layer $8BSH$ bytes, and the dropout mask with size BSH. This results in a total memory consumption of $19BSH$ bytes (see Korthikanti et al., 2022 for a detailed computation). With gradient checkpointing, we could choose to only keep the original input tensor of size $2BSH$ and recompute the rest of the activations during the backward pass. This

would reduce the memory consumption of the activations by almost 90%, at the cost of recomputing the activations during the backward pass. This shows the potential of gradient checkpointing to reduce the memory footprint of the activations. We visualize the idea of gradient checkpointing in the figure below. For simplicity, we do not show the residual connections and layer normalization, but the idea is the same.

In JAX and Flax, we can implement gradient checkpointing using the `remat` function. The `remat` function allows us to control which intermediate arrays should be saved on the forward pass, and which are recomputed on the backward pass. As a simple example, consider the following function that computes the GELU activation function manually with its approximation (see e.g. Hendrycks and Gimpel, 2016). Note that in practice, we would use the `gelu` function from the `flax.nn` module which is already optimized, but we use this example to illustrate the concept of gradient checkpointing:

[6]:
```
def gelu(x: jax.Array) -> jax.Array:
    """GeLU activation function with approximate tanh."""
    # This will be printed once every time the function is executed.
    jax.debug.print("Executing GeLU")
    # See https://arxiv.org/abs/1606.08415 for details.
    x3 = jnp.power(x, 3)
    tanh_input = np.sqrt(2 / np.pi) * (x + 0.044715 * x3)
    return 0.5 * x * (1 + jnp.tanh(tanh_input))
```

In this function, we instantiate several intermediate tensors, which we may need to store during the backward pass and can be expensive for large tensors. Meanwhile, the computation is relatively cheap, such that we would want to compute these tensors during the backward pass instead of storing them. We can use the `remat` function to control which tensors are stored and which are recomputed during the backward pass. We can use the `remat` function as follows:

[7]:
```
def loss_fn(x: jax.Array, remat: bool) -> jax.Array:
    act_fn = gelu
    if remat:
        act_fn = jax.remat(act_fn)
    return jnp.mean(act_fn(x))
```

If we now transform this function with a `jax.grad` call, we will see that JAX is executing the function twice (we see the `Executing GeLU` print statement twice). This is because JAX is computing the forward pass, then releases all intermediate tensors, and then recomputes them again in the backward pass.

[8]:
```
x = jax.random.normal(jax.random.PRNGKey(0), (100,))
grad_fn = jax.grad(loss_fn)
_ = grad_fn(x, remat=True)
```

```
Executing GeLU
Executing GeLU
```

If we would run the same function without the `remat` function, we would only see the `Executing GeLU` print statement once, as JAX would not need to recompute the intermediate tensors during the backward pass.

[9]:
```
_ = loss_fn(x, remat=False)
```

```
Executing GeLU
```

This shows that the `remat` function is controlling which tensors are stored and which are recomputed during the backward pass. We will see in the later Transformer example how we can use it in a neural network layer.

In JAX, the XLA compiler can also automatically apply rematerialization to the forward pass when we jit the function. In that case, we do not need to use the `remat` function explicitly, as the XLA compiler will automatically apply rema-

terialization to the forward pass. However, it can still be beneficial to use the `remat` function in some cases, like in `scans` (see practical notes on remat) or to manually control which tensors are stored and which are recomputed.

4.6.3 Gradient Accumulation

A common trade-off in training large models is the batch size. A larger batch size can lead to a more accurate estimate of the gradient, but it also requires more memory. In some cases, the batch size is limited by the memory of the accelerator, and we cannot increase the batch size further. In these cases, we can use gradient accumulation to simulate a larger batch size by accumulating the gradients over multiple sub-batches. Each sub-batch is independently processed, and we perform an optimizer step once all sub-batches have been processed. Gradient accumulation can be useful when the memory consumption of the activations is the limiting factor for the model's size, but we require a larger batch size for training. However, a disadvantage of gradient accumulation is that each sub-batch is processed independently and sequentially, such that nothing is parallelized and we need to ensure that we can still utilize the accelerator to its full potential with the small batch size. The figure below gives an overview of the gradient accumulation process:

In the figure, we have a batch size of 8, and we accumulate the gradients over 4 sub-batches (we refer to sub-batches as minibatches here). Each sub-batch is of size 2, and we process them one by one. After we obtain the gradients for the first minibatch, we can free up all intermediate arrays of the forward and backward pass, and start processing the next minibatch. Once we have processed all minibatches, we can perform an optimizer step. This allows us to simulate a batch size of 8, while only requiring the memory of a batch size of 2.

In JAX and Flax, we have easy control over the gradient accumulation process, since we explicitly calculate the gradients via `jax.grad`. Let's implement this process for our simple classification MLP from the mixed precision training. We first create a train state from Flax, which we extend by an RNG for easier handling of dropout.

[10]:
```
class TrainState(train_state.TrainState):
    rng: jax.Array
```

We also create a dataclass to store all elements of a batch. In classification, this is usually the input (e.g. an image) and the target (e.g. a label).

[11]:
```
@dataclass
class Batch:
    inputs: jax.Array
    labels: jax.Array
```

We now define a loss function, which is still independent of gradient accumulation. The loss function applies the model and computes the cross-entropy loss. We also return a dictionary with metrics, where the key is the name of the metric, and the value is a tuple of the metric (summed over elements) and the number of elements seen. This allows us to compute the average of the metric later.

[12]:
```
def classification_loss_fn(
    params: PyTree, apply_fn: Any, batch: Batch, rng: jax.Array
) -> Tuple[PyTree, Metrics]:
    """Classification loss function with cross-entropy."""
    logits = apply_fn({"params": params}, batch.inputs, train=True, rngs={"dropout": rng}
↪)
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, batch.labels)
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), batch.labels)
    batch_size = batch.inputs.shape[0]
    step_metrics = {"loss": (loss.sum(), batch_size), "accuracy": (correct_pred.sum(),␣
↪batch_size)}
```

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```
    loss = loss.mean()
    return loss, step_metrics
```

With this set up, we can implement the gradient accumulation process. Given a batch, we split it into multiple sub-batches, and execute the gradient function of the loss function for each sub-batch. We then accumulate the gradients and return the accumulated gradients. We also accumulate the metrics, such that we can compute the average of the metrics later. Note that we do not need to explicitly free up the memory of the forward and backward pass, as the XLA compiler will automatically release the memory after the gradient function has been executed. We implement it below with an for-loop over the sub-batches:

[13]:
```
def accumulate_gradients_loop(
    state: TrainState,
    batch: Batch,
    rng: jax.random.PRNGKey,
    num_minibatches: int,
    loss_fn: Callable,
) -> Tuple[PyTree, Metrics]:
    """Calculate gradients and metrics for a batch using gradient accumulation.

    Args:
        state: Current training state.
        batch: Full training batch.
        rng: Random number generator to use.
        num_minibatches: Number of minibatches to split the batch into. Equal to the␣
↪number of gradient accumulation steps.
        loss_fn: Loss function to calculate gradients and metrics.

    Returns:
        Tuple with accumulated gradients and metrics over the minibatches.
    """
    batch_size = batch.inputs.shape[0]
    minibatch_size = batch_size // num_minibatches
    rngs = jax.random.split(rng, num_minibatches)
    # Define gradient function for single minibatch.
    grad_fn = jax.value_and_grad(loss_fn, has_aux=True)
    # Prepare loop variables.
    grads = None
    metrics = None
    for minibatch_idx in range(num_minibatches):
        with jax.named_scope(f"minibatch_{minibatch_idx}"):
            # Split the batch into minibatches.
            start = minibatch_idx * minibatch_size
            end = start + minibatch_size
            minibatch = jax.tree_map(lambda x: x[start:end], batch)
            # Calculate gradients and metrics for the minibatch.
            (_, step_metrics), step_grads = grad_fn(
                state.params, state.apply_fn, minibatch, rngs[minibatch_idx]
            )
            # Accumulate gradients and metrics across minibatches.
            if grads is None:
                grads = step_grads
                metrics = step_metrics
```

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```
            else:
                grads = jax.tree_map(jnp.add, grads, step_grads)
                metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    # Average gradients over minibatches.
    grads = jax.tree_map(lambda g: g / num_minibatches, grads)
    return grads, metrics
```

A disadvantage of the implementation above is that we need to compile the gradient function for each sub-batch, which can be slow. We can avoid this by using the `scan` transformation in JAX (docs), which allows us to write a for-loop with a single compilation of the inner step. The `scan` transformation requires the function to take two inputs: the `carry` and the input `x`. The `carry` is the state that is passed between the steps, and the `x` input is the input to the current step. The function returns the new `carry` and any output that we want to gather per step. In our case, the `carry` is the accumulated gradients and the accumulated metrics of all previous steps, and the `x` input is the current minibatch index, with which we select the minibatch and RNG to use. As the new carry, we return the updated accumulated gradients and metrics, and do not require a per-step output. We implement the gradient accumulation with `scan` below:

[14]:
```
def accumulate_gradients_scan(
    state: TrainState,
    batch: Batch,
    rng: jax.random.PRNGKey,
    num_minibatches: int,
    loss_fn: Callable,
) -> Tuple[PyTree, Metrics]:
    """Calculate gradients and metrics for a batch using gradient accumulation.

    In this version, we use `jax.lax.scan` to loop over the minibatches. This is more␣
↪efficient in terms of compilation time.

    Args:
        state: Current training state.
        batch: Full training batch.
        rng: Random number generator to use.
        num_minibatches: Number of minibatches to split the batch into. Equal to the␣
↪number of gradient accumulation steps.
        loss_fn: Loss function to calculate gradients and metrics.

    Returns:
        Tuple with accumulated gradients and metrics over the minibatches.
    """
    batch_size = batch.inputs.shape[0]
    minibatch_size = batch_size // num_minibatches
    rngs = jax.random.split(rng, num_minibatches)
    grad_fn = jax.value_and_grad(loss_fn, has_aux=True)

    def _minibatch_step(minibatch_idx: jax.Array | int) -> Tuple[PyTree, Metrics]:
        """Determine gradients and metrics for a single minibatch."""
        minibatch = jax.tree_map(
            lambda x: jax.lax.dynamic_slice_in_dim(  # Slicing with variable index (jax.
↪Array).
                x, start_index=minibatch_idx * minibatch_size, slice_size=minibatch_size,
↪ axis=0
            ),
```

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```
            batch,
        )
        (_, step_metrics), step_grads = grad_fn(
            state.params, state.apply_fn, minibatch, rngs[minibatch_idx]
        )
        return step_grads, step_metrics

    def _scan_step(
        carry: Tuple[PyTree, Metrics], minibatch_idx: jax.Array | int
    ) -> Tuple[Tuple[PyTree, Metrics], None]:
        """Scan step function for looping over minibatches."""
        step_grads, step_metrics = _minibatch_step(minibatch_idx)
        carry = jax.tree_map(jnp.add, carry, (step_grads, step_metrics))
        return carry, None

    # Determine initial shapes for gradients and metrics.
    grads_shapes, metrics_shape = jax.eval_shape(_minibatch_step, 0)
    grads = jax.tree_map(lambda x: jnp.zeros(x.shape, x.dtype), grads_shapes)
    metrics = jax.tree_map(lambda x: jnp.zeros(x.shape, x.dtype), metrics_shape)
    # Loop over minibatches to determine gradients and metrics.
    (grads, metrics), _ = jax.lax.scan(
        _scan_step, init=(grads, metrics), xs=jnp.arange(num_minibatches), length=num_
↪minibatches
    )
    # Average gradients over minibatches.
    grads = jax.tree_map(lambda g: g / num_minibatches, grads)
    return grads, metrics
```

Especially for very large models, where the compilation time will be significant, the `scan` transformation can lead to a significant speedup of the compilation. However, for the small model in this example, the speedup may be small. We add a small wrapper below to allow for both versions, although we will mainly use the `scan` version.

[15]:
```
def accumulate_gradients(*args, use_scan: bool = False, **kwargs) -> Tuple[PyTree,␣
↪Metrics]:
    if use_scan:
        return accumulate_gradients_scan(*args, **kwargs)
    else:
        return accumulate_gradients_loop(*args, **kwargs)
```

After having accumulated the gradients of all batches, we can perform the optimizer step. We implement this in the final training step below:

[16]:
```
def train_step(
    state: TrainState,
    metrics: Metrics | None,
    batch: Batch,
    num_minibatches: int,
) -> Tuple[TrainState, Metrics]:
    """Training step function.

    Executes a full training step with gradient accumulation.
```

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```
    Args:
        state: Current training state.
        metrics: Current metrics, accumulated from previous training steps.
        batch: Training batch.
        num_minibatches: Number of minibatches to split the batch into. Equal to the␣
↪number of gradient accumulation steps.

    Returns:
        Tuple with updated training state (parameters, optimizer state, etc.) and␣
↪metrics.
    """
    # Split the random number generator for the current step.
    rng, step_rng = jax.random.split(state.rng)
    # Determine gradients and metrics for the full batch.
    grads, step_metrics = accumulate_gradients(
        state, batch, step_rng, num_minibatches, loss_fn=classification_loss_fn, use_
↪scan=True
    )
    # Optimizer step.
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Accumulate metrics across training steps.
    if metrics is None:
        metrics = step_metrics
    else:
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

Let's now test the implementation for training our small classifier on a single batch. We first define the random number generator keys and hyperparameters, and generate the example batch. Feel free to change the hyperparameters to see how the model behaves with different settings.

[17]:
```
batch_size = 512
num_inputs = 128
num_classes = 100
rng_seed = 0

rng = jax.random.PRNGKey(rng_seed)
data_input_rng, data_label_rng, model_rng, state_rng = jax.random.split(rng, 4)
batch = Batch(
    inputs=jax.random.normal(data_input_rng, (batch_size, num_inputs)),
    labels=jax.random.randint(data_label_rng, (batch_size,), 0, num_classes),
)
```

We can now create the model and optimizer, and initialize the parameters as usual. We set the dropout rate to 0 to compare the training with and without gradient accumulation.

[18]:
```
# Zero dropout for checking later equality between training with and without gradient␣
↪accumulation.
model = MLPClassifier(dtype=jnp.bfloat16, dropout_rate=0.0)
params = model.init(model_rng, batch.inputs, train=False)["params"]
state = TrainState.create(
    apply_fn=model.apply,
```

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```
    params=params,
    tx=optax.adam(1e-3),
    rng=state_rng,
)
```

Before we can train, we need to initialize the metric PyTree which we want to pass to the train step. While we could start with `metrics=None`, as the train step supports, it would be inefficient since we need to compile twice: once for `metrics=None`, and once for `metrics` being a PyTree. We can avoid this by inferring the shape and structure of the metric PyTree via `jax.eval_shape`, which only evaluates the shapes of the `train_step` without executing the function or compilation. Once we have the shape, we can initialize a metric PyTree with zeros and pass it to the train step. We implement this below:

[19]:
```
_, metric_shapes = jax.eval_shape(
    functools.partial(train_step, num_minibatches=4),
    state,
    None,
    batch,
)
print("Metric shapes:")
pprint(metric_shapes)
```

```
Metric shapes:
{'accuracy': (ShapeDtypeStruct(shape=(), dtype=int32),
              ShapeDtypeStruct(shape=(), dtype=int32)),
 'loss': (ShapeDtypeStruct(shape=(), dtype=float32),
          ShapeDtypeStruct(shape=(), dtype=int32))}
```

We then jit the train step, but define the number of minibatches to be a static argument. This means that for every different value of `num_minibatches`, we will need to recompile the train step, but keep them in cache for the same value of `num_minibatches`. This is useful in this case where we want to train the model with different number of gradient accumulation steps and compare the outputs.

[20]:
```
train_step_jit = jax.jit(
    train_step,
    static_argnames="num_minibatches",
)
```

We finally write a small training loop to train the model.

[21]:
```
def train_with_minibatches(
    state: TrainState,
    batch: Batch,
    num_minibatches: int,
    num_train_steps: int,
) -> Tuple[TrainState, Metrics]:
    """Small helper function for training loop."""
    train_metrics = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
    for _ in range(num_train_steps):
        state, train_metrics = train_step_jit(state, train_metrics, batch, num_
↪minibatches)
    return state, train_metrics
```

We also add a small function to print the metrics nicely.

[22]:
```
def print_metrics(metrics: Metrics, title: str | None = None) -> None:
    """Prints metrics with an optional title."""
    metrics = jax.device_get(metrics)
    lines = [f"{k}: {v[0] / v[1]:.6f}" for k, v in metrics.items()]
    if title:
        title = f" {title} "
        max_len = max(len(title), max(map(len, lines)))
        lines = [title.center(max_len, "=")] + lines
    print("\n".join(lines))
```

To validate our gradient accumulation implementation, we can compare the results of the model trained with and without gradient accumulation.

[23]:
```
state_mini1, metrics_mini1 = train_with_minibatches(
    state, batch, num_minibatches=1, num_train_steps=5
)
state_mini4, metrics_mini4 = train_with_minibatches(
    state, batch, num_minibatches=4, num_train_steps=5
)
print_metrics(metrics_mini1, "Minibatch 1")
print_metrics(metrics_mini4, "Minibatch 4")
```

```
== Minibatch 1 ===
accuracy: 0.026953
loss: 4.593200
== Minibatch 4 ===
accuracy: 0.026953
loss: 4.593173
```

We find that the model trained with gradient accumulation has the same loss and accuracy as the model trained without gradient accumulation. Note that small differences can occur due to using limited precision and we have different reduce operations happening in the two setups. In the gradient accumulation, we add the gradients one by one, while in the single batch, we calculate the gradients at once. However, the differences should be small and not affect the overall performance of the model. Additionally, if we would use dropout, we would expect the models to slightly differ due to the different dropout masks being used in the two setups, but the overall performance should be similar.

We could also compare the memory consumption of the two training processes to see the impact of gradient accumulation on the memory footprint, but due to the small model size, the memory consumption is not significantly different. We will see the impact of gradient accumulation on the memory footprint in the later Transformer example.

4.6.4 JAX-Specific Structures

In JAX, we can also use some JAX-specific structures to reduce the memory footprint of the model and help training larger models. These may not be useful for other frameworks like PyTorch, but good to keep in mind for JAX users. We cover two aspects: donating buffers and scanning.

Donating buffers

In JAX, we follow the idea of functional programming where all functions need to be stateless and pure. This means that we cannot modify the input arguments, and we cannot modify other global variables. This is also true for the model parameters, which are passed as arguments to the training step and returned with updated values. This enforces the device to have memory for at least twice the model parameters and optimizer state. However, as the model grows in size, this can become a significant limitation. To mitigate this, JAX provides a mechanism to donate buffers, which allows us to reuse the memory of the input arguments for the output arguments. This can be useful when the input and output arguments have the same shape and data type, and we do not need the input arguments after the function has been executed. This is often the case for the model parameters and optimizer state, where we do not need the input arguments after the optimizer step has been executed. We can use the `jax.jit` function with the `donate_argnums`/`donate_argnames` argument to donate buffers. We can donate buffers for the model parameters and optimizer state, which can reduce the memory footprint of the model and help training larger models. We implement this below for the training step:

[24]:
```
train_step_donated = jax.jit(
    train_step,
    static_argnames="num_minibatches",
    donate_argnames=(
        "state",
        "metrics",
    ),
)
```

If we now execute the training step with the `donate_argnames` argument, JAX will try to reuse the input buffers whenever possible. If the buffers are not usable, for instance because the output has different shapes or data types, JAX will allocate new memory for the output and we will see a warning (see more in here). For large models, we want to make sure that JAX can reuse the model parameter and optimizer state buffers, as this can significantly reduce the memory footprint of the model.

Scanning layers for faster compilation

In JAX, the compilation time can be a significant bottleneck, especially for large models. In the gradient accumulation section, we already have seen how we can use the `scan` transformation to reduce the compilation time. However, we can also use the lifted `scan` transformation from Flax to scan over the layers of the model to reduce the compilation time (docs). This can be useful when we have a large model with many layers, and we want to reduce the compilation time. We can use the `scan` transformation to compile the forward and backward pass of the individual layer only once, and reuse it throughout the model execution. This can significantly reduce the compilation time, especially for large models. We can implement this for the Transformer model in the later section.

4.6.5 Intermediate Summary

In this notebook, we have discussed several techniques to train larger models on a single device. We have implemented mixed precision training, gradient accumulation, and gradient checkpointing on a simple MLP model. We have also discussed JAX-specific structures to reduce the memory footprint of the model and help training larger models. In the next part (Part 1.2), we will combine these techniques to train a larger Transformer model on a single GPU, and explore the benefits and trade-offs of each technique. We will also profile the model to get further insights into the efficiency of these techniques.

4.6.6 References and Resources

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[Kalamkar et al., 2019] Kalamkar, D., Mudigere, D., Mellempudi, N., Das, D., Banerjee, K., Avancha, S., Vooturi, D.T., Jammalamadaka, N., Huang, J., Yuen, H. and Yang, J., 2019. A study of BFLOAT16 for deep learning training. arXiv preprint arXiv:1905.12322. Paper link

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[Weng et al., 2022] Weng, L., Brockman, G., 2022. Techniques for training large neural networks. Blog link

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[HuggingFace, 2024] HuggingFace, 2024. Performance and Scalability: How To Fit a Bigger Model and Train It Faster. Tutorial link

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[NVIDIA, 2024] NVIDIA, 2024. Performance Guide for Training. Documentation link

[Google, 2024] JAX Team Google, 2024. Control autodiff's saved values with jax.checkpoint (aka jax.remat). Tutorial link

[Google, 2024] JAX Team Google, 2024. Profiling JAX programs. Tutorial link

[Google, 2024] JAX Team Google, 2024. GPU peformance tips. Tutorial link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.7 Part 1.2: Profiling and Scaling Single-GPU Transformer Models

Filled notebook:

Author: Phillip Lippe

In the previous part, we have seen how to implement mixed precision training, gradient accumulation, and gradient checkpointing on a simple MLP model. In this part, we will apply these techniques to a transformer model and see how they can help us to train large models with limited resources. We will also see how to profile the model to identify bottlenecks and optimize the performance. It is recommended to go through Part 1.1 before starting this part, as we will be using the same techniques and concepts. We also assume that you are familiar with the transformer model and its components. If you are not, you can refer to the transformer model paper by Vaswani et al. and our transformer tutorial.

This notebook is designed to run on an accelerator, such as a GPU or TPU. If you are running this notebook on Google Colab, you can enable the GPU runtime. You can do this by clicking on `Runtime` in the top menu, then `Change runtime type`, and selecting `GPU` from the `Hardware accelerator` dropdown. If the runtime fails, feel free to disable the GPU and run the notebook on the CPU. In that case, we recommend to adjust the configuration of the model to fit the available resources.

4.7.1 Prerequisites

To reduce code duplication between notebooks, we import functions from the previous notebook. For this, we have converted the most important functions into a python script and uploaded it to the same repository. If you run on Google Colab, we need to download the python script before importing the functions. If you the notebook locally, it will be already available.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = ["single_gpu.py", "utils.py"]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

The file `utils.py` contains some simple functionalities, such as setting the XLA flags we have seen in the previous tutorial. Let's do that first.

[2]:
```
from utils import install_package, set_XLA_flags_gpu

set_XLA_flags_gpu()
```

We import our standard libraries below.

[3]:
```
import functools
from typing import Any, Dict, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from tqdm.auto import tqdm

# Install ml_collections on colab
try:
    from ml_collections import ConfigDict
except ModuleNotFoundError:
    install_package("ml_collections")
    from ml_collections import ConfigDict

# Type aliases
PyTree = Any
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

Finally, we import the functions and modules from our previous tutorial. If you are not familiar with any of these, check out Part 1.1.

[4]:
```
from single_gpu import Batch, TrainState, accumulate_gradients, print_metrics
```

4.7.2 Building an Optimized Transformer Model

In the following section, we will combine mixed precision, gradient checkpointing and gradient accumulation to train a larger Transformer model on a single GPU.

Model Definition

For passing hyperparameters and configurations to our modules, we will make use of ml-collections' `ConfigDict` class (docs). A config dict is a dict-like data structure that supports dot access to its keys, and provides a 'frozen' version which is useful for JAX.

We start with implementing the MLP layer in the Transformer model. We support mixed precision from before.

[5]:
```
class MLPBlock(nn.Module):
    config: ConfigDict
    train: bool

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        input_features = x.shape[-1]
```

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```
        x = nn.LayerNorm(dtype=self.config.dtype, name="pre_norm")(x)
        x = nn.Dense(
            features=self.config.mlp_expansion * input_features,
            dtype=self.config.dtype,
            name="input_layer",
        )(x)
        x = nn.gelu(x)
        x = nn.Dense(
            features=input_features,
            dtype=self.config.dtype,
            name="output_layer",
        )(x)
        x = nn.Dropout(rate=self.config.dropout_rate, deterministic=not self.train)(x)
        return x
```

Next, we turn to the attention block. To support mixed precision with numerical stability, we cast the attention weights to `float32` before the softmax operation, as discussed before. In cases where we would use `float16` precision, the dot product could occasionally go out of range, leading to numerical instability (see e.g. Karras et al., 2023). Thus, we cast the query and key tensors to `float32` before the softmax operation, and cast the attention weights back to `bfloat16` after the softmax operation. Alternatively, one could also keep the query and key tensors in `bfloat16` if we are just short of GPU memory. We implement the adjusted dot product attention below:

[6]:
```
def dot_product_attention(
    query: jax.Array,
    key: jax.Array,
    value: jax.Array,
    mask: jax.Array | None,
    softmax_dtype: jnp.dtype = jnp.float32,
):
    """Dot-product attention.

    Follows the setup of https://flax.readthedocs.io/en/latest/api_reference/flax.linen/
↪layers.html#flax.linen.dot_product_attention,
    but supports switch to float32 for numerical stability during softmax.

    Args:
        query: The query array, shape [..., num queries, num heads, hidden size].
        key: The key array, shape [..., num keys, num heads, hidden size].
        value: The value array, shape [..., num keys, num heads, hidden size].
        mask: The boolean mask array (0 for masked values, 1 for non-masked). If None,␣
↪no masking is applied.
        softmax_dtype: The dtype to use for the softmax and dot-product operation.

    Returns:
        The attention output array, shape [..., num queries, num heads, hidden size].
    """
    num_features = query.shape[-1]
    dtype = query.dtype
    scale = num_features**-0.5
    query = query * scale
    # Switch dtype right before the dot-product for numerical stability.
    query = query.astype(softmax_dtype)
```

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```
    key = key.astype(softmax_dtype)
    weights = jnp.einsum("...qhd,...khd->...hqk", query, key)
    if mask is not None:
        weights = jnp.where(mask, weights, jnp.finfo(softmax_dtype).min)
    weights = nn.softmax(weights, axis=-1)
    # After softmax, switch back to the original dtype
    weights = weights.astype(dtype)
    new_vals = jnp.einsum("...hqk,...khd->...qhd", weights, value)
    new_vals = new_vals.astype(dtype)
    return new_vals
```

With that, we can implement the attention block below. We use `nn.DenseGeneral` to implement the linear projections. Depending on the size of the hidden size, it may be beneficial to split the query, key and value projections into multiple smaller projections, also to give the XLA compiler more flexibility to schedule the computation. For simplicity, we use a single layer projection here, which is commonly more efficient for small model sizes.

[7]:
```
class AttentionBlock(nn.Module):
    config: ConfigDict
    mask: jax.Array | None
    train: bool

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        input_features = x.shape[-1]
        x = nn.LayerNorm(dtype=self.config.dtype, name="pre_norm")(x)
        qkv = nn.DenseGeneral(
            features=(self.config.num_heads, self.config.head_dim * 3),
            dtype=self.config.dtype,
            name="qkv",
        )(x)
        q, k, v = jnp.split(qkv, 3, axis=-1)
        x = dot_product_attention(q, k, v, mask=self.mask, softmax_dtype=self.config.
↪softmax_dtype)
        x = nn.DenseGeneral(
            features=input_features,
            axis=(-2, -1),
            dtype=self.config.dtype,
            name="output_layer",
        )(x)
        x = nn.Dropout(rate=self.config.dropout_rate, deterministic=not self.train)(x)
        return x
```

We can now combine the two blocks to implement a full Transformer block. In this block, we want to support gradient checkpointing around the two individual blocks. For this, we consider the config to have a `remat` key, which contains a sequence of names, indicating the functions/modules to remat. We implement the Transformer block below:

[8]:
```
class TransformerBlock(nn.Module):
    config: ConfigDict
    mask: jax.Array | None
    train: bool

    @nn.compact
```

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```
    def __call__(self, x: jax.Array) -> jax.Array:
        # MLP block
        mlp = MLPBlock
        if "MLP" in self.config.remat:
            mlp = nn.remat(mlp, prevent_cse=False)
        x = x + mlp(config=self.config, train=self.train, name="mlp")(x)
        # Attention block
        attn = AttentionBlock
        if "Attn" in self.config.remat:
            attn = nn.remat(attn, prevent_cse=False)
        x = x + attn(config=self.config, mask=self.mask, train=self.train, name="attn
↪")(x)
        return x
```

With that, we are ready to implement the full Transformer model. We use the `scan` transformation to scan over the layers of the model to reduce the compilation time. We implement a text-based GPT-style autoregressive model, which uses an embedding layer to embed the input tokens, and a stack of Transformer blocks to process the tokens. We also add a final dense layer to map the output tokens to the vocabulary size. We implement the model below:

[9]:
```
class Transformer(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(
        self, x: jax.Array, mask: jax.Array | None = None, train: bool = True
    ) -> jax.Array:
        if mask is None and self.config.causal_mask:
            mask = nn.make_causal_mask(x, dtype=jnp.bool_)
        # Input layer.
        x = nn.Embed(
            num_embeddings=self.config.vocab_size,
            features=self.config.hidden_size,
            dtype=self.config.dtype,
            name="embed",
        )(x)
        pos_emb = self.param(
            "pos_emb",
            nn.initializers.normal(stddev=0.02),
            (self.config.max_seq_len, self.config.hidden_size),
        )
        pos_emb = pos_emb.astype(self.config.dtype)
        x = x + pos_emb[None, : x.shape[1]]
        # Transformer blocks.
        block_fn = functools.partial(TransformerBlock, config=self.config, mask=mask,␣
↪train=train)
        if "Block" in self.config.remat:
            block_fn = nn.remat(block_fn, prevent_cse=False)
        if self.config.scan_layers:
            block = block_fn(name="block")
            x, _ = nn.scan(
                lambda module, carry, _: (module(carry), None),
                variable_axes={"params": 0},
```

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```
                split_rngs={"params": True, "dropout": True},
                length=self.config.num_layers,
            )(block, x, ())
        else:
            for l_idx in range(self.config.num_layers):
                x = block_fn(name=f"block_{l_idx}")(x)
        # Output layer.
        x = nn.LayerNorm(dtype=self.config.dtype, name="post_norm")(x)
        x = nn.Dense(
            features=self.config.num_outputs,
            dtype=self.config.dtype,
            name="output_layer",
        )(x)
        x = x.astype(jnp.float32)
        return x
```

Initialization

With the model set up, we can continue with the initialization. The initialization process is as usual, besides that we create a more detailed config dict below to specify all hyperparameters in the model. By default, we run with `bfloat16` precision and remat the MLP and Attention block. The model has 12 layers with a hidden size of 1024. We also create a config for the data, which we will use to create the example batch. We create batches with 64k tokens, which is large for a single GPU, but language models often train with ~1M tokens per batch. Feel free to change the hyperparameters to see how the model behaves with different settings.

[10]:
```
data_config = ConfigDict(
    dict(
        batch_size=64,
        seq_len=512,
        vocab_size=2048,
    )
)
model_config = ConfigDict(
    dict(
        hidden_size=1024,
        dropout_rate=0.1,
        mlp_expansion=4,
        num_layers=12,
        head_dim=128,
        causal_mask=True,
        max_seq_len=data_config.seq_len,
        vocab_size=data_config.vocab_size,
        num_outputs=data_config.vocab_size,
        dtype=jnp.bfloat16,
        softmax_dtype=jnp.float32,
        scan_layers=True,
        remat=("MLP", "Attn"),
    )
)
model_config.num_heads = model_config.hidden_size // model_config.head_dim
optimizer_config = ConfigDict(
```

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```
    dict(
        learning_rate=4e-4,
        num_minibatches=4,
    )
)
config = ConfigDict(
    dict(
        model=model_config,
        optimizer=optimizer_config,
        data=data_config,
        seed=42,
    )
)
```

We now create the model and initialize the parameters. We set the optimizer to be Adam with a warmup exponential decay schedule, although the optimizer is not really relevant for the simple example at hand.

[11]:
```
model = Transformer(config=config.model)
optimizer = optax.adam(
    learning_rate=optax.warmup_exponential_decay_schedule(
        init_value=0,
        peak_value=config.optimizer.learning_rate,
        warmup_steps=10,
        transition_steps=1,
        decay_rate=0.99,
    )
)
```

We train the model again on a single example batch. Since we perform autoregressive language modeling as the task, the input are the tokens shifted by one, and the target are the original tokens. We also use a causal mask, specified in the config, to prevent the model from attending to future tokens.

[12]:
```
tokens = jax.random.randint(
    jax.random.PRNGKey(0),
    (config.data.batch_size, config.data.seq_len),
    1,
    config.data.vocab_size,
)
batch_transformer = Batch(
    inputs=jnp.pad(tokens[:, :-1], ((0, 0), (1, 0)), constant_values=0),
    labels=tokens,
)
```

Finally, we initialize the parameters of the model, in the same way as before.

[13]:
```
model_rng, state_rng = jax.random.split(jax.random.PRNGKey(config.seed))
params = model.init(
    model_rng,
    batch_transformer.inputs[: config.data.batch_size // config.optimizer.num_
↪minibatches],
    train=False,
)["params"]
state = TrainState.create(
```

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```
    apply_fn=model.apply,
    params=params,
    tx=optimizer,
    rng=state_rng,
)
```

Let's check the number of parameters below.

[14]:
```
def get_num_params(state: TrainState) -> int:
    return sum(np.prod(x.shape) for x in jax.tree_util.tree_leaves(state.params))


print(f"Number of parameters: {get_num_params(state):_}")
```

```
Number of parameters: 155_877_376
```

With 150M parameters, the model is still relatively small compared to today's language models, but still challenging to fit on a single GPU. Furthermore, with a batch size of 64k tokens, the memory consumption of the activations is already significant.

Training

We can now train the model with gradient accumulation. We set the number of gradient accumulation steps to 4, which means that we accumulate the gradients over 4 sub-batches. We first define a loss function, which is very similar to the classification loss we have seen before, adjusted to allow for sequences.

[15]:
```
def next_token_pred_loss(
    params: PyTree, apply_fn: Any, batch: Batch, rng: jax.Array
) -> Tuple[PyTree, Metrics]:
    """Next token prediction loss function."""
    logits = apply_fn({"params": params}, batch.inputs, train=True, rngs={"dropout": rng}
↪)
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, batch.labels)
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), batch.labels)
    batch_size = np.prod(batch.labels.shape)
    step_metrics = {"loss": (loss.sum(), batch_size), "accuracy": (correct_pred.sum(),␣
↪batch_size)}
    loss = loss.mean()
    return loss, step_metrics
```

We also adjust the train step to use the new loss function. Everything else remains unchanged in the train step.

[16]:
```
@functools.partial(
    jax.jit,
    donate_argnames=(
        "state",
        "metrics",
    ),
)
def train_step_transformer(
    state: TrainState,
    metrics: Metrics | None,
```

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```
    batch: Batch,
) -> Tuple[TrainState, Metrics]:
    """Training step function.

    Executes a full training step with gradient accumulation for the next-token␣
↪prediction task.

    Args:
        state: Current training state.
        metrics: Current metrics, accumulated from previous training steps.
        batch: Training batch.

    Returns:
        Tuple with updated training state (parameters, optimizer state, etc.) and␣
↪metrics.
    """
    # Split the random number generator for the current step.
    rng, step_rng = jax.random.split(state.rng)
    # Determine gradients and metrics for the full batch.
    grads, step_metrics = accumulate_gradients(
        state,
        batch,
        step_rng,
        config.optimizer.num_minibatches,
        loss_fn=next_token_pred_loss,
        use_scan=True,
    )
    # Optimizer step.
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Accumulate metrics across training steps.
    if metrics is None:
        metrics = step_metrics
    else:
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

We now determine the metric shapes and initialize the metric PyTree, as we did before.

[17]:
```
_, metric_shapes = jax.eval_shape(
    train_step_transformer,
    state,
    None,
    batch_transformer,
)
metrics = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
```

Now, we can finally train the model. The goal of the training is not to show the model's performance, but to show the impact of the different techniques on the memory footprint and training speed. Feel free to experiment with different hyperparameters to see how the model behaves with different settings.

[18]:
```
for _ in tqdm(range(4)):
    state, metrics = train_step_transformer(state, metrics, batch_transformer)
```

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```
final_metrics = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
state, final_metrics = train_step_transformer(state, final_metrics, batch_transformer)
print_metrics(final_metrics, "Final metrics - Transformer")
```

```
  0%|          | 0/4 [00:00<?, ?it/s]
```

```
 Final metrics - Transformer
accuracy: 0.000916
loss: 7.776346
```

4.7.3 Profiling

To gain further insights into the model execution and see the individual operations, we can profile the model (documentation). In JAX, profiling the model creates a trace file which we can view in tools like Chrome's Trace Viewer or TensorBoard. We can start the profiling via `jax.profiler.start_trace`, and stop it with `jax.profiler.stop_trace`. Alternatively, one can use a context manager to start and stop the profiling. For the profiling, we run three training steps to get a good overview of the model execution and reduce the potential impact of the profiler on the model execution. Further, we can annotate operations in the trace via `jax.profiler.StepTraceAnnotation` or `jax.named_scope`, to better understand the model execution. Finally, before stopping the trace, we wait for the last train step to finish by blocking the execution until the metrics are ready. We implement the profiling below:

[19]:
```
jax.profiler.start_trace("traces/")
for i in range(3):
    with jax.profiler.StepTraceAnnotation("train_step", step_num=i + 1):
        state, metrics = train_step_transformer(state, metrics, batch_transformer)
metrics["loss"][0].block_until_ready()
jax.profiler.stop_trace()
```

With the trace generated, we can now visualize the model execution in TensorBoard. For this, we switch to the tab `Profiler` and load the newest trace file. Under `trace_viewer@`, we can see the individual operations and their execution time. Additionally, we can inspect the used memory in the `memory_viewer` tab (select `jit_train_step_transformer` under modules). The cell below is commented out, as it may take a while to start the TensorBoard, but feel free to run it to inspect the trace on your local machine.

[20]:
```
# %load_ext tensorboard
# %tensorboard --logdir traces/single_gpu_transformer
```

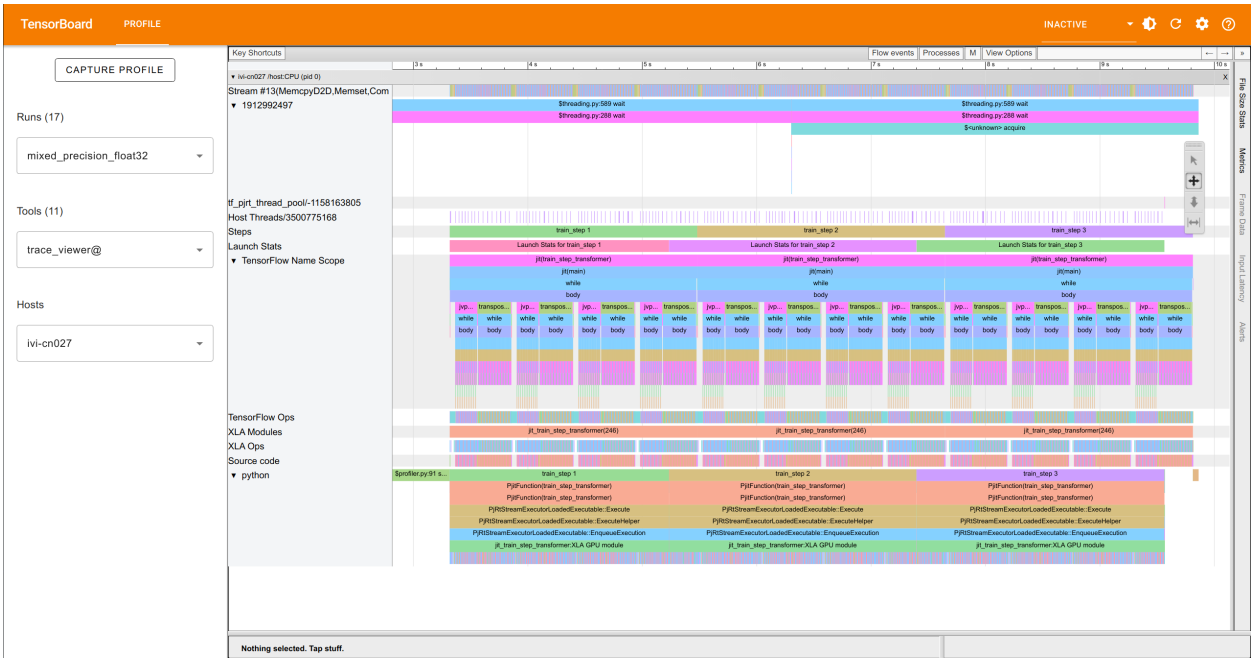
Since the trace will be different for different hyperparameters and different hardware configurations, we have uploaded some example runs here. Feel free to download them and investigate the models yourself. All experiments were run on a single A5000 GPU, which has up to 24GB of memory. Below, we go through some example traces to show the impact of the individual techniques on the model execution, and explain how to read the profiler output.

Profiler Overview

The profiler in TensorBoard is a powerful tool to find understand your model execution and find bottlenecks. For a full overview of the profiler, we recommend the official documentation. Here, we give a brief overview of the most important tabs and how to read the profiler output.

Trace Viewer

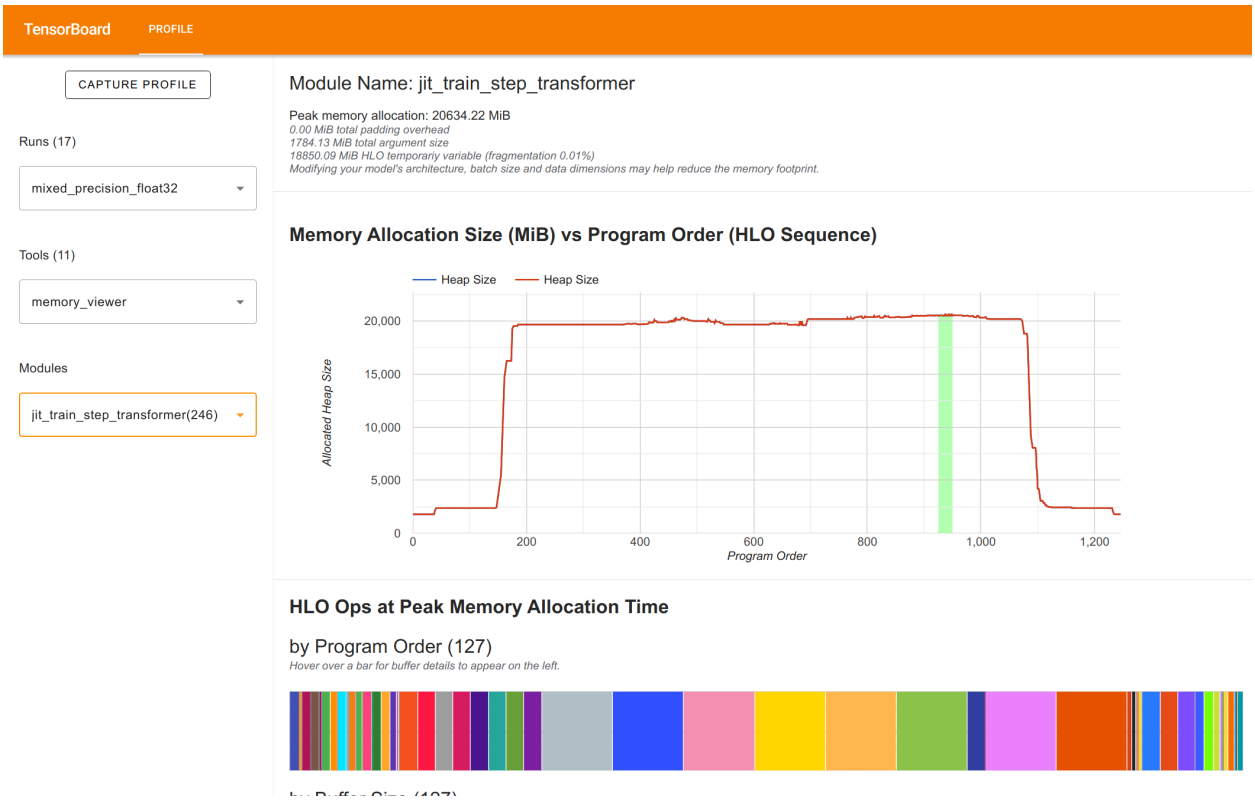
The trace viewer is the main tab to inspect the model execution. It shows the individual operations and their execution time. The operations are grouped by the JAX transformation, such as `jit`, `vmap`, or `scan`. We can inspect the execution time of the individual operations, and see which operations take the most time. This can help us to identify potential bottlenecks in the model execution, and optimize the model accordingly. Below is an example view of the trace viewer:



On the left, you have tabs to select the run and hosts if you have multiple nodes. In the middle, you have the individual operations. Here, we are mainly looking at the `TensorFlow Name Scope` which shows operations with their annotated names (and are most easily understandable for us). On the right, you see the toolbar. The single cursor allows you to select individual blocks and see more details on them (wall clock duration, start time, etc.). The four-way arrow allows you to move around the trace. The up-down arrow allows to zoom into the trace by clicking and dragging up (zoom in) or dragging down (zoom out). This helps us to focus on specific parts of the trace and get down to the individual operations. The left-right arrow allows us to select a subset of the trace and measure the time from one to the other operation. This is helpful for finding the joint execution time of multiple operations together. Overall, in this view, we can see the individual operations and their execution time, and identify potential bottlenecks in the model execution.

Memory Viewer

The memory viewer shows the memory consumption of the model. It shows the memory consumption over operations during the model execution, and how the memory consumption changes over time. This can help us to identify potential memory bottlenecks in the model execution, and optimize the model accordingly. Below is an example view of the memory viewer:

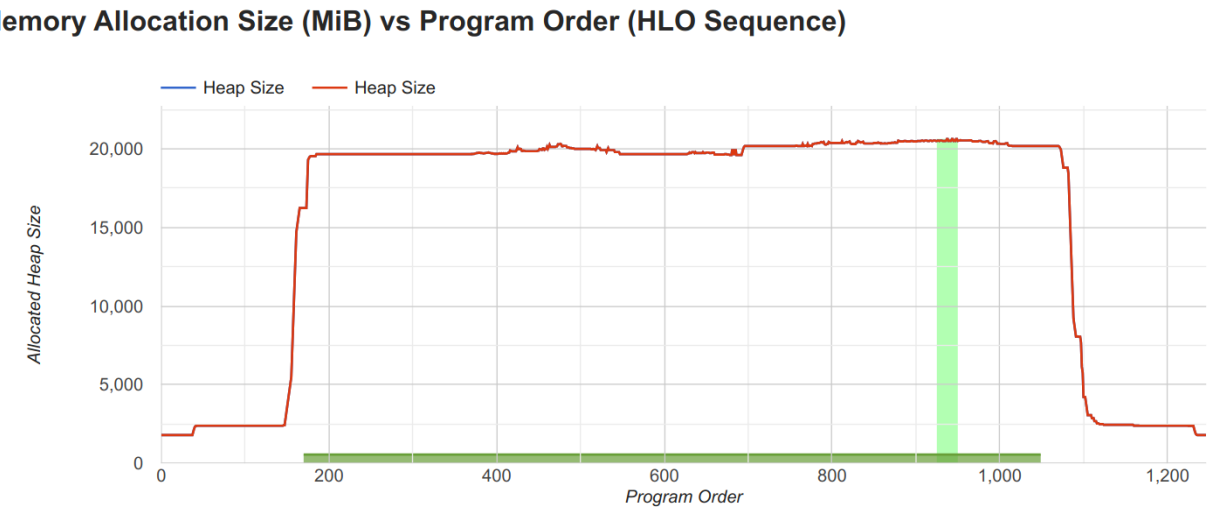


You can hover over the memory graph to find the memory consumption at a specific point in time. Further, on the bottom, you can find the individual arrays that make up the memory consumption. This is very helpful to find the largest memory consumers, and check whether your arrays are all in the right precision and we didn't forget somewhere to cast them to `bfloat16`. Overall, in this view, we can see the memory consumption of the model and identify potential memory bottlenecks in the model execution.

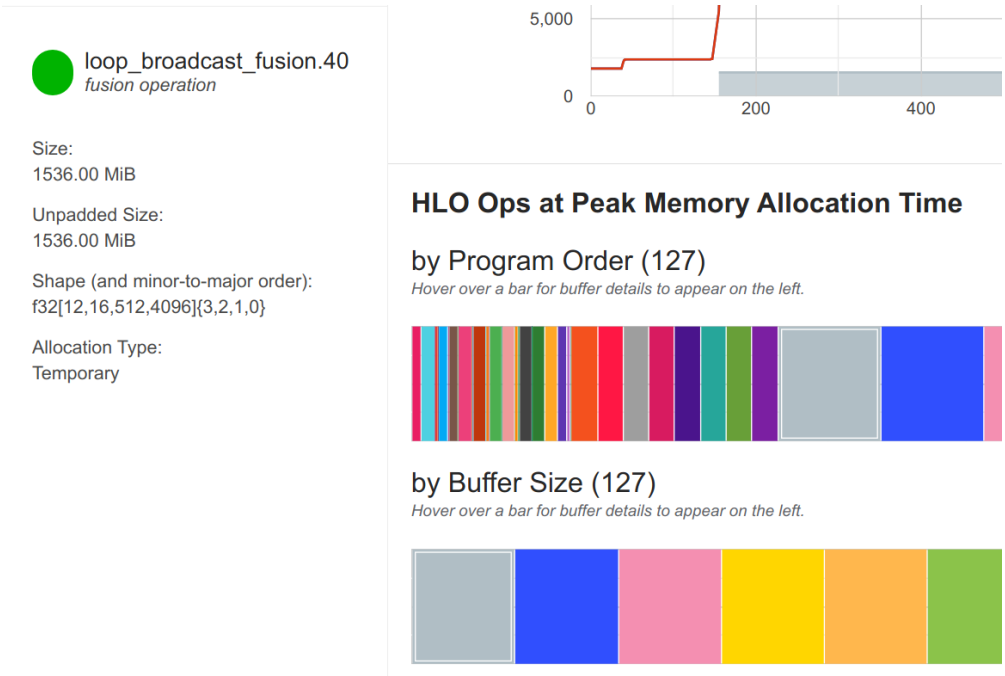
We will use both views to understand the impact of the individual techniques on the model execution.

Mixed Precision Training

First, we compare a model in `float32` versus `bfloat16` precision. For this, we adjust above's config to remove all remats and set the batch size to 64, to fit in memory. We then profile the model with `float32` and `bfloat16` precision. In the trace, we look at the memory viewer to get an idea of the memory usage:

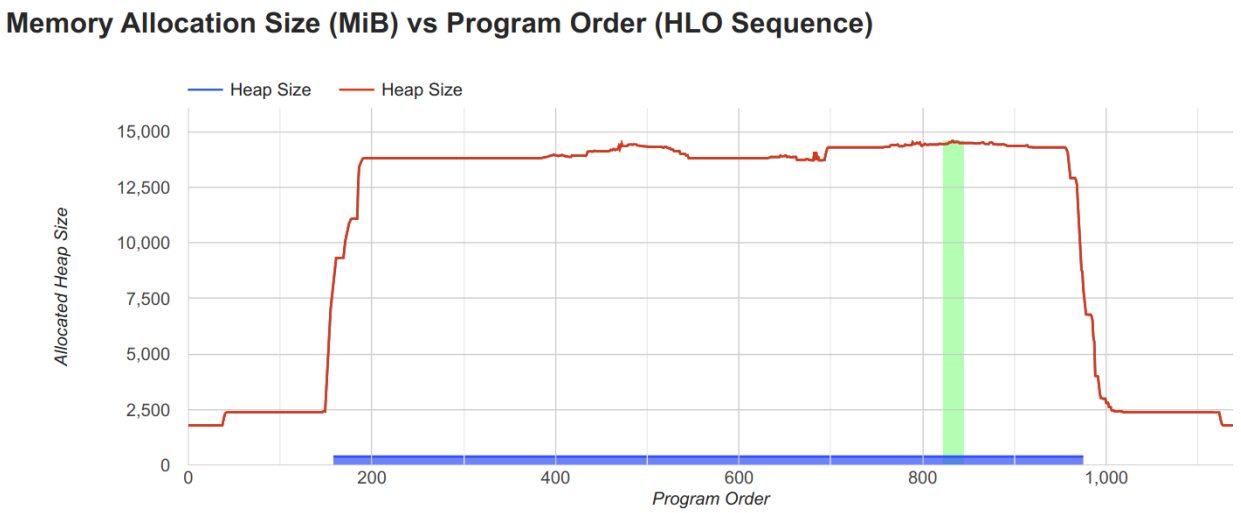


The `float32` model is at the maximum of the GPU memory with 20.6GB, while we also already see warnings of JAX that is had to perform automatic rematting. This is a sign that the model is too large to fit into memory. We can further investigate the arrays that take up the most memory in the view below the memory trace.

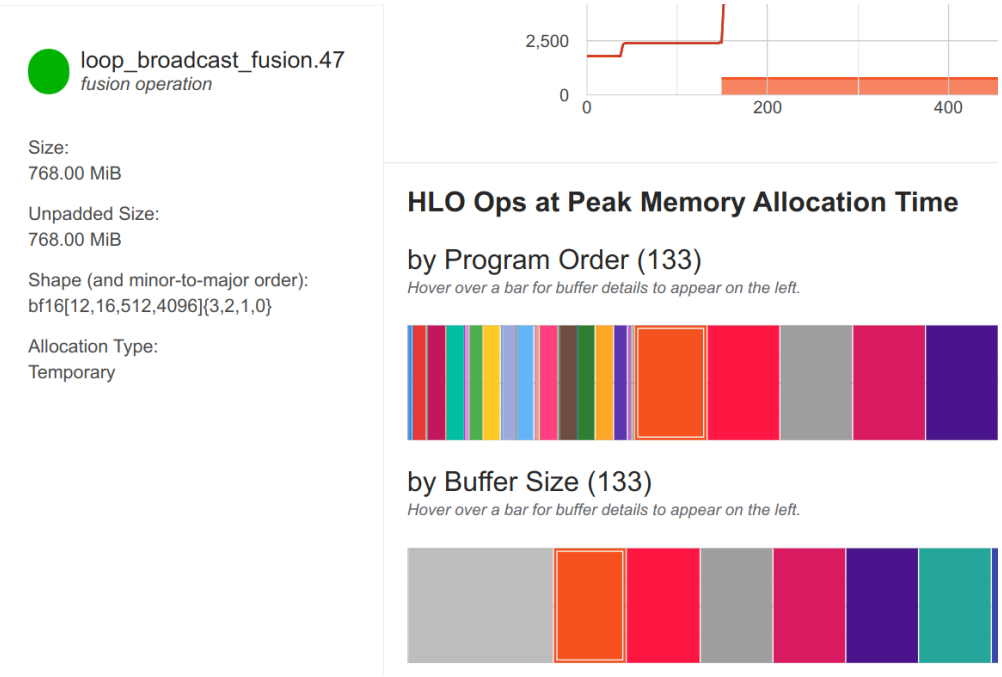


The arrays with largest memory usage are of shape `[12, 16, 512, 4096]`, which are the activations within the MLP block (12 layers, minibatch size 16, 512 sequence length, 4096 hidden size). We can also see that the activations are in `float32` precision, which is the main reason for the large memory consumption.

We can now compare this to the `bfloat16` model. The memory trace of the `bfloat16` model is shown below:



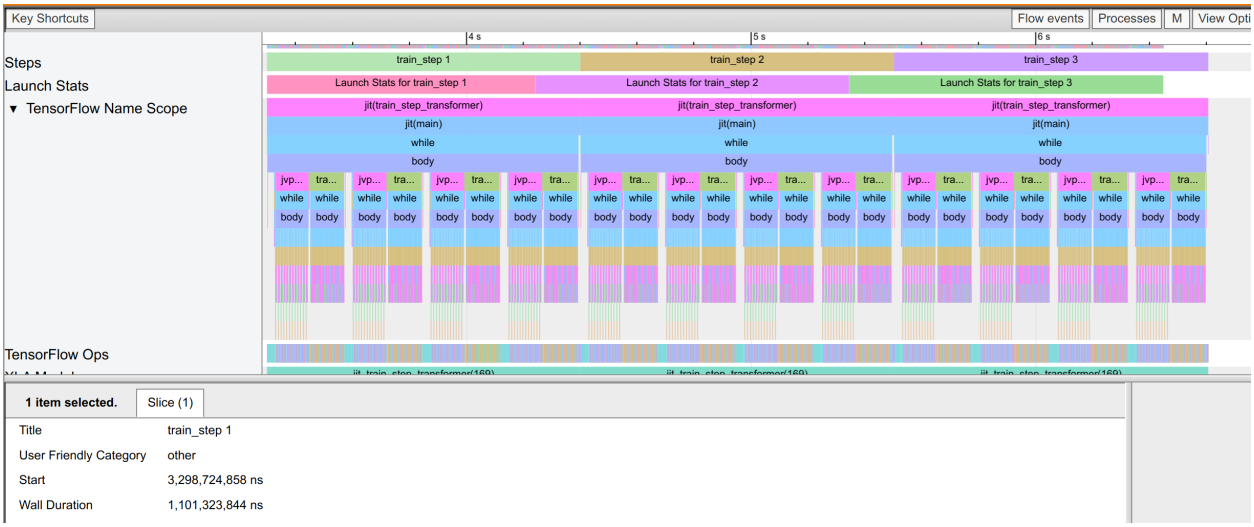
The `bfloat16` model is at 14.6GB, which is significantly less than the `float32` model. We can also see that the activations are in `bfloat16` precision, which is the main reason for the reduced memory consumption. Further, when looking at the largest arrays again, we see that most activations are in `bfloat16` precision, and previously largest arrays of shape `[12, 16, 512, 4096]` are now only half the size in memory (768MB).



The largest array remaining are the softmax logits in the attention, which with shape `[12, 16, 8, 512, 512]` are 1.5GB (12 layers, minibatch size 16, 8 attention heads, 512 sequence length). This remains in `float32` to prevent numerical instabilities. Overall, this comparison shows the potential of mixed precision training to reduce the memory footprint of the model.

Memory is not the only aspect mixed precision improves. If we look at the `trace_viewer` tab, we can see that the execution time of the model is also significantly reduced. The `float32` precision model takes 2.1 seconds per training step (see wall duration in the picture below). Note that this training step consists of 4 minibatch steps, which we can see in the 4 `jvp` and `transpose` blocks per train step.

The `bfloat16` precision model only takes 1.1 seconds per training step, which is a significant reduction in training time. Each operation can take advantage of the `bfloat16` supports of the GPUs tensor cores, which allows for the significant speed up. This shows the potential of mixed precision training to reduce the training time of the model, as well as the memory footprint.



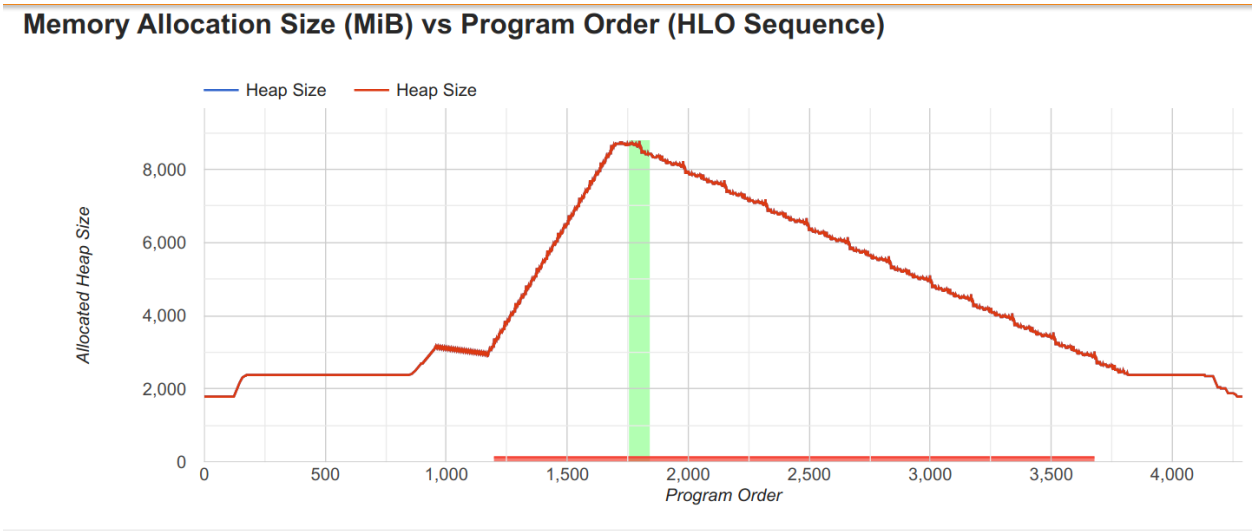
Scanning Layers

Before we continue with the other techniques, we take a closer look at the trace to identify potential model inefficiencies. For this, we zoom in to the `trace_viewer` tab and look at the individual operations. We see the operation within the block (e.g. `mlp` and `attn`), but also that there is quite some gap between the execution of subsequent layers. At closer inspection, many of these gaps are due to the reoccuring operation `dynamic_update_slice`:

This operation is used to copy one array into another, and is often used in the `scan` transformation to update the global state of the loop with the buffers of the individual layers. However, we can see that this operation is quite slow since we have to copy large arrays within the GPU memory compared to a fast layer execution. This is a sign that the `scan` transformation is not optimal for the model, and we should consider sacrificing some compilation time for a more efficient model execution, especially since the model is not extremely deep.

Hence, we test our model with `scan_layers=False`. While the compilation time increases, it stays within a few seconds, which is negligible for the overall training time. We show the trace of the new model below. We can see that the execution time of the model is significantly reduced to 0.73 seconds instead of 1.1 seconds, and the `dynamic_update_slice` operations are gone.

Furthermore, the peak memory is also reduced to 8.8GB instead of 14.6GB, which is a significant reduction in memory consumption. This is because we do not enforce the model anymore to keep the full activations of all layers in memory and can release the memory of a layer as soon as the gradients have been calculated:

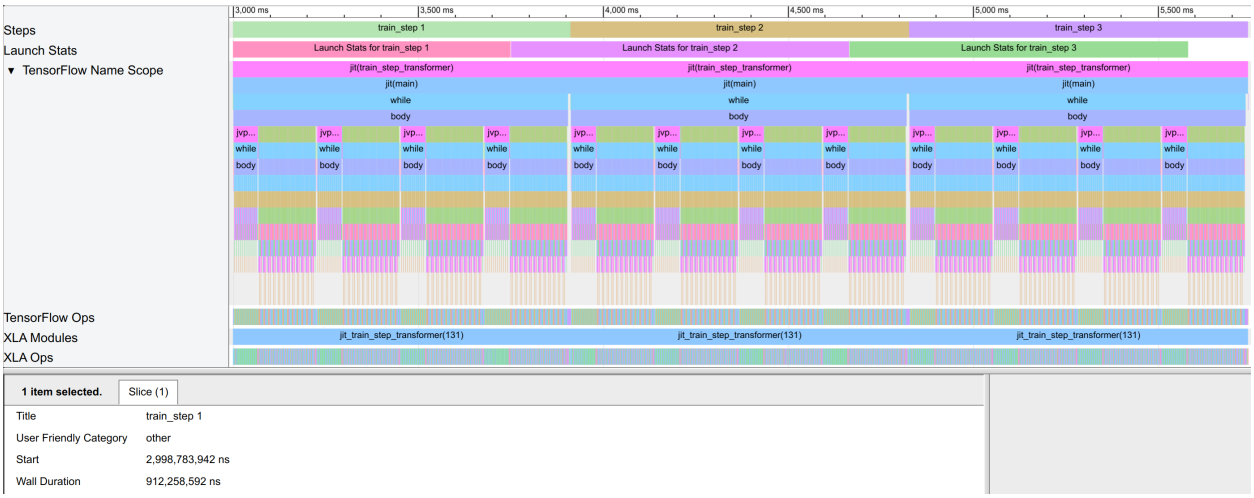


As a result, we find many more small arrays in our buffer, which are the activations of the individual layers. While this can give the compiler more freedom to schedule the computation, we may suffer more from memory fragmentation. However, for the model at hand, this is not a significant issue and we find a significant reduction in memory consumption and execution time when not scanning the layers.

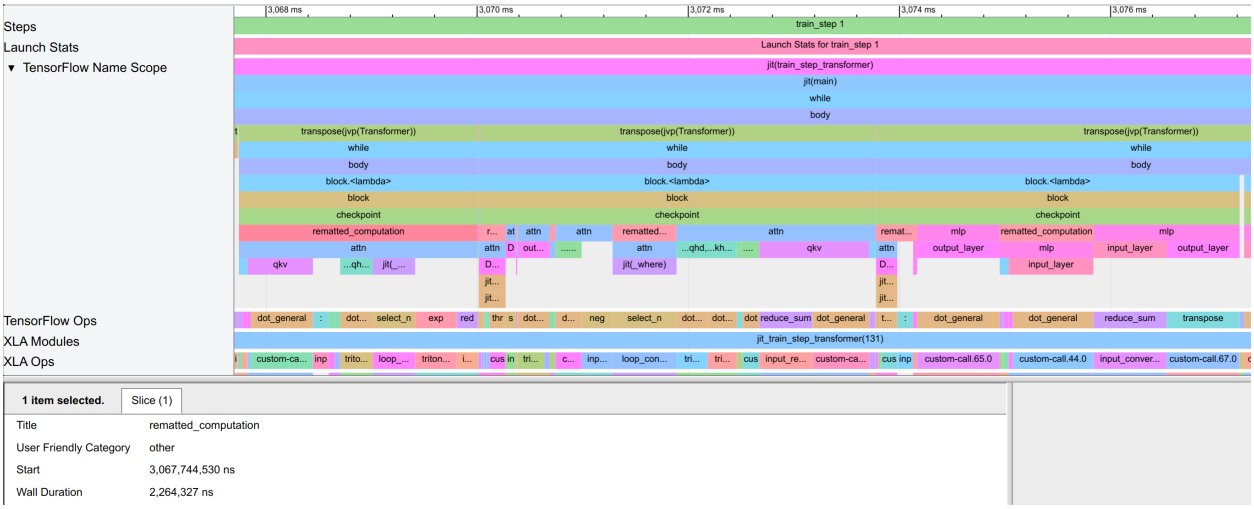
This insight should not be taken as a general rule, but as a reminder to always profile the model and consider the trade-offs of different techniques. For larger models, the `scan` transformation can be beneficial to reduce the compilation time, but for smaller models, it can be more beneficial to not scan the layers to reduce the memory consumption and execution time.

Gradient Checkpointing

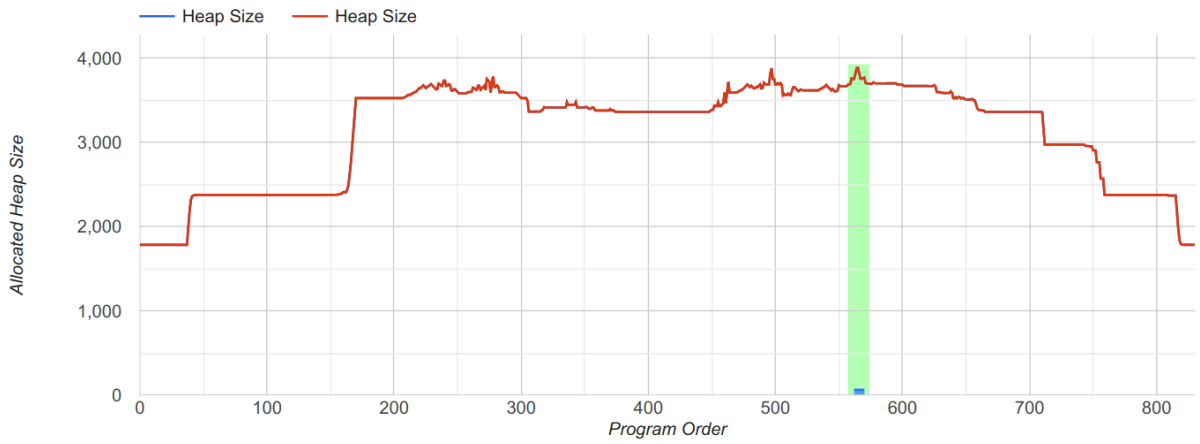
Another situation where scanning the layers become efficient again is when we combine it with gradient checkpointing. When recomputing most activations, we reduce the memory that needs to be kept between loop iterations in the scan and thus significantly reduce the dynamic slice operations. For instance, we trace a model using scan and `config.remat=("MLP", "Attn")`. This corresponds to checkpointing the input activations of the MLP and Attention Block, but recomputing the inner activations of both blocks. We show the trace below:



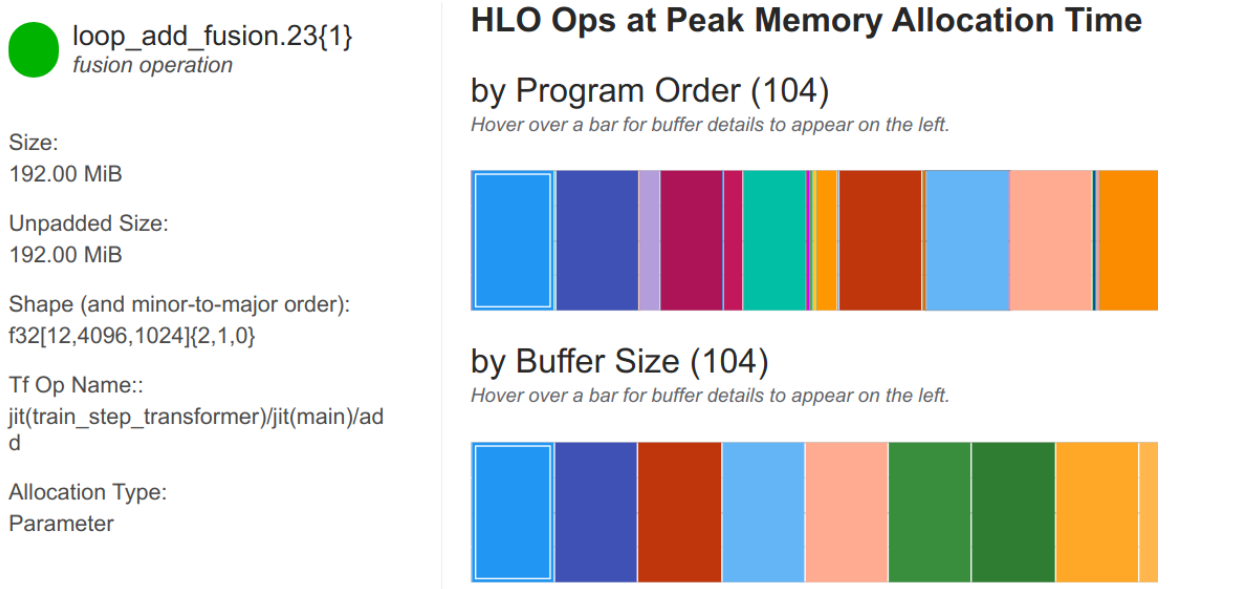
The model takes 0.91 seconds per training step, which is 25% slower than the model without scanning and rematting. Still, the model execution is faster than the scanned model without rematting, since we reduce the memory that needs to be kept between loop iterations. In the trace, the dynamic slice operations take a negligible amount of time now. To also verify that the model is performing the gradient checkpointing as intended, we can zoom into the backward pass of the model. There, we see that in each block, the model is performing `remated_computation` blocks, which corresponds to recomputing the activations during the backward pass:



Let's also check the memory consumption of the model, since this is the main goal of gradient checkpointing. The peak memory, shown below, is reduced to only 3.9GB, which is significantly less than the 14.6GB of the model without rematting.



Furthermore, the largest array left in the buffer is the MLP parameters of the model. This indicates that we can significantly increase the model size and batch size with gradient checkpointing, which we could not do with the model without rematting.

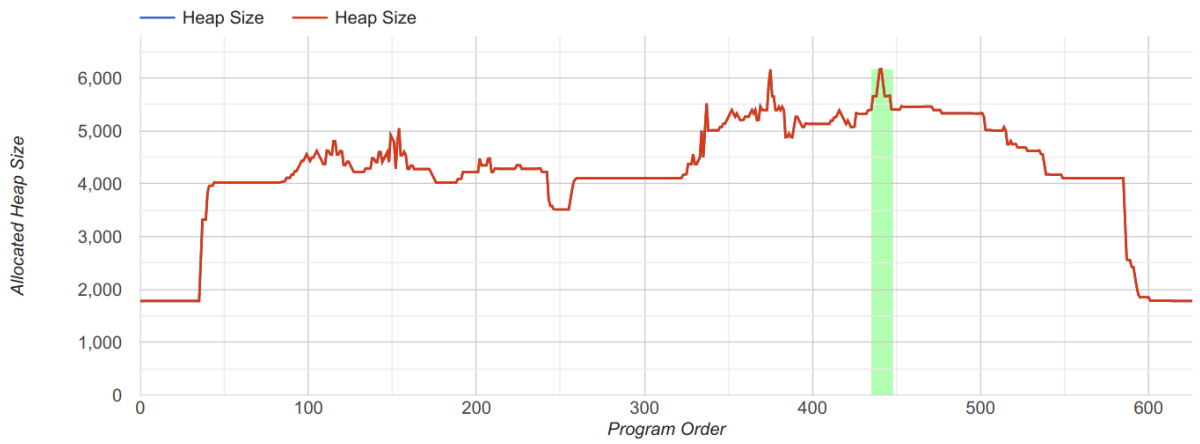


Besides rematting the MLP and Attention block, we could also remat the full block. However, since the activations are not the limiting factor for the memory consumption anymore, there is no significant benefit in rematting the full block. We find the model to use 3.8GB of memory, which is only slightly less than the model with rematting the MLP and Attention block. Further, the execution time is also slightly slower with 0.96 seconds per training step, which is likely not worth the small reduction in memory consumption in our case.

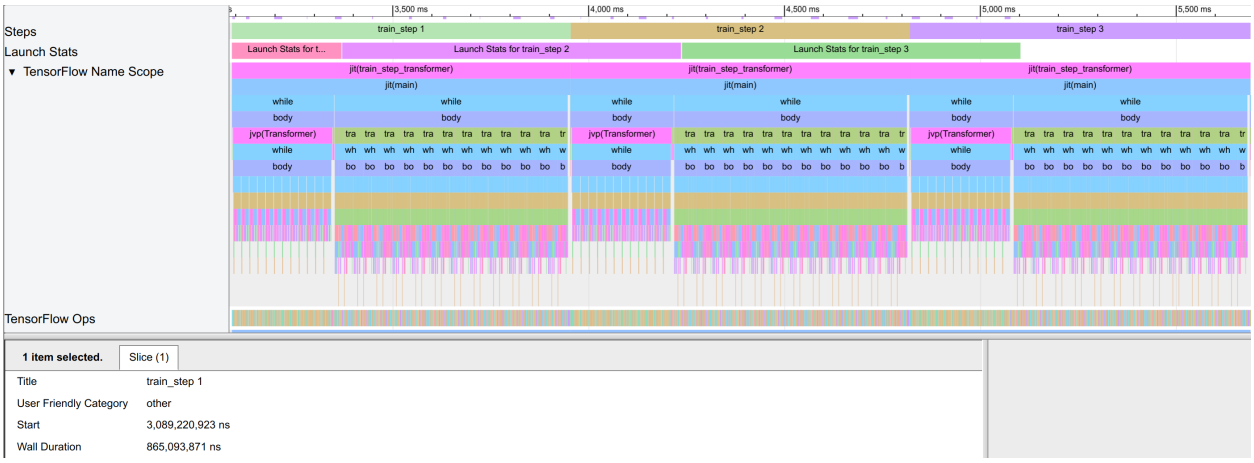
Nonetheless, these experiments show the potential of gradient checkpointing to reduce the memory footprint of the model and allow for larger models and batch sizes.

Gradient Accumulation

With mixed precision and gradient checkpointing, we saved so much memory that we do not need gradient accumulation anymore. To check this, we run a model with `bfloat16`, `remat=("MLP","Attn")`, and set the number of minibatches to 1, i.e. no gradient accumulation. We first show the memory consumption below:



The model takes 6.2GB of memory, which is an increase of the gradient accumulation model, but still significantly less than the maximum GPU memory of 24GB. Further, we can check the execution time of the model by looking at the trace:



With 0.86 seconds per training step, the model is slightly faster than the model with gradient accumulation. This is because the model can parallelize operations better and utilize the GPU more efficiently. Hence, we may want to reduce the usage of gradient accumulation if we have the GPU memory to fit the full batch into it.

Furthermore, we can scale the batch size well beyond 64. For instance, a batch size of 256 fits well into the memory (15GB usage), while the initial model hit the memory limit with a minibatch size of 16. This shows the potential of the combined techniques to reduce the memory footprint of the model and allow for larger models and batch sizes even on a single GPU.

4.7.4 Conclusion

In this notebook, we have explored several techniques to train larger models on a single device. We have implemented mixed precision training, gradient accumulation, and gradient checkpointing on a simple MLP model, and discussed JAX-specific structures to reduce the memory footprint of the model. We have also trained a larger Transformer model with these techniques and profiled the model to gain further insights into the model execution. We have seen that these techniques can significantly reduce the memory footprint of the model and help training larger models. However, these techniques also come with trade-offs, such as increased training time and reduced numerical precision. It is important to carefully consider these trade-offs when training larger models, and to experiment with different techniques to find the best setup for the specific model and hardware configuration. We have also seen that JAX provides a powerful backend with the XLA compiler to optimize our computations on the available hardware, and that we can use the profiler to gain further insights into the model execution. We hope that this notebook has provided a good overview of the techniques to train larger models on a single GPU, and has given a good starting point for further exploration of these techniques. In the following notebooks, we will explore how to train larger models on multiple GPUs and TPUs, and discuss the different parallelization strategies to scale the training to multiple devices.

4.7.5 References and Resources

[Bulatov, 2018] Bulatov, Y., 2018. Fitting larger networks into memory. Blog post link

[Kalamkar et al., 2019] Kalamkar, D., Mudigere, D., Mellempudi, N., Das, D., Banerjee, K., Avancha, S., Vooturi, D.T., Jammalamadaka, N., Huang, J., Yuen, H. and Yang, J., 2019. A study of BFLOAT16 for deep learning training. arXiv preprint arXiv:1905.12322. Paper link

[Ahmed et al., 2022] Ahmed, S., Sarofeen, C., Ruberry, M., et al., 2022. What Every User Should Know About Mixed Precision Training in PyTorch. Tutorial link

[Raschka, 2023] Raschka, S., 2023. Optimizing Memory Usage for Training LLMs and Vision Transformers in PyTorch. Tutorial link (gives more details for the topics here in PyTorch)

[HuggingFace, 2024] HuggingFace, 2024. Performance and Scalability: How To Fit a Bigger Model and Train It Faster. Tutorial link

[NVIDIA, 2024] NVIDIA, 2024. Mixed Precision Training. Documentation link

[NVIDIA, 2024] NVIDIA, 2024. Performance Guide for Training. Documentation link

[Google, 2024] JAX Team Google, 2024. Control autodiff's saved values with jax.checkpoint (aka jax.remat). Tutorial link

[Google, 2024] JAX Team Google, 2024. Profiling JAX programs. Tutorial link

[Google, 2024] JAX Team Google, 2024. GPU peformance tips. Tutorial link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.8 Part 2.1: Introduction to Distributed Computing in JAX

Filled notebook:

Author: Phillip Lippe

Recent success in deep learning has been driven by the availability of large datasets and the ability to train large models on these datasets. However, training large models on large datasets is computationally expensive and usually goes beyond the capability of a single accelerator like a GPU. To speed up training, we can use parallelism to distribute the computation across multiple devices. This is especially important as the size of the models and datasets continues to grow.

Before diving into different parallelism strategies for training large neural networks, this notebook will introduce the basic concepts of distributed, multi-device processing in JAX. In Part 2.2, we then implement different data parallelism strategies to train a small neural network on multiple devices. If you are already familiar with the basics of distributed computing in JAX, you can skip this notebook and move to Part 2.2.

While the intention of this notebook is to provide an implementation to run on multiple devices like GPUs or TPUs, not everyone will have easily access to such hardware. Luckily enough, in JAX, it is very easy to simulate multiple devices on a single CPU. This is done by adding the flag `xla_force_host_platform_device_count=8` to the XLA environment variable `XLA_FLAG`. This will simulate 8 devices on a single CPU, which we can use to design and test our parallelized implementation. Once tested, we can remove the flag and could run the implementation without changes on the actual hardware if available.

Let's set these environment variables below. If you are running on Google Colab, you do not need to select a GPU runtime, as we will simulate multiple devices on a single CPU. If you are running on your local machine and have multiple GPUs available, you can set `USE_CPU_ONLY` to False and run the implementation on the actual hardware.

[1]:
```
import os

# Set this to True to run the model on CPU only.
USE_CPU_ONLY = True

flags = os.environ.get("XLA_FLAGS", "")
if USE_CPU_ONLY:
    flags += " --xla_force_host_platform_device_count=8"  # Simulate 8 devices
    # Enforce CPU-only execution
    os.environ["CUDA_VISIBLE_DEVICES"] = ""
else:
    # GPU flags
    flags += (
        "--xla_gpu_enable_triton_softmax_fusion=true "
        "--xla_gpu_triton_gemm_any=false "
        "--xla_gpu_enable_async_collectives=true "
        "--xla_gpu_enable_latency_hiding_scheduler=true "
        "--xla_gpu_enable_highest_priority_async_stream=true "
    )
os.environ["XLA_FLAGS"] = flags
```

With the environment variables set, we can import our required libraries and start with the implementation.

[2]:
```
import functools
from typing import Any, Dict, Tuple

import flax.linen as nn
```

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```
import jax
import jax.numpy as jnp
import numpy as np
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh, NamedSharding
from jax.sharding import PartitionSpec as P

PyTree = Any
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

4.8.1 Distributed Computing in JAX

This section will quickly introduce the basic concepts of distributed computing in JAX. We will focus on the basic building blocks which are essential for implementing data parallelism and other parallelism strategies in the following tutorials. For a more detailed introduction to distributed computing in JAX, we refer to the official documentation. If you are already familiar with parallelization strategies and shard map in JAX, you can skip this section and directly jump to the next part.

Basics

JAX supports distributed computation across multiple devices. We can check which devices we have access to by using the `jax.devices()` function. If we set up the environment variable `xla_force_host_platform_device_count=8`, we should see 8 (CPU) devices below:

[3]:
```
jax.devices()
```

```
2024-03-07 10:46:09.748770: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

[3]:
```
[CpuDevice(id=0),
 CpuDevice(id=1),
 CpuDevice(id=2),
 CpuDevice(id=3),
 CpuDevice(id=4),
 CpuDevice(id=5),
 CpuDevice(id=6),
 CpuDevice(id=7)]
```

If we would have many more resources that are placed in different servers or hosts, we can distinguish between the devices our process has access to and the devices that are available globally. We can check the local devices by using `jax.local_devices()` and the global devices by using `jax.devices()`. Since we only run a single process here, both will return the same devices. For now, we mainly focus on parallelization within a single process/machine since this is easiest in a tutorial notebook setting. However, the same concepts can be applied to parallelization across multiple processes/machines, and more details on JAX with multiple processes can be found in the official documentation.

When creating an array with JAX, we usually place it on a device directly. For instance, let's create a simple array below and check its placement:

[4]:
```
a = jnp.arange(8)
print("Array", a)
```

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```
print("Device", a.device())
print("Sharding", a.sharding)
```

```
Array [0 1 2 3 4 5 6 7]
Device TFRT_CPU_0
Sharding SingleDeviceSharding(device=CpuDevice(id=0))
```

The array is placed on the first CPU device by default. The attribute `sharding` describes how the array is laid out across devices. In this case, the array is placed on a single device. If we would now run any operation on this array, it would be executed on the first CPU device and the remaining devices would be idle. To distribute the computation across multiple devices, we need to shard the array. We can do this by first defining a `Mesh`. A mesh organizes the devices into a grid and assigns a logical name to each axis of the grid. Let's create a mesh of our 8 CPU devices below, where we organize them all in a single axis with name `i`:

[5]:
```
mesh = Mesh(np.array(jax.devices()), ("i",))
mesh
```

[5]:
```
Mesh(device_ids=array([0, 1, 2, 3, 4, 5, 6, 7]), axis_names=('i',))
```

We can now use this mesh to shard our array. We first define a sharding using `NamedSharding` which takes as input the mesh and a specification of how the array should be sharded. This `PartitionSpec` (here abbreviated to `P`) takes as input a tuple of axis names, one value per dimension of the array. To shard an array axis over a certain mesh axis, we add the axis name at the corresponding position in the tuple. For instance, to shard the first dimension of our array over the `i` axis of our mesh, we would use the tuple `P('i',)`:

[6]:
```
sharding = NamedSharding(
    mesh,
    P("i"),
)
```

To not shard an axis, we can use `None` in the tuple. Any axis that we do not shard will be replicated across all devices in the mesh. For instance, to shard the second dimension of another array over the `i` axis of our mesh, we would use the tuple `P(None, 'i')`. Any axis that is not specified in the tuple will be considered as `None`, i.e. replicated across all devices.

To set this sharding on an array, we use the `jax.device_put` function, but pass the sharding object instead of a single device:

[7]:
```
a_sharded = jax.device_put(a, sharding)
print("Sharded array", a_sharded)
print("Device", a_sharded.devices())
print("Sharding", a_sharded.sharding)
```

```
Sharded array [0 1 2 3 4 5 6 7]
Device {CpuDevice(id=5), CpuDevice(id=1), CpuDevice(id=0), CpuDevice(id=7),␣
↪CpuDevice(id=6), CpuDevice(id=4), CpuDevice(id=3), CpuDevice(id=2)}
Sharding NamedSharding(mesh=Mesh('i': 8), spec=PartitionSpec('i',))
```

The array is now sharded across all 8 CPU devices, each device holding a different part of the array. We can also visualize the sharding of the array using `jax.debug.visualize_array_sharding`:

[8]:
```
jax.debug.visualize_array_sharding(a_sharded)
```

If we apply any operation on this sharded array, the computation will be distributed across all devices and the return value is again a sharded array. For instance, let's apply a simple operation to the sharded array:

[9]:
```
out = nn.tanh(a_sharded)
print("Output array", out)
jax.debug.visualize_array_sharding(out)
```

```
Output array [0.         0.7615942  0.9640276  0.9950547  0.9993292  0.99990916
 0.9999876  0.99999833]
```

If we now write a function and jit it, the computation will also follow the sharding and be distributed across all devices.

Multi-axis mesh

In many of our parallelism strategies, we will use multi-axis meshes. For instance, over a certain group of devices, we may apply data parallelism, while over another group of devices, we may apply pipeline parallelism. We can define a multi-axis mesh by reshaping our devices into a multi-dimensional grid, and naming each axis. For instance, let's reshape our 8 CPU devices into a 4x2 grid and name the axes `i` and `j`:

[10]:
```
mesh = Mesh(np.array(jax.devices()).reshape(4, 2), ("i", "j"))
mesh
```

[10]:
```
Mesh(device_ids=array([[0, 1],
       [2, 3],
       [4, 5],
       [6, 7]]), axis_names=('i', 'j'))
```

We can see that device 0 and device 1 are on the axis along dimension 1, and device 0, 2, 4, and 6 along dimension 0. The specific placement of each device in the mesh will depend on communication links between devices, e.g. which GPUs are connected via an NVLink. The benefit of using a multi-axis mesh is that we can shard arrays over different axes. For instance, consider a simple matmul operation with bias: `y = x @ w + b`. To maximize the parallelism of this operation, we can shard the batch dimension of the input `x` over the `i` axis, and the output dimension of the weight matrix `w` and bias `b` over the `j` axis. Let's set this up below:

[11]:
```
batch_size = 192
input_dim = 64
output_dim = 128
x = jax.random.normal(jax.random.PRNGKey(0), (batch_size, input_dim))
w = jax.random.normal(jax.random.PRNGKey(1), (input_dim, output_dim))
b = jax.random.normal(jax.random.PRNGKey(2), (output_dim,))
```

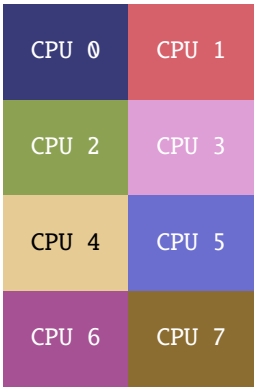
We specify the shardings and apply them to the corresponding arrays.

[12]:
```
x_sharded = jax.device_put(x, NamedSharding(mesh, P("i", None)))
w_sharded = jax.device_put(w, NamedSharding(mesh, P(None, "j")))
b_sharded = jax.device_put(b, NamedSharding(mesh, P("j")))
```

If we now apply the matmul operation, each device will compute the matmul between its part of the input and its part of the weight matrix. The result will be a sharded array across the `i` and `j` axes. We can visualize the sharding of the result below:

[13]:
```
out = jnp.dot(x_sharded, w_sharded) + b_sharded
print("Output shape", out.shape)
jax.debug.visualize_array_sharding(out)
```

```
Output shape (192, 128)
```



Note that when we check the shape of the array, it returns the global shape of the array and not the shape of the array on a single device. Hence, for some operations where we need to know the shape of the array on a single device, we need to adjust our code from single to multi-device execution. Alternatively, we can use one of JAX's transformation functions like `jax.pmap` or `shard_map` which we will introduce in the next section.

Shard map

When using `jax.jit` directly on distributed arrays, we give the compiler the task to automatically parallelize the computation. For instance, if we compute a matmul where the features of `x` are distributed over devices, the compiler will automatically parallelize the computation and organize the communication between devices. However, in some cases like scaling deep learning models, we want to have more explicit control over the parallelization and communication. This is where `shard_map` comes into play. The transformation `shard_map` has been developed as an alternative to `jax.pmap` which was found to have flaws (see more here), and allows us to write simple and efficient parallelized code. In contrast to `jit`, we write per-device code with local array shapes and explicit communications. Besides being useful in scaling models in general, it is also well suited for our tutorials to discuss the different parallelization strategies and their explicit implementation.

Shard map is a transformation that takes a function, a mesh, and a sharding specification for the input and outputs. It then applies the function to the sharded inputs and outputs in a single-program multiple-data (SPMD) fashion. This means that the function is executed on each device with the local input and output arrays. As a first example, let's reimplement the matmul operation from the previous section using `shard_map`. We first define the function `matmul` which takes as input the sharded arrays `x` and `w` and returns the sharded array `y`:

[14]:
```
def matmul_fn(x: jax.Array, w: jax.Array, b: jax.Array) -> jax.Array:
    print("Local x shape", x.shape)
    print("Local w shape", w.shape)
    print("Local b shape", b.shape)
    return jnp.dot(x, w) + b
```

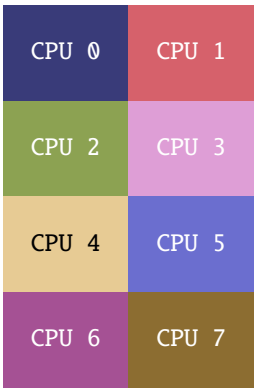
The print statements in the function are only for demonstration purposes to show the local shapes of the arrays on each device. We then apply `shard_map` to the function and pass the mesh and the sharding specifications for the input and output:

[15]:
```
matmul_sharded = shard_map(
    matmul_fn, mesh, in_specs=(P("i", None), P(None, "j"), P("j")), out_specs=P("i", "j")
)
```

The input specification is a tuple with three elements, corresponding to our three input arrays `x`, `w`, and `b`. The output specification is a single element, corresponding to our output array `y`. We can now apply the function to the sharded arrays and check the result:

[16]:
```
y = matmul_sharded(x_sharded, w_sharded, b_sharded)
print("Output shape", y.shape)
jax.debug.visualize_array_sharding(y)
```

```
Local x shape (48, 64)
Local w shape (64, 64)
Local b shape (64,)
Output shape (192, 128)
```

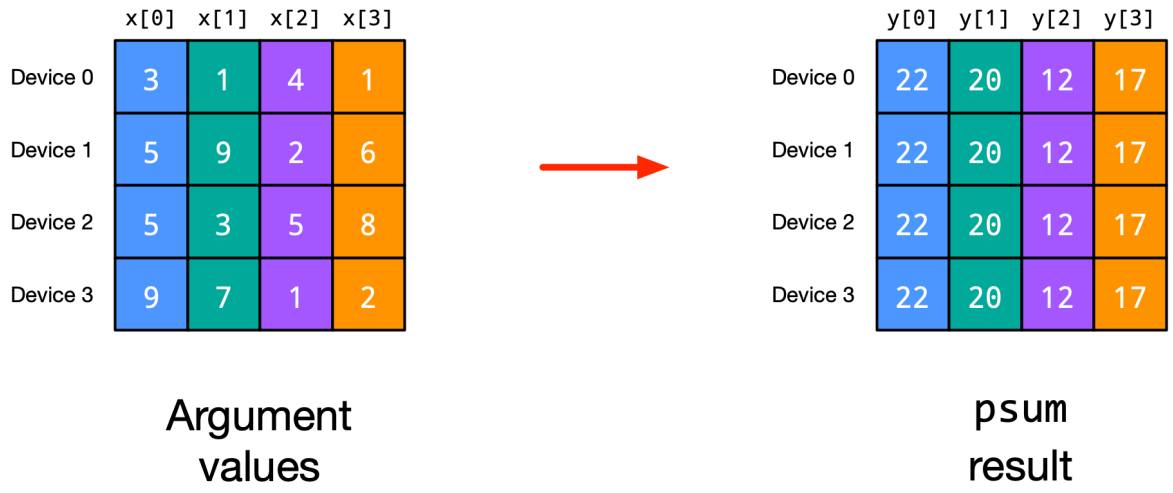


In comparison to `jax.jit`, we see that within the function, we have access to the local shapes of the arrays on each device. The final output is again in a global `jax.Array` format, which we can use for further operations and even combine with `jax.jit` operations. Note that we will also jit the `shard_map` operation in the following tutorials to speed up the computation.

Axis Communication

We will encounter many situations where we need to communicate between devices. For instance, in data parallelism, we need to aggregate the gradients from each device to update the model. In pipeline parallelism, we need to communicate the intermediate results between devices. JAX provides a set of communication operations to facilitate this. Here, we will go over some basic communication operations which we will use in the following tutorials. More details on the communication operations can be found in the official documentation.

Mean/Sum: One of the most common communication operations is `jax.lax.psum` which computes the parallel sum of an array across devices. Take for instance the following example (figure credit: JAX documentation):



The mean operation averages over all values on both devices. These operations will be frequently used in our parallelization strategies. For instance, in normalization layers like LayerNorm where the features are sharded over different devices, we need to sum/average the statistics of each individual device. Let's create a function that normalizes the values of a sharded array with `jax.lax.pmean`:

[17]:
```
@functools.partial(shard_map, mesh=mesh, in_specs=P("i", "j"), out_specs=P("i", "j"))
def parallel_normalize(x: jax.Array) -> jax.Array:
    mean = jax.lax.pmean(x, axis_name="j")
    std = jax.lax.pmean((x - mean) ** 2, axis_name="j") ** 0.5
    return (x - mean) / std
```

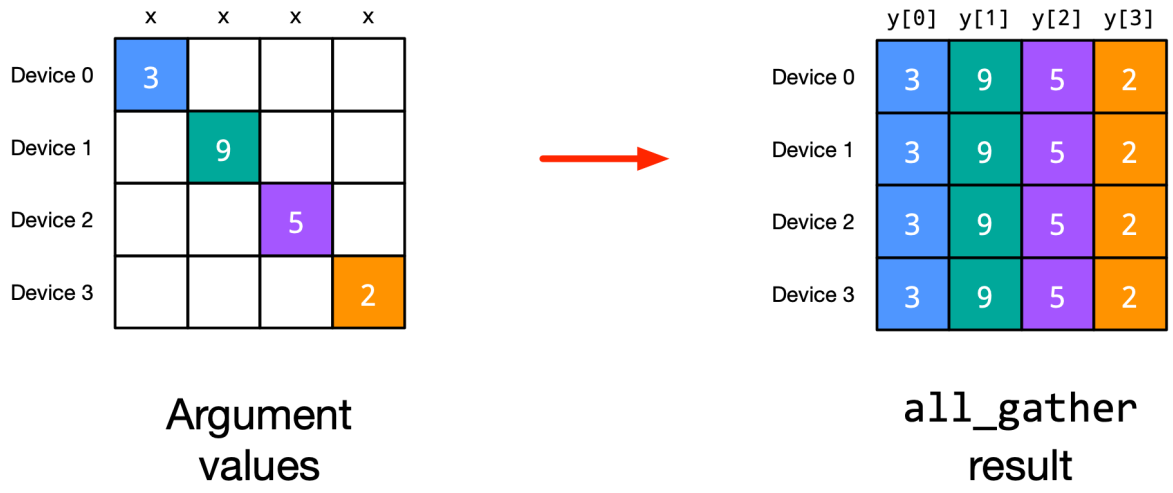
As an example, we used shard map as a decorator to the function. We can now apply it to the array `x` and verify its global mean and standard deviation:

[18]:
```
out = parallel_normalize(x)
out = jax.device_get(out)
print("Mean", out.mean())
print("Std", out.std())
```

```
Mean -4.162818e-08
Std 1.0
```

Another usage of `jax.lax.psum` is to identify the size of a mesh axis in sub-modules when we have no direct axis to the mesh object. The line `jax.lax.psum(1, axis_name)` will return the size of the axis `axis_name` of the mesh, since we add 1 per device on the mesh axis. Since this operation is independent of any input, the compiler can optimize it away when jitted and we get the size of the axis without any runtime cost.

All-gather: Another common communication operation is `jax.lax.all_gather` which gathers, i.e. collects and concatenates/stacks, the values of an array from all devices. After this operation, all devices will have the same data over the gathered axis. For instance, consider the following example (figure credit: JAX documentation):



One case where we will need to use gathering is if a weight matrix is sharded over different devices, but we need the full weight matrix to compute the output on each device. We implement an example below where the weight matrix `w` is sharded over the `i` axis, and we want to gather the full weight matrix on each device before computing the matmul:

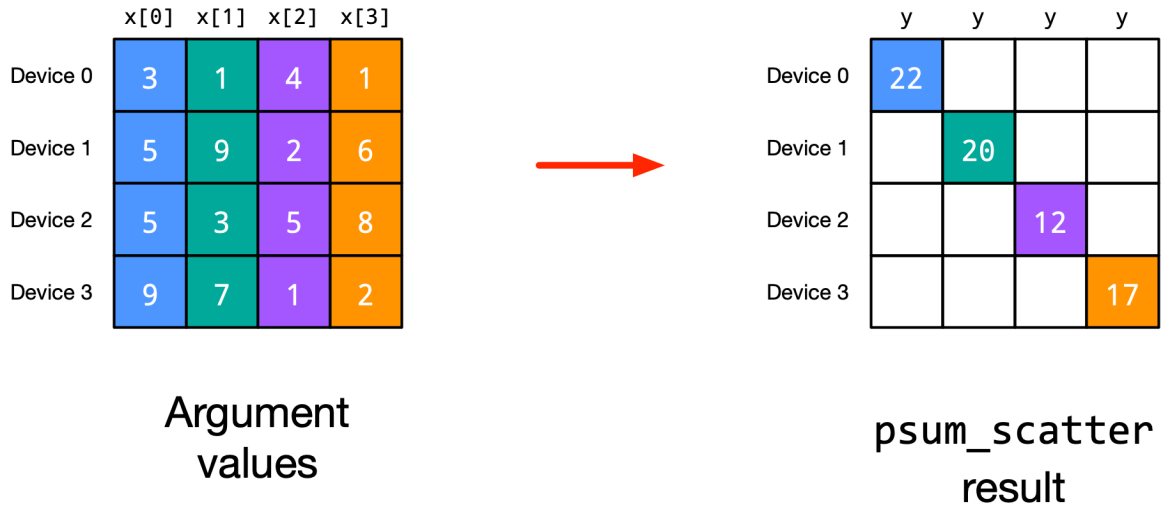
[19]:
```
@functools.partial(
    shard_map, mesh=mesh, in_specs=(P("i", None), P("i", None)), out_specs=P("i", None)
)
def matmul_with_weight_gather(x: jax.Array, w: jax.Array) -> jax.Array:
    print("Original w shape", w.shape)
    w_gathered = jax.lax.all_gather(w, axis_name="i", axis=0, tiled=True)
    print("Gathered w shape", w_gathered.shape)
    y = jnp.dot(x, w_gathered)
    return y


out = matmul_with_weight_gather(x, w)
out = jax.device_get(out)
np.testing.assert_array_equal(out, jnp.dot(x, w))
```

```
Original w shape (16, 128)
Gathered w shape (64, 128)
```

On input, each device only has a subpart of the weight matrix. After the all-gather operation, each device has the full weight matrix. With the full matrix, we can compute the matmul operation on each device and obtain the same result as if we would have computed the matmul on a single device.

Scatter sum: When taking the sum, we sometimes do not want to keep the full sum on all devices, but shard it again over the devices. This is where `jax.lax.psum_scatter` comes into play. It takes the sum of an array across devices and scatters the result across devices. For instance, consider the following example (figure credit: JAX documentation):



The sum of the array is computed across devices, and device n gets the sum of the values $x[n]$. We can re-implement the example from the figure using `jax.lax.psum_scatter`:

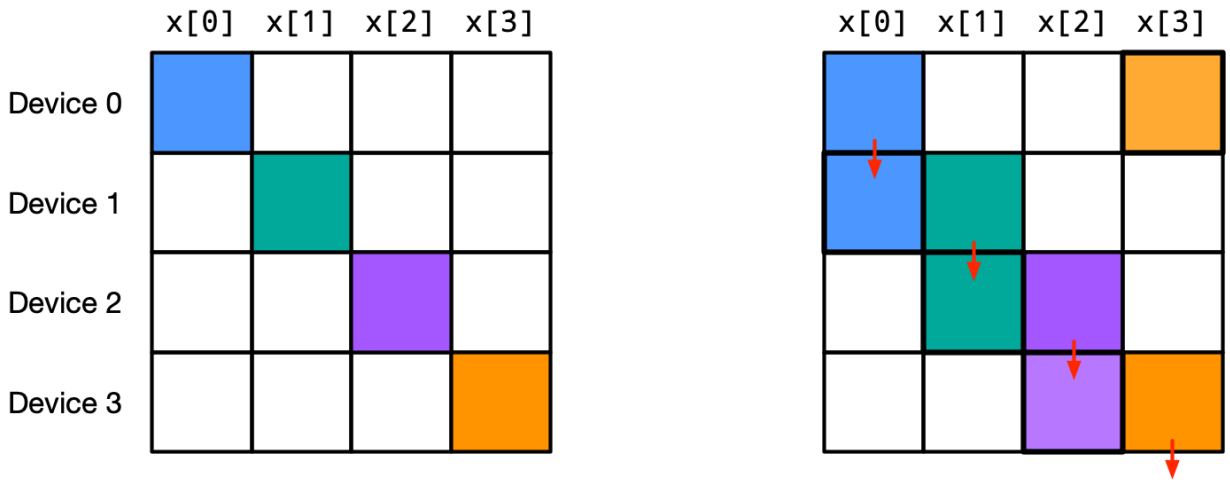
[20]:
```
@functools.partial(shard_map, mesh=mesh, in_specs=P("i", None), out_specs=P("i", None))
def scatter_example(x: jax.Array) -> jax.Array:
    x_scatter = jax.lax.psum_scatter(x, axis_name="i", scatter_dimension=1)
    return x_scatter


x_exmp = np.array(
    [
        [3, 1, 4, 1],
        [5, 9, 2, 6],
        [5, 3, 5, 8],
        [9, 7, 1, 2],
    ]
)
out = scatter_example(x_exmp)
print("Output", out)
```

```
Output [22 20 12 17]
```

A frequent usage of this operation is as the grad function of `jax.lax.all_gather`: each device originally held only $x[n]$ and gathered x in the forward pass. In the backward pass, each device gets a gradient for every element in x, and we need to sum the gradients of $x[n]$ across all devices and place it back to device n. This is done by using `jax.lax.psum_scatter` on the gradients. In contrast to `jax.lax.psum`, `jax.lax.psum_scatter` does not keep the full sum on all devices and requires fewer communications. We will use this operation later in the tutorial.

ppermute: Another useful operation is `jax.lax.ppermute` which communicates an array in a round robin fashion. If given a mesh axis with 4 devices, device 0 sends its data to device 1, device 1 sends its data to device 2, and so on. Device 3 sends its data to device 0, completing the loop. The operation looks something similar to the following figure (figure credit: JAX documentation):



The equivalent operation on a single device is `np.roll`. We can show an example of `jax.lax.ppermute` below:

[21]:
```
@functools.partial(shard_map, mesh=mesh, in_specs=P("i"), out_specs=P("i"))
def ppermute_example(x: jax.Array) -> jax.Array:
    axis_size = mesh.shape["i"]
    x_perm = jax.lax.ppermute(
        x, axis_name="i", perm=[(i, (i + 1) % axis_size) for i in range(axis_size)]
    )
    return x_perm


x_exmp = np.arange(4)
out = ppermute_example(x_exmp)
print("Output", out)
```

```
Output [3 0 1 2]
```

For `jax.lax.ppermute`, we need to specify the permutation in which we want to communicate. In a ring topology, we can usually communicate upwards (i.e. device 0 to device 1) or downwards (i.e. device 1 to device 0). Which one to use depends on the specific use case.

Example usages include the communication of the intermediate results in pipeline parallelism, where we send the output of device 0 to device 1, device 1 to device 2, and so on. Furthermore, `jax.lax.ppermute` is a basic building block with which we can implement other communication operations we have seen so far like `jax.lax.gather` (permute $N-1$ times and keep results) or `jax.lax.psum_scatter` (alternate permute and sum between adjacent devices). We will use this property of `jax.lax.ppermute` extensively in the tensor parallelism tutorial.

Axis Indexing

While a lot of deep learning modules can be implemented nicely in a single-program multiple-data (SPMD) fashion, there are some operations that require slightly adjusted operations per device. For instance, in pipeline parallelism, each device will have a slightly different processing pattern for which we need to adjust the compute graph. JAX provides for this purpose the `jax.lax.axis_index` function which returns the index of the current device along a certain axis. With that, we can identify the current device and adjust the computation accordingly. For instance, we can write a small function that returns the index of every device:

[22]:
```
axis_idx_fn = jax.jit(
    shard_map(
        lambda: jnp.stack(
            [
                jax.lax.axis_index("i"),  # Device index in mesh along the "i" axis
                jax.lax.axis_index("j"),  # Device index in mesh along the "j" axis
            ],
            axis=-1,
        )[None],
        mesh,
        in_specs=P(),
        out_specs=P(
            ("i", "j"),
        ),
    )
)
out = axis_idx_fn()
out = jax.device_get(out)
for i in range(out.shape[0]):
    print(f"Device {i}: i-axis={out[i, 0]}, j-axis={out[i, 1]}")
```

```
Device 0: i-axis=0, j-axis=0
Device 1: i-axis=0, j-axis=1
Device 2: i-axis=1, j-axis=0
Device 3: i-axis=1, j-axis=1
Device 4: i-axis=2, j-axis=0
Device 5: i-axis=2, j-axis=1
Device 6: i-axis=3, j-axis=0
Device 7: i-axis=3, j-axis=1
```

As we can see, the index of each device within the mesh is returned, as we had originally specified in the mesh. Note that at the moment of writing this notebook (March 2024, jax version 0.4.25), `jax.lax.axis_index` is only supported within a jitted function of shard map, and eager compilation is not supported yet. However, since we anyways will jit our shard map operations, this is not a big limitation for us.

A common application of `jax.lax.axis_index` is the RNG handling. For instance, when using dropout, we want to have different dropout masks on each device when performing data parallelism. We can use `jax.lax.axis_index` to select a different RNG split per device. However, other RNG operations like the parameter initialization needs to use the same RNG key on all devices. This is why we cannot pass a different RNG key to each device in the shard map, but instead pass the same RNG key to all devices, and use `jax.lax.axis_index` to split the RNG keys across devices where it is needed. We implement this RNG splitting in the function below:

[23]:
```
def fold_rng_over_axis(rng: jax.random.PRNGKey, axis_name: str) -> jax.random.PRNGKey:
    """Folds the random number generator over the given axis.

    This is useful for generating a different random number for each device
    across a certain axis (e.g. the model axis).

    Args:
        rng: The random number generator.
        axis_name: The axis name to fold the random number generator over.

    Returns:
        A new random number generator, different for each device index along the axis.
```

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```
    """
    axis_index = jax.lax.axis_index(axis_name)
    return jax.random.fold_in(rng, axis_index)
```

Let's try out the function below:

[24]:
```
fold_fn = jax.jit(
    shard_map(
        functools.partial(fold_rng_over_axis, axis_name="i"),
        mesh,
        in_specs=P(),
        out_specs=P(
            ("i", "j"),
        ),
    )
)
rng = jax.random.PRNGKey(0)
out = fold_fn(rng)
out = jax.device_get(out)
for i in range(out.shape[0] // 2):
    print(f"Device {i}: RNG={out[2*i:2*i+2]}")
```

```
Device 0: RNG=[1797259609 2579123966]
Device 1: RNG=[1797259609 2579123966]
Device 2: RNG=[ 928981903 3453687069]
Device 3: RNG=[ 928981903 3453687069]
Device 4: RNG=[4146024105 2718843009]
Device 5: RNG=[4146024105 2718843009]
Device 6: RNG=[2467461003 3840466878]
Device 7: RNG=[2467461003 3840466878]
```

By folding the RNG key over the `i` axis, each device with a different index will have a different RNG key, but shares the same RNG key across the `j` axis. For instance, device 0 and device 1 share the same RNG key because they have the same index along the `i` axis, but device 0 and device 2 have different RNG keys because they have different indices along the `i` axis. We will use this property in the following tutorials to implement data parallelism with different dropout masks on each device.

With that, we have covered the basic building blocks of distributed computing in JAX. We will use these building blocks to implement data parallelism in the following section.

4.8.2 Intermediate Summary

In this section, we have introduced the basic building blocks of distributed computing in JAX. We have learned how to shard arrays over a mesh, how to use `shard_map` to write per-device code, and how to communicate between devices. We have also learned how to use `jax.lax.axis_index` to identify the current device and adjust the computation accordingly. In the next part (Part 2.2), we will use these building blocks to implement data parallelism to train a neural network on multiple devices.

4.8.3 References and Resources

[Rajbhandari et al., 2020] Rajbhandari, S., Rasley, J., Ruwase, O. and He, Y., 2020. Zero: Memory optimizations toward training trillion parameter models. In SC20: International Conference for High Performance Computing, Networking, Storage and Analysis (pp. 1-16). Paper link

[Wang and Komatsuzaki, 2021] Wang, B., and Komatsuzaki, A., 2021. Mesh transformer jax. GitHub link

[Beyer et al., 2022] Beyer, L., Zhai, X., and Kolesnikov, A., 2022. Big Vision. GitHub link

[Google, 2024] JAX Team Google, 2024. Distributed arrays and automatic parallelization. Notebook link

[Google, 2024] JAX Team Google, 2024. SPMD multi-device parallelism with shard_map. Notebook link

[Google, 2024] JAX Team Google, 2024. Using JAX in multi-host and multi-process environments. Notebook link

[DeepSpeed, 2024] DeepSpeed, 2024. Zero Redundancy Optimizer. Tutorial link

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For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.9 Part 2.2: (Fully-Sharded) Data Parallelism

Filled notebook:

Author: Phillip Lippe

In the following series of tutorials, we will explore different parallelism strategies for training large deep learning models. Our focus will be on three common parallelism strategies: data parallelism, pipeline parallelism, and tensor parallelism. Data parallelism, as the name suggests, focuses on parallelizing the data processing of the model. If we are given a very large batch, we divide the batch into smaller batches and distribute them across multiple devices. Each device will process a different batch of data in parallel. Afterwards, we will aggregate the results from each device to update the model. Data parallelism is the most common parallelism strategy used in deep learning and well supported in most frameworks. Thus, we will start with data parallelism in this tutorial. In later tutorials, we will explore pipeline and tensor parallelism which focus on parallelizing the computation of the model itself. A short overview of the three parallelism strategies is shown in the figure below.

We will focus on implementing data parallelism in JAX, but a lot of the concepts can be easily transferred to other frameworks like PyTorch or TensorFlow. With distributed computing introduced in Part 2.1, we can now implement a simple data parallelism strategy to train a small neural network on multiple devices. We then discuss fully-sharded data parallelism (FSDP), which distributes the model parameters across multiple devices and reduces memory consumption (also known as part of the ZeRO optimizer).

4.9.1 Prerequisites

First, let's start with setting up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = ["single_gpu.py", "utils.py"]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

As in the previous part, we set up the notebook such that it can be run on a CPU with 8 simulated devices and no expensive hardware is required. If you are running on Google Colab, you do not need to select a GPU runtime, as we will simulate multiple devices on a single CPU. If you are running on your local machine and have multiple GPUs available, you can comment out the line below and use `set_XLA_flags_gpu` instead to set the XLA flags we have seen in the previous parts.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

With the environment variables set, we can import our required libraries and start with the implementation.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Sequence, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from absl import logging
from jax import lax
from jax.experimental.shard_map import shard_map
```

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```
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict

PyTree = Any
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We again use some small utilities from the previous notebook (Part 1.1) to reduce the code duplication in this notebook.

[4]:
```
from single_gpu import Batch, TrainState, accumulate_gradients, print_metrics
```

Additionally, in Part 2.1, we have already implemented the `fold_rng_over_axis`, which allows us to create mesh-axis specific RNGs. In this notebook, we will use this utility in our data parallelism implementation.

[5]:
```
def fold_rng_over_axis(rng: jax.random.PRNGKey, axis_name: str) -> jax.random.PRNGKey:
    """Folds the random number generator over the given axis.

    This is useful for generating a different random number for each device
    across a certain axis (e.g. the model axis).

    Args:
        rng: The random number generator.
        axis_name: The axis name to fold the random number generator over.

    Returns:
        A new random number generator, different for each device index along the axis.
    """
    axis_index = jax.lax.axis_index(axis_name)
    return jax.random.fold_in(rng, axis_index)
```

4.9.2 Data Parallelism

In data parallelism, we aim to use our multiple devices to increase our batch size. Each device will hold the same model and parameters, and process a different batch of data in parallel. After processing the data and obtaining the gradients for each batch, we aggregate the gradients over the devices and update our model. The main advantage of data parallelism is that it is easy to implement and scales well with the number of devices, since the devices need to communicate only once per batch. However, the main disadvantage is that the model size is limited by the memory of a single device, which can be a bottleneck for very large models and we will discuss how to overcome this in the next section.

For now, let's start with plain data parallelism. By using shard map, we can focus on writing single-device code and shard map will take care of the parallelization. Hence, we can simply write our model and training loop as if we would run it on a single device. We use our example, small classifier from the previous tutorial below:

[6]:
```
class DPClassifier(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array, train: bool) -> jax.Array:
        x = nn.Dense(
            features=self.config.hidden_size,
            dtype=self.config.dtype,
```

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```
            name="input_dense",
        )(x)
        x = nn.silu(x)
        x = nn.Dropout(rate=self.config.dropout_rate, deterministic=not train)(x)
        x = nn.Dense(
            features=self.config.num_classes,
            dtype=self.config.dtype,
            name="output_dense",
        )(x)
        x = x.astype(jnp.float32)
        return x
```

We again specify all hyperparameters in a config. Feel free to adjust the hyperparameters to your needs. As only addition to the previous tutorial, we add the `data_axis_name` attribute, which will denote the mesh axis over which we want to perform data parallelism. We will use this attribute in the following sections to coordinate communications over the data axis.

[7]:
```
data_config = ConfigDict(
    dict(
        batch_size=128,
        num_classes=10,
        input_size=784,
    )
)
model_config = ConfigDict(
    dict(
        hidden_size=512,
        dropout_rate=0.1,
        dtype=jnp.bfloat16,
        num_classes=data_config.num_classes,
        data_axis_name="data",
    )
)
optimizer_config = ConfigDict(
    dict(
        learning_rate=1e-3,
        num_minibatches=4,
    )
)
config = ConfigDict(
    dict(
        model=model_config,
        optimizer=optimizer_config,
        data=data_config,
        data_axis_name=model_config.data_axis_name,
        seed=42,
    )
)
```

Initialization

We start by initializing the model and optimizer. Also here, we can continue to write the initialization as if we would run it on a single device. We create the objects below:

[8]:
```
model_dp = DPClassifier(config=config.model)
optimizer = optax.adamw(
    learning_rate=config.optimizer.learning_rate,
)
```

We also create an example batch of data to test the model. Since shard map will take care of the parallelization and sharding of the inputs, we can simply create the batch as if we would run it on a single device:

[9]:
```
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng, data_labels_rng = jax.random.split(rng, 3)
batch = Batch(
    inputs=jax.random.normal(data_inputs_rng, (config.data.batch_size, config.data.input_
↪size)),
    labels=jax.random.randint(
        data_labels_rng, (config.data.batch_size,), 0, config.data.num_classes
    ),
)
```

```
2024-03-07 10:46:28.299510: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

Each device will process a batch size of `config.data.batch_size // num_devices`. In a full training run, you may want to prefetch the array to the devices in the correct sharding to avoid the initial transfer time. This can be done via `flax.jax_utils.prefetch_to_device`, which supports async placement of arrays on devices, and is especially useful for large arrays in a dataset. However, for the purpose of this tutorial, we will keep the array on the first device and let shard map take care of the transfer.

We can now write an initialization function. Again, this is the same function as we have seen for single-device training:

[10]:
```
def init_dp(rng: jax.random.PRNGKey, x: jax.Array, model: nn.Module) -> TrainState:
    init_rng, rng = jax.random.split(rng)
    variables = model.init({"params": init_rng}, x, train=False)
    params = variables.pop("params")
    state = TrainState.create(
        apply_fn=model.apply,
        params=params,
        tx=optimizer,
        rng=rng,
    )
    return state
```

Before we can execute the initialization, we need to define the mesh and wrap the initialization function with `shard_map`. We define the mesh below:

[11]:
```
device_array = np.array(jax.devices())
mesh = Mesh(device_array, (config.data_axis_name,))
```

We create a single-dimensional mesh, with all devices along the data axis. Hence, we will perform data parallelism over all devices.

For wrapping the initialization function with `shard_map`, we need to specify the mesh and the sharding specifications for the input and output. For generating the parameters, we input an RNG which we want to replicate across all devices. This ensures that all devices have the same parameters. The input batch on the other hand will be sharded over the data axis. As an output, we expect a train state which is identical on all devices. We wrap the initialization function with `shard_map` below:

[12]:
```
init_dp_fn = jax.jit(
    shard_map(
        functools.partial(init_dp, model=model_dp),
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=P(),
        check_rep=False,
    ),
)
```

The jitting is optional, but may be necessary in models where we make use of `jax.lax.axis_index` or other operations that are only supported within a jitted function of shard map. We can now execute the initialization function and check the resulting train state:

[13]:
```
state_dp = init_dp_fn(model_init_rng, batch.inputs)
print("DP Parameters")
pprint(jax.tree_map(lambda x: (x.shape, x.sharding), state_dp.params))
```

```
DP Parameters
{'input_dense': {'bias': ((512,), GSPMDSharding({replicated})),
                 'kernel': ((784, 512), GSPMDSharding({replicated}))},
 'output_dense': {'bias': ((10,), GSPMDSharding({replicated})),
                  'kernel': ((512, 10), GSPMDSharding({replicated}))}}
```

We find all parameters have the expected shape and are replicated across all devices. We can now move on to the training loop.

Train Step

We can write the train step almost as if we would run it on a single device. The only difference is the dropout RNG. As mentioned before, we want each device to use a different dropout mask. However, the RNG in the train state is replicated across all devices. We can use our function `fold_rng_over_axis` to split the RNG key across devices on the data axis. This device-specific key can then be passed to the dropout layers. We implement the train step below:

[14]:
```
def loss_fn(
    params: PyTree, apply_fn: Any, batch: Batch, rng: jax.Array
) -> Tuple[jax.Array, Dict[str, Any]]:
    # Since dropout masks vary across the batch dimension, we want each device to␣
↪generate a
    # different mask. We can achieve this by folding the rng over the data axis, so that␣
↪each
    # device gets a different rng and thus mask.
    dropout_rng = fold_rng_over_axis(rng, config.data_axis_name)
    # Remaining computation is the same as before for single device.
    logits = apply_fn({"params": params}, batch.inputs, train=True, rngs={"dropout":␣
↪dropout_rng})
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, batch.labels)
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), batch.labels)
```

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```
    batch_size = batch.inputs.shape[0]
    step_metrics = {"loss": (loss.sum(), batch_size), "accuracy": (correct_pred.sum(),␣
↪batch_size)}
    loss = loss.mean()
    return loss, step_metrics
```

In the previous tutorial, we explored the option of accumulating the gradients of multiple batches before updating the model, to reduce memory footprint. While in data parallelism, we usually can already run a much larger batch due to parallelization across multiple devices, we can still use this option to further increase the batch size. Since the forward step and backward pass do not require any communication between devices, we can use the same function `accumulate_gradients` as for the single-device training and scan over smaller splits of the batch per device. We can then accumulate the gradients over subbatches on each device, and only communicate the final aggregated gradients to update the model.

In the train step, we need to communicate the gradients over the data axis. After obtaining the gradients and metrics per device, we want to average the gradients over all devices and update the model. We can use `jax.lax.pmean` to average the gradients over the data axis, and then apply the optimizer step to update the model on each device in parallel. Similarly, we use `jax.lax.psum` to sum the statistics in the metrics over the data axis. Alternatively, we could sync the metrics only before we want to log them, to reduce the communication overhead. However, since the metrics are usually just a few scalars compared to millions or billions of parameters, the communication overhead is usually negligible. The returned state and metrics will be the same on all devices, and we can use them to continue the training loop.

[15]:
```
def train_step_dp(
    state: TrainState,
    metrics: Metrics | None,
    batch: Batch,
) -> Tuple[TrainState, Metrics]:
    rng, step_rng = jax.random.split(state.rng)
    grads, step_metrics = accumulate_gradients(
        state,
        batch,
        step_rng,
        config.optimizer.num_minibatches,
        loss_fn=loss_fn,
    )
    # Update parameters. We need to sync the gradients across devices before updating.
    with jax.named_scope("sync_gradients"):
        grads = jax.tree_map(lambda g: jax.lax.pmean(g, axis_name=config.data_axis_name),
↪ grads)
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Sum metrics across replicas. Alternatively, we could keep the metrics separate
    # and only synchronize them before logging. For simplicity, we sum them here.
    with jax.named_scope("sync_metrics"):
        step_metrics = jax.tree_map(
            lambda x: jax.lax.psum(x, axis_name=config.data_axis_name), step_metrics
        )
    if metrics is None:
        metrics = step_metrics
    else:
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

We can now wrap the train step with `shard_map` and jit it. We need to specify the mesh and the sharding specifications for the input and output. The input batch will be sharded over the data axis. All other arrays, i.e. the input/output train state and metrics, will be replicated across all devices. Further, we can specify the state and metrics as donatable to avoid unnecessary memory overhead. We wrap the train step with `shard_map` below:

[16]:
```
train_step_dp_fn = jax.jit(
    shard_map(
        train_step_dp,
        mesh,
        in_specs=(P(), P(), P(config.data_axis_name)),
        out_specs=(P(), P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
```

Before running the training step, we want to find the shape and PyTree structure of the metrics. We use `jax.eval_shape` or `flax.jax_utils.partial_eval_by_shape` to find the shape of the metrics without running the full computation. Otherwise, we would need to compile the training step twice, once for the input metrics being None, and once for the input metrics being the correct shape. We avoid this overhead by the shape evaluation below:

[17]:
```
_, metric_shapes = jax.eval_shape(
    train_step_dp_fn,
    state_dp,
    None,
    batch,
)
metrics_dp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
```

Finally, we can run the training loop for a few steps and check the resulting metrics:

[18]:
```
for _ in range(15):
    state_dp, metrics_dp = train_step_dp_fn(state_dp, metrics_dp, batch)
final_metrics_dp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_dp, final_metrics_dp = train_step_dp_fn(state_dp, final_metrics_dp, batch)
print_metrics(final_metrics_dp)
```

```
accuracy: 1.000000
loss: 0.003343
```

As we can see, the model is training as expected and is able to overfit on the single batch of data. Let's once more check how the parameters are distributed across the devices:

[19]:
```
print("DP Parameters")
pprint(jax.tree_map(lambda x: (x.shape, x.sharding), state_dp.params))
print("Metrics")
pprint(jax.tree_map(lambda x: (x.shape, x.sharding), final_metrics_dp))
```

```
DP Parameters
{'input_dense': {'bias': ((512,), GSPMDSharding({replicated})),
                 'kernel': ((784, 512), GSPMDSharding({replicated}))},
 'output_dense': {'bias': ((10,), GSPMDSharding({replicated})),
                  'kernel': ((512, 10), GSPMDSharding({replicated}))}}
Metrics
```

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```
{'accuracy': ((), GSPMDSharding({replicated})),
              ((), GSPMDSharding({replicated}))),
 'loss': (((), GSPMDSharding({replicated})), ((), GSPMDSharding({replicated})))}
```

Both parameters and metrics are still replicated over all devices, suggesting our implementation works as expected. We can now move on to the next section.

4.9.3 Parameter Sharding

So far, we have implemented data parallelism where the model parameters are replicated across all devices. This is a simple and effective way to parallelize the training of a model. However, as the model size continues to grow, the memory consumption of the model parameters can become a bottleneck. For instance, if we have a model with 1 billion parameters and 8 devices, each device would need to hold the full 1 billion parameters. With each parameter being in float32 and using an optimizer like Adam with two additional float32 values per parameter (first- and second-order momentum), the model itself already takes up 12GB of the device memory. This can be a problem for devices with limited memory, like taking already half the memory of an A5000 GPU with 24GB. To overcome this, we can shard the model parameters across multiple devices. This is known as fully-sharded data parallelism (FSDP) and is part of the ZeRO optimizer. In FSDP, each device holds a different part of the model parameters and their optimizer state. Before executing a layer or module, we communicate the respective parameters across devices such that we can process the data in parallel. In the backward pass, we communicate the gradients back to the respective devices and update the model. This way, we can significantly reduce the memory consumption of the model parameters and scale to very large models. The ZeRO optimizer further extends this concept by allowing for different stages of sharding, such as only sharding the optimizer state (P_{os}), sharding the gradients as well (P_{os+g}), or sharding the model parameters as well (P_{os+g+p}, FSDP). The figure below shows the different stages of ZeRO (figure credit: Rajbhandari et al., 2019). Here, Ψ represents the number of parameters in the model, and K the number of bytes in the optimizer state per parameter. In the mixed precision training setup shown, we use bfloat16 for the model parameters (2 bytes) and the gradients (2 bytes), and float32 for the Adam optimizer state (8 bytes) with a float32 copy of the parameters (4 bytes). Thus, our memory is 16 bytes per parameter. By using different stages of ZeRO, we can reduce the memory consumption of the model parameters and optimizer state by up to $1/N_d$ where N_d is the number of devices.

We will focus on the basic concept of FSDP in this tutorial, but the other ZeRO stages can also be implemented in similar ways. We will start by sharding the model parameters across multiple devices and then implement the forward and backward pass accordingly. We will also discuss the communication of the optimizer state and gradients in the backward pass.

Sharding setup

We start by sharding the model parameters across multiple devices. The strategy we follow is as follows: - During initialization, we create the full parameters on each device. - We then use `jax.lax.axis_index` to split the parameters across devices and only keep a shard of the parameters on each device. - We annotate the parameters with the sharding specification, so we know how to put the parameters back together in the forward pass.

For annotating the sharding specification of parameters, Flax provides a wrapper called `nn.Partitioned` (docs). This wrapper takes as input a parameter and a list of axis names, similar to the `PartitionSpec` we have seen before. We can then use the parameter as before, but can use the axis name specification to determine the communication needed between devices, the shard map specification, and more. Further, whenever we apply transformations on modules with partitioned parameters, e.g. vmap or scan, the partitioned parameters will be transformed accordingly and the annotated axis adjusted to the new shapes. From now on, we consider parameters to be either a `jax.Array` if fully replicated, or a `flax.linen.Partitioned` if sharded across devices. We create a small type annotation for this case below.

[20]:
```
Parameter = jax.Array | nn.Partitioned
```

We now need to write a function that shards the parameters across devices for FSDP. We can take as input a PyTree of parameters and a mesh axis name, and determine for each parameter the sharding specification. To keep the global shape of a parameter untouched, we look for an axis which can be equally split across the number of devices present. If multiple are present, we select the largest possible axis, to keep the sharding consistent when varying the number of devices. We then use this axis as the sharding axis, and wrap the parameter in a `nn.Partitioned` with the axis name and position. For some parameters that are very small, sharding may not be beneficial since the communication time may outweigh the memory costs. For instance, we are likely interested in sharding large weight matrices while the bias and scaling parameter in a normalization layer have negligible memory costs. We can specify a minimum size for sharding, and only shard parameters that are larger than this size. We implement the function below:

[21]:
```
@jax.named_scope("shard_params")
def shard_params(params: PyTree, axis_name: str, min_weight_size: int = 2**18) -> PyTree:
    """Shard parameters across the given mesh axis.

    Args:
        params: The parameters to shard.
        axis_name: The axis to shard parameters across.
        min_weight_size: The minimum size of a parameter to shard. Parameters with fewer␣
↪values will not be sharded.

    Returns:
        PyTree of same structure as params, but with leaves sharded over new axis if␣
↪possible.
    """
    axis_idx = jax.lax.axis_index(axis_name)
    axis_size = jax.lax.psum(1, axis_name)

    def _split(x: Parameter) -> Parameter:
        if isinstance(x, nn.Partitioned):
            value, names = x.value, x.names
        else:
            value = x
            names = (None,) * value.ndim
        if axis_name in names:
            logging.warning(
                f"Parameter {value.shape} with names {names} already sharded on axis
↪{axis_name}."
            )
            return x
        elif value.size <= min_weight_size:
            logging.info(
                f"Parameter {value.shape} with names {names} too small to shard, size
↪{value.size} < {min_weight_size}."
            )
            return x
        else:
            shape = value.shape
            idx = np.argsort(shape)[::-1]  # Shard along largest possible axis.
            for i in idx:
                if shape[i] % axis_size == 0 and names[i] is None:
                    split_size = shape[i] // axis_size
```

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```
                    p_sharded = nn.Partitioned(
                        value=lax.dynamic_slice_in_dim(  # Shard to keep on present␣
↪device.
                            value, axis_idx * split_size, split_size, axis=i
                        ),
                        names=names[:i] + (axis_name,) + names[i + 1 :],
                    )
                    return p_sharded
            logging.warning(
                f"Could not shard {value.shape} with names {names} on axis {axis_name},␣
↪no suitable axis found."
            )
            return x

    return jax.tree_util.tree_map(
        _split,
        params,
        is_leaf=lambda x: isinstance(
            x, nn.Partitioned
        ),  # Consider a nn.Partitioned object as a leaf.
    )
```

In the split function, we check for each parameter wether it has been already sharded over the data axis. This case should usually not occur, since we cannot shard a parameter twice over the same mesh axis (otherwise information must get lost). However, it can occur if we shard a parameter over the data axis, and then want to shard it over another axis. Hence, we allow for `nn.Partitioned` objects with other axis names, and find a new axis to shard over. We then shard the parameter over the new axis and return the new `nn.Partitioned` object. Note that the logging statements are only evaluated during the first run of the function when jitted, and can give us a hint when something went wrong.

With the parameters sharded, we now need to write a function to gather the parameters back to a single device. This is necessary for the forward pass, where we want to compute the output of the model on a single device. We can use `jax.lax.all_gather` to gather the parameters from all devices and concatenate them along the sharding axis. In the backward pass, we will use `jax.lax.psum_scatter` to scatter the gradients back to the respective devices. However, one subtle difference to a non-sharded parameter is that in our previous data parallelism training step, we averaged the gradients of different devices. The `jax.lax.psum_scatter` would instead sum the gradients over the devices. To keep the behavior consistent, we adjust the backward pass to average the gradients over the devices. We implement the adjusted gather operation below:

[22]:
```
def gather_array_with_mean_grads(x: jax.Array, axis: int, axis_name: str):
    """Gathering with averaging gradients across replicas."""
    axis_size = jax.lax.psum(1, axis_name)

    # Define a custom gradient for the gather operation.
    @jax.custom_gradient
    def f(x):
        def grad_fn(g):
            # pmean_scatter
            return (
                jax.lax.psum_scatter(g, axis_name, scatter_dimension=axis, tiled=True) /␣
↪axis_size
            )

        return jax.lax.all_gather(x, axis_name, axis=axis, tiled=True), grad_fn
```

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```
    return f(x)
```

We can now write a function that takes as input a PyTree of the sharded parameters and gathers them back to a single device. This will be our reverse operation of `shard_params` function. We implement the function below:

[23]:
```
@jax.named_scope("gather_params")
def gather_params(params: PyTree, axis_name: str) -> PyTree:
    """Gather parameters from all replicas across the given axis.

    Args:
        params: The parameters to gather.
        axis_name: The axis to gather parameters across.

    Returns:
        PyTree of same structure as params, but with leaves gathered if they were a nn.
↪Partitioned object.
    """

    def _gather(p: Parameter) -> Parameter:
        if isinstance(p, nn.Partitioned) and axis_name in p.names:
            param_shard = p.names
            shard_axis = param_shard.index(axis_name)
            value = gather_array_with_mean_grads(p.value, axis=shard_axis, axis_
↪name=axis_name)
            # If there are any other axes that are sharded, we need to keep the␣
↪partitioned structure.
            # Otherwise, we can return the value directly.
            param_shard = param_shard[:shard_axis] + (None,) + param_shard[shard_axis +␣
↪1 :]
            if any([name is not None for name in param_shard]):
                return nn.Partitioned(value, param_shard)
            else:
                return value
        else:
            return p

    return jax.tree_util.tree_map(_gather, params, is_leaf=lambda x: isinstance(x, nn.
↪Partitioned))
```

Whenever we call a module, we want to gather the parameters back to a single device, and then shard them again once the module is done computing (i.e. free the memory of the full parameters). For this, we wrap a module into a `nn.map_variables` transformation, which allows for transformations on the parameter before and after the module is called. We can use this to gather the parameters before the module is called, and shard them again after the module is done. We implement the function below:

[24]:
```
def shard_module_params(
    target: nn.Module | Callable, axis_name: str, min_weight_size: int = 2**18
) -> nn.Module | Callable:
    """Shard parameters of a module across replicas.

    Args:
```

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```
        target: The module to shard.
        axis_name: The axis name to shard parameters across.
        min_weight_size: The minimum size of a parameter to shard. Parameters with fewer␣
↪values will not be sharded.

    Returns:
        The module with sharded parameters.
    """
    return nn.map_variables(
        target,
        trans_in_fn=functools.partial(gather_params, axis_name=axis_name),
        trans_out_fn=functools.partial(
            shard_params, axis_name=axis_name, min_weight_size=min_weight_size
        ),
        mapped_collections="params",
        mutable=True,
    )
```

Another aspect in the design of FSDP is how we deal with the gathered parameters during the training step. If we use the function as is, we would gather the parameters and we keep the full parameters as intermediate arrays on a single device until the backward step is completed. We may have situations where the full parameters do not fit on a single device. In that case, we can remat the gather operation, such that after the forward pass of a module, we free up the memory of the full parameters of the module, and only keep the sharded parameters. We can then gather the parameters again before the backward pass, and scatter the gradients back to the respective devices. This can be done by using the `remat` transformation directly on `gather_params`, or by rematting the whole forward pass with a policy to remat all `all_gather` operations: `@partial(jax.remat, policy=lambda op, *_, **__: str(op) != 'all_gather')` (see official documentation for more details). The final option is to remat the whole module, which we have seen in the previous tutorial. In that case, it matters whether we shard the parameters of every individual module, or the global module, since in the individual case, we also remat the gather, while in the other case, we only remat the forward pass. All these options trade off memory and communication cost, and need to be chosen based on the hardware at hand. We will provide both options in our code, such that depending on the model size, the corresponding setup can be chosen.

Let's now use the sharding function to shard our simple classifier below:

[25]:
```
class FSDPClassifier(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array, train: bool) -> jax.Array:
        sharded_dense = shard_module_params(
            nn.Dense,
            axis_name=self.config.data_axis_name,
            min_weight_size=self.config.min_weight_size,
        )
        x = sharded_dense(
            features=self.config.hidden_size,
            dtype=self.config.dtype,
            name="input_dense",
        )(x)
        x = nn.silu(x)
        x = nn.Dropout(rate=self.config.dropout_rate, deterministic=not train)(x)
        x = sharded_dense(
```

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```
            features=self.config.num_classes,
            dtype=self.config.dtype,
            name="output_dense",
        )(x)
        x = x.astype(jnp.float32)
        return x
```

Note that we only shard the dense layers here, since all other layers (activation function, dropout) do not have any parameters.

Initialization

We can now initialize the model. First, we set the `min_weight_size` at which we want to shard the parameters. The original value of 2^{18} is chosen based on parameters being greater than 1MB (assuming 4 bytes per parameter), inspired by the Big Vision repository. However, for demonstration purposes, we set it much lower here such that some weights are sharded for our small example model.

[26]:
```
config.model.min_weight_size = 2**4
```

The model is then created as usual. If we want to shard the parameters of the whole model, we would use `model_fsdp = shard_module_params(FSDPClassifier, axis_name=config.data_axis_name, min_weight_size=config.model.min_weight_size)(config.model)` instead.

[27]:
```
model_fsdp = FSDPClassifier(config=config.model)
```

While we can reuse our initialization function, we need to adjust the shard map. This is because some parameters are now sharded across devices, and we need to specify the mesh and the sharding specifications for the input and output. The partitioning is determined within the model initialization, so we cannot manually specify it as before. Instead, we can first wrap the initialization function with `shard_map` and an unknown output specification (i.e. simply set to all replicated `P()` and `check_rep` to False), and evaluate the shapes which is independent of the output specification. Since the shapes are also determined for the partitioned parameters, we can then use the shapes to determine the sharding specification. An easy way of doing that is by using `nn.get_partition_spec` which returns the sharding specification of a PyTree with `nn.Partitioned` leafs. We can then use this specification to wrap the initialization function with `shard_map` and the correct output specification. We implement the function below:

[28]:
```
init_fsdp_fn = shard_map(
    functools.partial(init_dp, model=model_fsdp),
    mesh,
    in_specs=(P(), P(config.data_axis_name)),
    out_specs=P(),
    check_rep=False,
)
state_fsdp_shapes = jax.eval_shape(init_fsdp_fn, model_init_rng, batch.inputs)
state_fsdp_specs = nn.get_partition_spec(state_fsdp_shapes)
```

We can check the specification before plugging it into the `shard_map` function. Since the output of the initialization function is a train state, `state_fsdp_specs` is a train state as well, but with each element being a partition spec instead. We can print out the specs below.

[29]:
```
print("RNG", state_fsdp_specs.rng)
print("\nParameters")
pprint(state_fsdp_specs.params)
```

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```
print("\nOptimizer state")
pprint(state_fsdp_specs.opt_state[0])
```

```
RNG PartitionSpec()

Parameters
{'input_dense': {'bias': PartitionSpec('data',),
                 'kernel': PartitionSpec('data', None)},
 'output_dense': {'bias': PartitionSpec(),
                  'kernel': PartitionSpec('data', None)}}

Optimizer state
ScaleByAdamState(count=PartitionSpec(), mu={'input_dense': {'bias': PartitionSpec('data',
↪), 'kernel': PartitionSpec('data', None)}, 'output_dense': {'bias': PartitionSpec(),
↪'kernel': PartitionSpec('data', None)}}, nu={'input_dense': {'bias': PartitionSpec(
↪'data',), 'kernel': PartitionSpec('data', None)}, 'output_dense': {'bias':␣
↪PartitionSpec(), 'kernel': PartitionSpec('data', None)}})
```

The random number generator is replicated across devices as before. The parameters have now different shardings. The kernels of both dense layers are sharded over the data axis, while the output bias is replicated across all devices due to its small size (only 10 parameters). Further, the optimizer state follows the same sharding as the parameters. The `mu` (first order momentum) and `nu` (second order momentum) are sharded over the data axis like the parameters, while the `step` (step counter) is replicated across all devices. We can now wrap the initialization function with the correct output specification and execute it.

[30]:
```
init_fsdp_fn = jax.jit(
    shard_map(
        functools.partial(init_dp, model=model_fsdp),
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_fsdp_specs,
        check_rep=False,
    )
)
state_fsdp = init_fsdp_fn(model_init_rng, batch.inputs)
```

We print the shapes of the parameters to verify that the sharding was successful and their global shape is as we expected.

[31]:
```
print("FSDP Parameters")
pprint(jax.tree_map(lambda x: x.shape, jax.device_get(state_fsdp.params)))
```

```
FSDP Parameters
{'input_dense': {'bias': Partitioned(value=(512,), names=('data',), mesh=None),
                 'kernel': Partitioned(value=(784, 512),
                                       names=('data', None),
                                       mesh=None)},
 'output_dense': {'bias': (10,),
                  'kernel': Partitioned(value=(512, 10),
                                        names=('data', None),
                                        mesh=None)}}
```

All parameters have the expected global shape, and are sharded on their largest axis if they are larger than the minimum weight size. The `mesh` attribute in `nn.Partitioned` can be set to a different mesh if we do not want to shard over the global mesh, as set by the `shard_map`. In most cases, however, we want to shard over the global mesh, and can leave

the `mesh` attribute as `None`. We can now move on to the training loop.

Train Step

In the training step, we need to adjust the synchronization of the gradients to take into account the parameter sharding. For a given parameter gradient in our PyTree, we want to average the gradients over a mesh axis if it was not partitioned over it, and leave it otherwise. We implement this strategy in the function below. Note that, in later tutorials, we will be dealing with multiple mesh axes. Hence, the function is written such that it can handle multiple mesh axes, and we can simply pass the mesh axis name over which we want to average the gradients.

[32]:
```
def sync_gradients(
    grads: PyTree,
    axis_names: Sequence[str],
) -> PyTree:
    """Synchronize gradients across devices.

    Gradients for parameters that are replicated over a given axis are averaged across␣
↪devices.
    Parameters that are partitioned over a given axis are considered to already have a␣
↪mean of
    the gradients on each device, and hence do not need to be altered.

    Args:
        grads: The gradients to synchronize.
        axis_names: The axis names to synchronize gradients across.

    Returns:
        The gradients averaged over the specified axes if they are replicated.
    """

    def sync_grad(g: Parameter) -> Parameter:
        if isinstance(g, nn.Partitioned):
            # Tree leaves for flattening potentially nested axis (multiple names can␣
↪exist for single array axis).
            replication_axis_names = [
                name for name in axis_names if name not in jax.tree_util.tree_leaves(g.
↪names)
            ]
            if len(replication_axis_names) == 0:
                # Parameters partitioned over all axes.
                return g
            else:
                # Average over remaining replicated axes.
                return g.replace(value=jax.lax.pmean(g.value, axis_name=replication_axis_
↪names))
        else:
            # Parameters are replicated over all axes.
            return jax.lax.pmean(g, axis_name=axis_names)

    return jax.tree_map(sync_grad, grads, is_leaf=lambda x: isinstance(x, nn.
↪Partitioned))
```

Besides the gradient averaging, we do not need to adjust anything else of our training step. One potential optimization is to cast the parameters to `bfloat16` before we execute the `apply_fn` in the `loss_fn`. This can reduce the communi-

cation overhead, since we only need to communicate half the amount of data. However, this only works if all parameters would need to be in `bfloat16`, and might be more tricky to handle if we have a mix of parameter precisions in our model. Hence, for simplicity, we will not implement this optimization here, and leave the loss function unchanged.

[33]:
```
def train_step_fsdp(
    state: TrainState,
    metrics: Metrics,
    batch: Batch,
) -> Tuple[TrainState, Metrics]:
    rng, step_rng = jax.random.split(state.rng)
    grads, step_metrics = accumulate_gradients(
        state,
        batch,
        step_rng,
        config.optimizer.num_minibatches,
        loss_fn=loss_fn,
    )
    # Update parameters. We need to sync the gradients across devices before updating.
    with jax.named_scope("sync_gradients"):
        grads = sync_gradients(grads, (config.data_axis_name,))
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Sum metrics across replicas. Alternatively, we could keep the metrics separate
    # and only synchronize them before logging. For simplicity, we sum them here.
    with jax.named_scope("sync_metrics"):
        step_metrics = jax.tree_map(
            lambda x: jax.lax.psum(x, axis_name=config.data_axis_name), step_metrics
        )
    if metrics is None:
        metrics = step_metrics
    else:
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

We can now wrap the train step with `shard_map` and jit it. We reuse our sharding specification of the train state, which we determined during the initialization, and specify the mesh and the sharding specifications for the metrics and batch as before.

[34]:
```
train_step_fsdp_fn = jax.jit(
    shard_map(
        train_step_fsdp,
        mesh,
        in_specs=(state_fsdp_specs, P(), P(config.data_axis_name)),
        out_specs=(state_fsdp_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
_, metric_shapes = jax.eval_shape(
    train_step_fsdp_fn,
    state_fsdp,
    None,
    batch,
)
metrics_fsdp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
```

Let's run it again for a few steps and check the resulting metrics:

[35]:
```
for _ in range(15):
    state_fsdp, metrics_fsdp = train_step_fsdp_fn(state_fsdp, metrics_fsdp, batch)
final_metrics_fsdp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_fsdp, final_metrics_fsdp = train_step_fsdp_fn(state_fsdp, final_metrics_fsdp,␣
↪batch)
print_metrics(final_metrics_fsdp, "FSDP - Final metrics")
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[64]),␣
↪ShapedArray(float32[98,512]), ShapedArray(float32[64,10]), ShapedArray(float32[64]),␣
↪ShapedArray(float32[98,512]), ShapedArray(float32[64,10]), ShapedArray(float32[64]),␣
↪ShapedArray(float32[98,512]), ShapedArray(float32[64,10]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

```
 FSDP - Final metrics
accuracy: 1.000000
loss: 0.003343
```

The model is training as expected and is able to overfit on the single batch of data.

Verify that FSDP gives same results as DP

Since the different parallelism strategies should result in the same model, we can verify that the FSDP model gives the same results as the data parallel model without sharding. Further, the initialization of the both models behave in the exact same way, such that in our example training runs above, they should have resulted in the same outputs. We can verify this by comparing the metrics of the FSDP and DP model below:

[36]:
```
metrics_dp = jax.device_get(metrics_dp)
metrics_fsdp = jax.device_get(metrics_fsdp)
for key in metrics_dp.keys():
    val_dp = metrics_dp[key][0] / metrics_dp[key][1]
    val_fsdp = metrics_fsdp[key][0] / metrics_fsdp[key][1]
    print(f"Metrics DP Avg {key}: {val_dp:.4f}")
    print(f"Metrics FSDP Avg {key}: {val_fsdp:.4f}")
    np.testing.assert_allclose(val_dp, val_fsdp, atol=1e-2)
```

```
Metrics DP Avg accuracy: 0.8844
Metrics FSDP Avg accuracy: 0.8844
Metrics DP Avg loss: 0.5102
Metrics FSDP Avg loss: 0.5102
```

Both models have resulted in the same metrics, suggesting that the FSDP model is training as expected. We can also compare parameters and optimizer state to verify that they are the same.

[37]:
```
params_dp = jax.device_get({"params": state_dp.params, "opt_state": state_dp.opt_state})
params_fsdp = jax.device_get({"params": state_fsdp.params, "opt_state": state_fsdp.opt_
↪state})
params_fsdp = jax.tree_map(
    lambda x: x.value if isinstance(x, nn.Partitioned) else x,
    params_fsdp,
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
```

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```
)
_ = jax.tree_map(lambda x, y: np.testing.assert_allclose(x, y, atol=1e-4), params_dp,␣
↪params_fsdp)
print("Parameters match between DP and FSDP")
```

```
Parameters match between DP and FSDP
```

We find that both methods result in the same output, verifying that we have implemented FSDP correctly. Note that very small differences can still occur due to different reductions in the gradient sync. However, these differences should be negligible and not affect the training of the model.

4.9.4 Conclusion

In this tutorial, we have introduced the basic building blocks of distributed computing in JAX, and implemented data parallelism and fully-sharded data parallelism. In data parallelism, we shard the input batch over the data axis, and the model parameters are replicated across all devices. This allows for a larger batch size and faster training. For large models, we further improved the memory footprint by sharding the model parameters across devices. In this fully-sharded data parallelism (FSDP), we have seen how to shard the model parameters, and how to gather and scatter the parameters and gradients in the forward and backward pass. Data parallelism is one of the most common parallelism strategies in deep learning, and FSDP is a powerful tool to scale to very large models. Still, we may come to situations where the model size is limited by the memory of a single device, and we need expensive remat strategies to overcome this. Alternatively, we can look at other parallelism strategies which shard the model execution itself over devices. These strategies, also called model parallelism, will be the focus in the next tutorials, specifically pipeline parallelism and tensor parallelism. With these, we can scale to even larger models and train billion-parameter models efficiently.

4.9.5 References and Resources

[Rajbhandari et al., 2020] Rajbhandari, S., Rasley, J., Ruwase, O. and He, Y., 2020. Zero: Memory optimizations toward training trillion parameter models. In SC20: International Conference for High Performance Computing, Networking, Storage and Analysis (pp. 1-16). Paper link

[Wang and Komatsuzaki, 2021] Wang, B., and Komatsuzaki, A., 2021. Mesh transformer jax. GitHub link

[Beyer et al., 2022] Beyer, L., Zhai, X., and Kolesnikov, A., 2022. Big Vision. GitHub link

[Google, 2024] JAX Team Google, 2024. Distributed arrays and automatic parallelization. Notebook link

[Google, 2024] JAX Team Google, 2024. SPMD multi-device parallelism with shard_map. Notebook link

[Google, 2024] JAX Team Google, 2024. Using JAX in multi-host and multi-process environments. Notebook link

[DeepSpeed, 2024] DeepSpeed, 2024. Zero Redundancy Optimizer. Tutorial link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.10 Part 3.1: Pipeline Parallelism

Filled notebook:

Author: Phillip Lippe

In the previous tutorial, we have seen data parallelism, which works well for intermediate large models and large batch sizes. However, as we continue to increase the model size, the batch size per device can become very small, which can lead to inefficient usage of the accelerators. This is because on the one hand, the time spent on communication between devices can become significant compared to the time spent on computation. On the other hand, small batch sizes can lead to poor utilization of the device's computational resources, since fewer operations can be performed in parallel.

In such cases, we need to consider parallelism strategies that can parallelize the model itself, rather than the data. Such strategies can lead to strong utilization, even if the batch size per device is small. In this notebook series, we will consider two such strategies: pipeline parallelism and tensor parallelism. Intuitively, pipeline parallelism splits the model across layers, while tensor parallelism splits the model across feature dimensions. We visualize these strategies in the figure below.

In this notebook, we will focus on pipeline parallelism. We will first discuss the concept of pipeline parallelism, and then show how to implement it in JAX.

Pipeline parallelism is a way to parallelize the forward and backward passes of a model across multiple devices. In comparison to data parallelism which replicates the model across devices, the model is instead split across its layers into multiple stages. Each stage consists of multiple layers of the model, and is placed on a different device. The output of each stage is passed to the next stage, and the final output is the result of the last stage. For example, consider a Transformer model with 12 layers and 4 devices. In this case, we can split the model into 4 stages, each consisting of 3 layers. The first three layers are placed on the first device, the next three on the second device, and so on. Given an input batch, we start by passing it to stage 1 on the first device. The output of stage 1 is then passed to stage 2, and so on, until the final output is produced by stage 4. The backward pass is performed in the reverse order, starting from the last stage and ending at the first stage. This way, each device only requires a subset of the model, reducing the memory requirements and allowing for larger models to be trained. At the same time, we introduce minimal communication between devices, as the output of each stage is only passed to the next stage. This leads to a computation graph similar as in the figure below (F_i - forward pass of stage i, B_i - backward pass of stage i, Update - optimizer step and gradient communication). We note that the precise timings may depend on additional factors, such as communication speed, cost of backward pass, additional data parallelism (especially for update step), etc. But for now, let's focus on the basic idea.

When looking at the figure, we can see that the forward pass of stage 1 can start as soon as the first layer is computed, and the backward pass of stage 4 can start as soon as the last layer is computed. However, for a large amount of time, the devices are idle, as they are waiting for the output of the previous stage. This can lead to the **"pipeline bubble"** problem, where the utilization of the devices is reduced due to the time spent waiting for the output of the previous stage. In this notebook, we will discuss and implement simple strategies to mitigate the pipeline bubble problem, and show how this can be done efficiently in JAX.

4.10.1 Prerequisites

First, let's start with setting up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = ["single_gpu.py", "data_parallel.py", "utils.py"]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

As before, we simulate 8 devices on CPU to demonstrate the parallelism without the need for multiple GPUs or TPUs. If you are running on your local machine and have multiple GPUs available, you can comment out the lines below.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

We now import our standard libraries.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from flax.core.frozen_dict import FrozenDict
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict
```

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```
# Helper types
PyTree = Any
Parameter = jax.Array | nn.Partitioned
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We also import the utility functions from the previous notebooks.

[4]:
```
from data_parallel import fold_rng_over_axis, sync_gradients
from single_gpu import (
    Batch,
    TrainState,
    accumulate_gradients,
    get_num_params,
    print_metrics,
)
```

4.10.2 Pipeline Parallelism with Micro-Batching

The first strategy to mitigate the pipeline bubble problem is to use micro-batching, as introduced in GPipe [Huang et al., 2019]. The idea is to split the input batch into smaller sub-batches (micro-batches), and processing them sequentially. At the end of each micro-batch, we communicate the outputs between stages, and start processing the next micro-batch. This way, we can keep the devices busy while waiting for the output of the previous stage, and reduce the pipeline bubble problem.

For example, consider a batch of size 32, and a pipeline with 4 stages. We can split the batch into 4 micro-batches (or any other factor of 32), each of size 8, and process them sequentially. As soon as the first micro-batch is processed by stage 1, we can communicate the output to stage 2, and start processing the second micro-batch, as so on. The figure below shows the computation graph for the forward and backward passes of the pipeline with this micro-batching strategy.

Compared to the original pipeline, we can see that the devices are kept busy for a larger portion of the time, as they are processing the micro-batches sequentially. However, we also note that the communication between stages is now more frequent, as we need to communicate the output of each micro-batch. This can lead to increased communication overhead, especially for small micro-batches. In practice, the choice of the micro-batch size is a trade-off between the pipeline bubble problem, the communication overhead, and the max utilization we can achieve per device with this micro-batch size.

In the following, we will show how to implement pipeline parallelism with micro-batching in JAX. We will use a simple MLP model for demonstration (to make it feasible on CPU), and show how to split the model across stages. For any other model such as larger Transformer, the same principles apply and can be implemented without changes to the pipeline wrapper below.

Module Preparation

We start with implementing a simple MLP model, which requires no changes compared to a non-pipeline model. The MLP consists of multiple residual blocks as in a Transformer model, just without the attention (for simplicity). As in the previous notebook, we use a `ConfigDict` to store the model hyperparameters, a scan for reducing compilation time, and support remat and mixed precision.

[5]:
```
class MLPBlock(nn.Module):
    config: ConfigDict
    train: bool

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        input_features = x.shape[-1]
        residual = x
        x = nn.LayerNorm(dtype=self.config.dtype, name="pre_norm")(x)
        x = nn.Dense(
            features=self.config.hidden_size * self.config.mlp_expansion,
            dtype=self.config.dtype,
            name="input_dense",
        )(x)
        x = nn.silu(x)
        x = nn.Dropout(rate=self.config.dropout_rate, deterministic=not self.train)(x)
        x = nn.Dense(features=input_features, dtype=self.config.dtype, name="output_dense
↪")(x)
        return x + residual
```

[6]:
```
class MLPLayers(nn.Module):
    config: ConfigDict
    train: bool

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        # Scan version
        block_class = MLPBlock
        if "MLP" in self.config.remat:
            block_class = nn.remat(block_class, prevent_cse=False)
        block = block_class(config=self.config, train=self.train, name="block")
        x, _ = nn.scan(
            lambda module, carry, _: (module(carry), ()),
            variable_axes={"params": 0},
            split_rngs={"params": True, "dropout": True},
            length=self.config.num_layers,
        )(block, x, ())
        # Non-scanned version
        # for i in range(self.config.num_layers):
        #     x = block_class(self.config, train=train, name=f"block_{i}")(x)
        return x
```

Similar to the previous notebook on data parallelism, we have parameters have different values on different devices. Note that we will be generally allowing for multiple axes in our mesh, since model parallelism is often combined with data parallelism. Thus, we will wrap the parameters in a `nn.Partitioned` class to annotate their sharding over the `model` axis (for simplicity, we do not consider FSDP here, but show how it can be easily added in a later notebook). This way, we can easily split the parameters across devices, and use the same model definition for all stages.

Compared to last time, we stack the parameters over a new axis that we create. While one could also concatenate them along the layer index that is introduced by `nn.scan`, it would be unintuitive and error-prone for settings or parameters that are not scanned over. Still, this is only a design choice and both ways can be used.

Below, we implement functions that will support the partitioning of parameters in this fashion via the `nn.map_variables` transform.

[7]:
```
def stack_params(
    params: PyTree, axis_name: str, axis: int = 0, mask_except: jax.Array | int | None =␣
↪None
) -> PyTree:
    """Stacks sharded parameters along a given axis name.

    Args:
        params: PyTree of parameters.
        axis_name: Name of the axis to stack along.
        axis: Index of the axis to stack along.
        mask_except: If not None, only the `mask_except`-th shard will be non-zero.

    Returns:
        PyTree of parameters with the same structure as `params`, but with the leaf
        nodes replaced by `nn.Partitioned` objects with sharding over axis name added
        to `axis`-th axis of parameters.
    """

    def _stack(x: Parameter) -> Parameter:
        if isinstance(x, nn.Partitioned):
            value, names = x.value, x.names
        else:
            value, names = x, (None,) * x.ndim
        if mask_except is not None:
            axis_index = jax.lax.axis_index(axis_name)
            value = jnp.where(axis_index == mask_except, value, 0.0)
        value = jnp.expand_dims(value, axis)
        names = names[:axis] + (axis_name,) + names[axis:]
        return nn.Partitioned(value, names=names)

    return jax.tree_map(_stack, params, is_leaf=lambda x: isinstance(x, nn.Partitioned))


def unstack_params(params: PyTree, axis_name: str) -> PyTree:
    """Unstacks parameters along a given axis name.

    Inverse operation to `stack_params`.

    Args:
        params: PyTree of parameters.
        axis_name: Name of the axis to unstack along.

    Returns:
        PyTree of parameters with the same structure as `params`, but
        with the leaf nodes having the sharding over the axis name removed.
    """
```

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```
    def _unstack(x: Parameter) -> Parameter:
        if isinstance(x, nn.Partitioned) and axis_name in x.names:
            value = x.value
            names = x.names
            axis_idx = names.index(axis_name)
            value = value.squeeze(axis_idx)
            names = names[:axis_idx] + names[axis_idx + 1 :]
            if all([n is None for n in names]):
                return value
            else:
                return nn.Partitioned(value, names=names)
        else:
            return x

    return jax.tree_map(_unstack, params, is_leaf=lambda x: isinstance(x, nn.
↪Partitioned))
```

Pipeline Implementation

The pipeline implementation is iterating over two simple steps: applying the stages per device on a micro-batch, and communicating the last output between devices to get the next input. Whenever there is no proper input ready, we still run the stage to follow the SPMD principle (single program multiple devices), but ignore the output. Our communication is performed using `jax.lax.ppermute` which transfers an array over a ring: stage 1 sends its output to stage 2, stage 2 to stage 3, stage 3 to stage 4, and finally, stage 4 to stage 1. The last communication between stage 4 and stage 1 can be ignored, as it is only used to close the ring and stage 1 uses the original micro-batches as input. Instead, we store the last N outputs of stage 4 and use them for the loss calculation in the final layers, since those are the outputs of the full model. In summary, the computation graph for the forward pass will look similar as in the figure below:

Note that for simplicity, we didn't visualize unused communications (e.g. stage 4 to stage 1). Finally, the backward pass will be automatically handled by JAX's `jax.grad` transformation.

We implement this loop with a `nn.scan` operation, which keeps the parameters across all steps the same, but allows for different inputs and outputs, as well as updating the RNGs (used in Dropout). First, we implement a single step of the loop below:

[8]:
```
def execute_pipeline_step(
    module: nn.Module,
    state: jax.Array,
    input: jax.Array,
    *args,
    model_axis_name: str,
    **kwargs,
) -> Tuple[jax.Array, jax.Array]:
    """Single micro-batch pipeline step.

    Args:
        module: Flax module representing the stage to execute.
        state: Last communicated features between stages. Used as input to the␣
↪for all stages except the first.
        input: Original micro-batch input to the pipeline stage. Used as input to the␣
↪module for the first stage.
```

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```
        *args: Additional arguments to the module.
        model_axis_name: Name of the model axis in the mesh/shard_map.
        **kwargs: Additional keyword arguments to the module.

    Returns:
        Tuple of the new state (after communication) and the output of the module.
    """
    num_stages = jax.lax.psum(1, model_axis_name)
    stage_index = jax.lax.axis_index(model_axis_name)
    # For the first stage, we use the microbatches as input.
    # For all other stages, we use the last state from the
    # previous stage as input.
    state = jnp.where(stage_index == 0, input, state)
    state = module(state, *args, **kwargs)
    # For the last stage, we return the state as output.
    # For all other stages, we return zeros.
    output = jnp.where(
        stage_index == num_stages - 1,
        state,
        jnp.zeros_like(state),
    )
    # Communicate the last state to the next stage.
    state = jax.lax.ppermute(
        state,
        model_axis_name,
        perm=[(i, (i + 1) % num_stages) for i in range(num_stages)],
    )
    return (state, output)
```

With the single step implemented, we can now wrap it in a `nn.scan` operation to iterate over the micro-batches. Compared to the scan over layers in the `MLPLayers` module, we now scan over the micro-batches, and keep the parameters the same. The latter is controlled by setting `variable_broadcast` to `{"params": True}`, and not splitting the params RNG over iterations. To scan over the input and output, we add `in_axes=0` and `out_axes=0`, which effectively unstacks the input and stacks the output over the first axis across iterations. In other words, the first iteration get the first micro-batch as input, the second iteration the second micro-batch, and so on. Additionally, the current `state` of the stages is communicated as a carry, which is passed between iterations.

The final difference in the `nn.scan` is that we do not want to scan a single module, but instead actually the function `execute_pipeline_step`. Flax allows for that by requiring the function to take a module as its first argument. This module is then scanned as specified by the other keyword arguments, but we execute the passed function at each iteration. This way, we can use our `execute_pipeline_step` function with the `nn.scan` operation. This results in the following pipeline function:

[9]:
```
@jax.named_scope("pipeline")  # Naming scope for profiling.
def execute_pipeline(
    module: nn.Module, x: jax.Array, *args, num_microbatches: int, model_axis_name: str,␣
↪**kwargs
) -> jax.Array:
    """Execute a pipeline of stages on a batch of data.

    Uses the principle of GPipe in splitting the batch into micro-batches
    and running the pipeline stages in parallel.
```

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```
    Args:
        module: Flax module representing the pipeline stage to execute.
        x: Batch of input data, only needed on device of the first stage. Data will be␣
↪split into micro-batches.
        *args: Additional arguments to the module.
        num_microbatches: Number of micro-batches to split the batch into.
        model_axis_name: Name of the model axis in the mesh/shard_map.
        **kwargs: Additional keyword arguments to the module.

    Returns:
        Output of the last stage of the pipeline. For devices that are not
        the last stage, the output is zeros.
    """
    num_stages = jax.lax.psum(1, model_axis_name)
    # Structure the input data into micro-batches.
    batch_size = x.shape[0]
    assert (
        batch_size % num_microbatches == 0
    ), f"Batch size {batch_size} must be divisible by number of microbatches {num_
↪microbatches}"
    microbatch_size = batch_size // num_microbatches
    microbatches = jnp.reshape(x, (num_microbatches, microbatch_size, *x.shape[1:]))
    inputs = jnp.concatenate(  # Add zeros for unused computation blocks in first stage.
        [
            microbatches,
            jnp.zeros((num_stages - 1, *microbatches.shape[1:]), dtype=microbatches.
↪dtype),
        ],
        axis=0,
    )
    state = jnp.zeros_like(microbatches[0])
    num_iterations = inputs.shape[0]
    # Run loop over pipeline steps.
    _, outputs = nn.scan(
        functools.partial(
            execute_pipeline_step,
            *args,
            model_axis_name=model_axis_name,
            **kwargs,
        ),
        variable_broadcast={"params": True},
        split_rngs={"params": False, "dropout": True},
        length=num_iterations,
        in_axes=0,
        out_axes=0,
    )(module, state, inputs)
    # Take last N outputs (first ones are zeros from unused computation blocks in last␣
↪stage).
    outputs = jnp.concatenate(outputs[-num_microbatches:], axis=0)
    return outputs
```

We can now use this pipeline function to define the model. First, we write a small module wrapper, that creates a module and executes it using the `execute_pipeline` function.

[10]:
```
class PipelineModule(nn.Module):
    model_axis_name: str
    num_microbatches: int
    module_fn: Callable[..., nn.Module]

    @nn.compact
    def __call__(self, *args, **kwargs):
        module = self.module_fn()
        return execute_pipeline(
            module,
            *args,
            **kwargs,
            num_microbatches=self.num_microbatches,
            model_axis_name=self.model_axis_name,
        )
```

Before we can use the pipeline model, we need to shard the parameters. As for the fully-sharded data parallel, we do this by wrapping the module in a `nn.map_variables`, in which we use our two previous functions `stack_params` and `unstack_params` to shard the parameters over the `model` axis. We also need to initialize the parameters on each device differently, which we do by folding the RNG of the parameters over the `model` axis. With that, each device uses a different RNG key, and thus generates different parameters. Since this is a module that can be used for almost any layer that should be sharded across the model axis, we refer to it as a `ModelParallelismWrapper`:

[11]:
```
class ModelParallelismWrapper(nn.Module):
    """Wrapper for adding model parallelism to a module.

    This wrapper adds sharding over the model axis to the parameters of the module
    and initializes the module with different parameters across the model axis.

    Args:
        model_axis_name: Name of the model axis to shard over.
        module_fn: Function that returns the Flax module to wrap.
        mask_except_model_idx: If not None, only the `mask_except_model_idx`-th shard␣
↪will be non-zero.
        split_rngs: If True, split the random number generators across the model axis.
        module_kwargs: Additional keyword arguments to pass to the module function.
    """

    model_axis_name: str
    module_fn: Callable[..., nn.Module]
    mask_except_model_idx: int | None = None
    split_rngs: bool = True
    module_kwargs: FrozenDict[str, Any] = FrozenDict({})

    @nn.compact
    def __call__(self, *args, **kwargs):
        if self.is_initializing() and self.split_rngs:
            # Initialize each module across the model axis with different parameters.
            self.scope.rngs["params"] = self.scope.rngs["params"].replace(
                rng=fold_rng_over_axis(self.scope.rngs["params"].rng, self.model_axis_
↪name)
            )
        # Wrap variables in nn.Partitioned objects to add sharding over the model axis.
```

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```
        module = nn.map_variables(
            target=functools.partial(
                self.module_fn,
                name="sharded",
                **self.module_kwargs,
            ),
            trans_in_fn=functools.partial(unstack_params, axis_name=self.model_axis_
↪name),
            trans_out_fn=functools.partial(
                stack_params,
                axis_name=self.model_axis_name,
                mask_except=self.mask_except_model_idx,
            ),
            mapped_collections="params",
            mutable=True,
        )()
        return module(
            *args,
            **kwargs,
        )
```

Combine Full Model with Pipeline

The pipeline structure assumes that each stage has the same layers and structures. However, commonly, we have an input layer, mapping the input to the first stage, and an output layer, mapping the output of the last stage to the final output. We can easily combine the pipeline model with these layers by using the pipeline model as a sub-module. We can then define the input and output layers as usual, and use the pipeline model to process the intermediate features.

Depending on the cost of the input and output layers, we can also consider to split them across devices. This is particularly of interest if the communication cost is comparatively low on the available devices. For instance, we could perform a data-parallel strategy over the model axis for the input layer and gather all outputs on the first device before executing the pipeline. However, for setups like language models, where the input layer mainly consists of an embedding lookup, the communication between devices may become more expensive than performing the lookup on a single device, or we may consider a tensor parallel approach (more on it in the next notebook). For simplicity, in this notebook, we will duplicate the computation of the input and output layers on all devices, and ignore the outputs of the input layers on all devices except the first one. Duplicating the weights across model devices would lead to unnecessary communication overhead during the optimization step, and we instead set all weights that are unused on certain devices to zero. Hence, the optimizer step will not change the weights on the unused devices, and we can avoid the communication overhead. We have already implemented this strategy in the `ModelParallelismWrapper` by supporting the `mask_except_model_idx` argument. For the input layer, we mask all model devices besides the first one, and for the output layer, we mask all model devices besides the last one.

With this wrapper in place, we can now define the full model, and use it to train the model on a simple task. We will use a simple MLP model to classify random data, and show how to train the model using the pipeline wrapper. Thus, our full model will consist of a linear input layer, the pipeline model, and a final norm plus the linear output layer. For language models, the input layer may be an embedding layer combined with positional embeddings, and the output layer may be the same as shown here, just applied on a per-token basis.

[12]:
```
class PPClassifier(nn.Module):
    config: ConfigDict
```

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```
    pipeline_module_class: Callable[..., nn.Module] = PipelineModule

    @nn.compact
    def __call__(self, x: jax.Array, train: bool) -> jax.Array:
        # Input layer. Only needed in the first stage.
        x = ModelParallelismWrapper(
            module_fn=functools.partial(
                nn.Dense,
                features=self.config.hidden_size,
                dtype=self.config.dtype,
            ),
            model_axis_name=self.config.model_axis_name,
            mask_except_model_idx=0,
            name="input_dense",
        )(x)
        # Pipeline
        stage_module_fn = functools.partial(
            MLPLayers, config=self.config, train=train, name="mlp_layers"
        )
        pipeline_module_fn = functools.partial(
            self.pipeline_module_class,
            model_axis_name=self.config.model_axis_name,
            num_microbatches=self.config.num_microbatches,
            module_fn=stage_module_fn,
        )
        module = ModelParallelismWrapper(
            module_fn=pipeline_module_fn,
            model_axis_name=self.config.model_axis_name,
            name="pipeline",
        )
        x = module(x)
        # Output layer. Only needed in the last stage.
        output_wrapper = functools.partial(
            ModelParallelismWrapper,
            model_axis_name=self.config.model_axis_name,
            mask_except_model_idx=self.config.model_axis_size - 1,
        )
        x = output_wrapper(
            module_fn=functools.partial(nn.LayerNorm, dtype=self.config.dtype), name=
↪"output_norm"
        )(x)
        x = output_wrapper(
            module_fn=functools.partial(
                nn.Dense, features=self.config.num_classes, dtype=self.config.dtype
            ),
            name="output_dense",
        )(x)
        x = x.astype(jnp.float32)
        return x
```

Initialization

With the model defined, we can now implement the initialization and training step. Most of the functions will be very similar to our previous notebook on data parallelism, since the model parallelism in handled within the model. This also suggest a simple composition of parallelization strategies, which we will further explore in a later notebook. For now, we will focus on the pipeline parallelism with simple data parallelism over the batch axis.

Let's start with defining the basic config of our model below. Feel free to adjust the parameters and experiment with different settings.

[13]:
```
data_config = ConfigDict(
    dict(
        batch_size=128,
        num_classes=10,
        input_size=784,
    )
)
model_config = ConfigDict(
    dict(
        hidden_size=512,
        mlp_expansion=1,
        dropout_rate=0.1,
        num_layers=8,
        dtype=jnp.float32,
        num_classes=data_config.num_classes,
        remat=(),
        data_axis_name="data",
        model_axis_name="model",
        model_axis_size=4,
        num_microbatches=8,
    )
)
model_config.num_layers //= model_config.model_axis_size  # Layers distributed over␣
↪model axis.
optimizer_config = ConfigDict(
    dict(
        learning_rate=1e-3,
        num_minibatches=1,
    )
)
config = ConfigDict(
    dict(
        model=model_config,
        optimizer=optimizer_config,
        data=data_config,
        data_axis_name=model_config.data_axis_name,
        model_axis_name=model_config.model_axis_name,
        model_axis_size=model_config.model_axis_size,
        seed=42,
    )
)
```

We can now create our device mesh. By default, we create a 2x4 mesh (for 8 devices), which means that we have a data parallel size of 2 and a model parallel size of 4. Hence, each device will process a batch of half the global size, and the model pipeline will be split into 4 stages.

[14]:
```
device_array = np.array(jax.devices()).reshape(-1, config.model_axis_size)
mesh = Mesh(device_array, (config.data_axis_name, config.model_axis_name))
```

```
2024-03-07 10:47:01.486665: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

We then create the model object and the optimizer. We stick with simple Adam in this example, but feel free to change the optimizer setup.

[15]:
```
model_pp = PPClassifier(config=model_config)
optimizer = optax.adamw(
    learning_rate=config.optimizer.learning_rate,
)
```

For simplicity, we will train the model on a simple random data classification task. This is mainly to demonstrate the pipeline parallelism, and not to achieve state-of-the-art results. In practice, one would instead create a dataset and dataloader at this point, and setup the data prefetching.

[16]:
```
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng, data_labels_rng = jax.random.split(rng, 3)
batch = Batch(
    inputs=jax.random.normal(data_inputs_rng, (config.data.batch_size, config.data.input_
↪size)),
    labels=jax.random.randint(
        data_labels_rng, (config.data.batch_size,), 0, config.data.num_classes
    ),
)
```

The initialization function follows the same principles as in the previous notebook, creating the parameters via `model.init` and the optimizer parameters in the `TrainState.create`.

[17]:
```
def init_fn(rng: jax.random.PRNGKey, x: jax.Array, model: nn.Module) -> TrainState:
    init_rng, rng = jax.random.split(rng)
    variables = model.init({"params": init_rng}, x, train=False)
    params = variables.pop("params")
    state = TrainState.create(
        apply_fn=model.apply,
        params=params,
        tx=optimizer,
        rng=rng,
    )
    return state
```

Before we can run the full initialization, we need to identify the partitioning of the parameters. Since we annotated the partitioning of all parameters via `nn.Partitioned` in the model, we can obtain the partitioning by calling `jax.eval_shape` on the init function. This will return the state shapes, as well as the `nn.Partitioned` parameter leafs. From those, we can read out the partitioning using `nn.get_partition_spec`. For the initial call, we can leave the `out_specs` of the shard map empty, since we do not create the actual parameters during shape evaluation.

[18]:
```
init_pp_fn = shard_map(
    functools.partial(init_fn, model=model_pp),
    mesh,
```

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```
    in_specs=(P(), P(config.data_axis_name)),
    out_specs=P(),
    check_rep=False,
)
state_pp_shapes = jax.eval_shape(init_pp_fn, model_init_rng, batch.inputs)
state_pp_specs = nn.get_partition_spec(state_pp_shapes)
```

Let's investigate the partitioning of the parameters below.

[19]:
```
pprint(state_pp_specs.params)
```

```
{'input_dense': {'sharded': {'bias': PartitionSpec('model', None),
                             'kernel': PartitionSpec('model', None, None)}},
 'output_dense': {'sharded': {'bias': PartitionSpec('model', None),
                              'kernel': PartitionSpec('model', None, None)}},
 'output_norm': {'sharded': {'bias': PartitionSpec('model', None),
                             'scale': PartitionSpec('model', None)}},
 'pipeline': {'sharded': {'mlp_layers': {'block': {'input_dense': {'bias': PartitionSpec(
↪'model', None, None),
                                                                   'kernel':␣
↪PartitionSpec('model', None, None, None)},
                                                   'output_dense': {'bias':␣
↪PartitionSpec('model', None, None),
                                                                    'kernel':␣
↪PartitionSpec('model', None, None, None)},
                                                   'pre_norm': {'bias': PartitionSpec(
↪'model', None, None),
                                                                'scale': PartitionSpec(
↪'model', None, None)}}}}}}
```

We can see that all parameters are partitioned over the model axis, as we expect. Note that if we would have performed data parallelism over the model devices in the input and output layers, those would not be partitioned over the model axis. Similarly, if we would have used FSDP, the parameters would be partitioned over the data axis as well. Finally, the pipeline parameters are partitioned over the model axis on their first axis, and have the scan axis as their second axis (i.e. the layer axis). This is why the biases are three dimensional (model, layers, features), and the weights are four dimensional (model, layers, features, features).

With the partitioning in place, we can now perform the full initialization of the model and optimizer.

[20]:
```
init_pp_fn = jax.jit(
    shard_map(
        functools.partial(init_fn, model=model_pp),
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_pp_specs,
        check_rep=False,
    ),
)
state_pp = init_pp_fn(model_init_rng, batch.inputs)
```

Let's inspect once more the shapes of the parameters to ensure that the initialization was successful.

[21]:
```
pprint(
    jax.tree_map(lambda x: x.shape, state_pp.params["pipeline"]["sharded"]["mlp_layers"][
↪"block"])
```

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```
)
```

```
{'input_dense': {'bias': Partitioned(value=(4, 2, 512),
                                     names=('model', None, None),
                                     mesh=None),
                 'kernel': Partitioned(value=(4, 2, 512, 512),
                                       names=('model', None, None, None),
                                       mesh=None)},
 'output_dense': {'bias': Partitioned(value=(4, 2, 512),
                                      names=('model', None, None),
                                      mesh=None),
                  'kernel': Partitioned(value=(4, 2, 512, 512),
                                        names=('model', None, None, None),
                                        mesh=None)},
 'pre_norm': {'bias': Partitioned(value=(4, 2, 512),
                                  names=('model', None, None),
                                  mesh=None),
              'scale': Partitioned(value=(4, 2, 512),
                                   names=('model', None, None),
                                   mesh=None)}}
```

As we expected, the first axis of the parameters is the model axis, thus being the same size as the model parallel size. The second axis is the layer axis, with the model in default configuration having 2 layers per stage, i.e. 8 layers in total.

We can also check that each model device has initialized its parameters differently, by comparing the parameters on different devices.

[22]:
```
pprint(
    state_pp.params["pipeline"]["sharded"]["mlp_layers"]["block"]["input_dense"]["kernel
↪"].value[
        :, :, 0, 0
    ]
)
```

```
Array([[ 0.01044598, -0.07416785],
       [-0.04605146,  0.0008348 ],
       [-0.00904123, -0.00018691],
       [ 0.00661926, -0.06117292]], dtype=float32)
```

The printed parameter values above are indeed different for each device, since different RNG keys were used for the initialization of the parameters on each device.

Additionally, we check the input and output layers to ensure that they are masked correctly.

[23]:
```
print("Input Layer")
pprint(state_pp.params["input_dense"]["sharded"]["kernel"].value[:, 0, 0])
print("\nOutput layer")
pprint(state_pp.params["output_dense"]["sharded"]["kernel"].value[:, 0, 0])
```

```
Input Layer
Array([-0.0754908,  0.       ,  0.       ,  0.       ], dtype=float32)

Output layer
Array([ 0.        ,  0.        ,  0.        , -0.07138917], dtype=float32)
```

The input layer only has non-zero weights on the first element of the first axis, which corresponds to the first model

device. For the output layer, we have the last element which is non-zero, corresponding to the last model device/pipeline stage. This is as expected, and completes our check of the initialization.

Training with Pipeline Parallelism

With the model and optimizer initialized, we can now define the training step and train the model. The training step is very similar to the previous notebook, with the main difference being that we now consider only the last model device to calculate the loss. Note that, for more expensive output layers, one could also consider to scatter the pipeline outputs over the model axis and calculate the loss of each sub-batch on all devices and average the results. This would lead to a more balanced computation load, but also to a higher communication overhead. For simplicity, we will stick with the last device for the loss calculation, such that we can ignore the losses on the other devices.

Another small difference is that we split the dropout RNG over the model axis, such that each device uses a different RNG key for the dropout. This is done by folding the RNG key over both the data and model axis. This way, each device uses a different RNG key for the dropout, and thus generates different dropout masks. For other random operations, we may want to fold the RNG key only over one of the two axes, depending on the operation and the desired behavior.

[24]:
```
def loss_fn(
    params: PyTree, apply_fn: Any, batch: Batch, rng: jax.Array
) -> Tuple[jax.Array, Dict[str, Any]]:
    # Since dropout masks vary across the batch dimension, we want each device to␣
↪generate a
    # different mask. We can achieve this by folding the rng over the data axis, so that␣
↪each
    # device gets a different rng and thus mask.
    dropout_rng = fold_rng_over_axis(rng, (config.data_axis_name, config.model_axis_
↪name))
    # Remaining computation is the same as before for single device.
    logits = apply_fn(
        {"params": params},
        batch.inputs,
        train=True,
        rngs={"dropout": dropout_rng},
    )
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, batch.labels)
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), batch.labels)
    batch_size = batch.inputs.shape[0]
    # Mask out loss and accuracy for pipeline stages except last one.
    model_idx = jax.lax.axis_index(config.model_axis_name)
    model_size = jax.lax.psum(1, config.model_axis_name)
    loss = jnp.where(model_idx != model_size - 1, 0.0, loss)
    correct_pred = jnp.where(model_idx != model_size - 1, False, correct_pred)
    batch_size = jnp.where(model_idx != model_size - 1, 0, batch_size)
    # Collect metrics and return loss.
    step_metrics = {
        "loss": (loss.sum(), batch_size),
        "accuracy": (correct_pred.sum(), batch_size),
    }
    loss = loss.mean()
    return loss, step_metrics
```

The training step is also very similar as before. While we support gradient accumulation, it is recommended to integrate those minibatches into the pipeline. This is because the pipeline parallelism improves efficiency with increasing number of micro-batches, and thus we want to keep the pipeline busy as much as possible.

[25]:
```
def train_step_pp(
    state: TrainState,
    metrics: Metrics | None,
    batch: Batch,
) -> Tuple[TrainState, Metrics]:
    rng, step_rng = jax.random.split(state.rng)
    grads, step_metrics = accumulate_gradients(
        state,
        batch,
        step_rng,
        config.optimizer.num_minibatches,
        loss_fn=loss_fn,
    )
    # Update parameters. We need to sync the gradients across data devices before␣
↪updating.
    with jax.named_scope("sync_gradients"):
        grads = sync_gradients(grads, (config.data_axis_name, config.model_axis_name))
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Sum metrics across replicas (both model and data axes).
    with jax.named_scope("sync_metrics"):
        step_metrics = jax.tree_map(
            lambda x: jax.lax.psum(x, axis_name=(config.data_axis_name, config.model_
↪axis_name)),
            step_metrics,
        )
    if metrics is None:
        metrics = step_metrics
    else:
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

Finally, we can compile the training step. As before, we first use the `jax.eval_shape` function to find the shapes of the metrics we want to keep track of. We then initialize those metrics, and compile the training step using the `jax.jit` function.

[26]:
```
train_step_pp_fn = jax.jit(
    shard_map(
        train_step_pp,
        mesh,
        in_specs=(state_pp_specs, P(), P(config.data_axis_name)),
        out_specs=(state_pp_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
_, metric_shapes = jax.eval_shape(
    train_step_pp_fn,
    state_pp,
    None,
    batch,
)
metrics_pp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
state_pp, metrics_pp = train_step_pp_fn(state_pp, metrics_pp, batch)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[1,512]),
↪ ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]), ShapedArray(float32[1,
↪512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]),␣
↪ShapedArray(float32[1,512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]),␣
↪ShapedArray(float32[1,512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

As a reference, we print the number of parameters of the model. Since we are running on CPU, we design the model extra small.

[27]:
```
print(f"Number of parameters: {get_num_params(state_pp):_}")
```

```
Number of parameters: 5_842_984
```

Let's check if our pipeline training step is working as expected by running it for a few steps on the randomized classification task.

[28]:
```
for _ in range(15):
    state_pp, metrics_pp = train_step_pp_fn(state_pp, metrics_pp, batch)
final_metrics_pp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_pp, final_metrics_pp = train_step_pp_fn(state_pp, final_metrics_pp, batch)
print_metrics(final_metrics_pp, title="Final Metrics - Pipeline")
```

```
 Final Metrics - Pipeline
accuracy: 1.000000
loss: 0.000185
```

As we can see, the model is training as expected and achieves a low loss after very few steps. This is mainly due to the simplicity of the task, and not due to the pipeline parallelism. However, the pipeline parallelism is working as expected, and the model is training on all devices in parallel. We will perform a closer test at the end of the notebook to verify that the model parallelized across devices works identically to the non-parallelized single-device model.

4.10.3 Intermediate Summary

In this notebook, we have discussed and implemented pipeline parallelism with micro-batching. We have shown how to split the model across stages, and how to implement the pipeline parallelism in JAX. We have also shown how to combine the pipeline model with input and output layers, and how to initialize and train the model. We have also discussed the trade-offs of the micro-batching strategy, and how to choose the micro-batch size. In the next part, we will implement another method to mitigate the pipeline bubble problem, namely looping pipelines.

4.10.4 References and Resources

[Huang et al., 2019] Huang, Y., Cheng, Y., Bapna, A., Firat, O., Chen, D., Chen, M., Lee, H., Ngiam, J., Le, Q.V. and Wu, Y., 2019. Gpipe: Efficient training of giant neural networks using pipeline parallelism. Advances in neural information processing systems, 32. Paper link

[Narayanan et al., 2021] Narayanan, D., Shoeybi, M., Casper, J., LeGresley, P., Patwary, M., Korthikanti, V., Vainbrand, D., Kashinkunti, P., Bernauer, J., Catanzaro, B. and Phanishayee, A., 2021, November. Efficient large-scale language model training on gpu clusters using megatron-lm. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (pp. 1-15). Paper link

[Lamy-Poirier, 2023] Lamy-Poirier, J., 2023. Breadth-First Pipeline Parallelism. Proceedings of Machine Learning and Systems, 5. Paper link

[McKinney, 2023] McKinney, A., 2023. A Brief Overview of Parallelism Strategies in Deep Learning. Blog post link

[Huggingface, 2024] Huggingface, 2024. Model Parallelism. Documentation link

[DeepSpeed, 2024] DeepSpeed, 2024. Pipeline Parallelism. Documentation link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.11 Part 3.2: Looping Pipelines

Filled notebook:

Author: Phillip Lippe

In Part 3.1, we have seen how we can use pipeline parallelism to distribute a model across multiple GPUs. A remaining difficulty in pipeline parallelism is the pipeline bubble, which is the time that devices are idle while waiting for the next stage to finish. Micro-batching, as discussed in Part 3.1, improves the efficiency of pipeline parallelism, but some drawbacks still remain. For example, while the pipeline bubble has been reduced, our devices are still idle for `model_axis_size - 1` stage executions of a single microbatch. One way of reducing this idle time is by making the microbatches smaller and execute more in sequence, but as discussed before, it becomes difficult to fully utilize the devices with tiny batch sizes. So, can we instead reduce the time of the second factor, i.e. the stage execution? As it turns out, we can, and one option for it are *Looping Pipelines* introduced by Narayanan et al., 2021, which will be the focus of this notebook.

So far, we have split the model into consecutive stages of layers. For instance, for a model with 8 layers and 4 model devices, we would place the first two layers on the first device, the next two layers on the second device, and so on.

However, we can also split the model into non-consecutive stages, and *loop* over our devices. For instance, we could place the first layer on the first device, the second layer on the second device, and so on, until we place the fifth layer on the first device again. This split of layers is shown in the figure below.

A microbatch is then passed through the looped pipeline in a similar way as before, but the output of the last stage, when it executes layer 4, is passed to the first stage again to continue with layer 5. Now, every stage execution takes only have the time as before, since we are executing half the layers. Furthermore, compared to reducing microbatch size, the stage reduction doesn't reduce efficiency since the layers would have been executed sequentially anyways.

As long as we have more or an equal number of microbatches as number of model devices, which we anyways need to keep the pipeline efficient, we can keep the devices busy for a large amount of the time. This is because the output of the first stage is passed to the second stage, and so on, until the output of the last stage is passed to the first stage again. This way, the looping does not introduce an additional bubble while reducing the execution of the individual stages. The computation graph for the forward pass will look similar as in the figure below:

Note that if we have more microbatches than model devices, we can either decide to first finish all microbatches of its earlier layer before moving on to the next layer (breadth-first), or start with the next layer as early as possible (depth-first). We will discuss the differences between the two approaches below, but support both in our implementation.

Compared to the estimated execution time of the original pipeline (shown in gray), the execution time of the looping pipeline is significantly reduced, and the devices are kept busy for a larger portion of the time. We have to note though, that this computation graph takes a strong simplification by ignoring the communication costs, which we discuss in more detail in the next section.

In this notebook, we will implement a looping pipeline for a simple model and compare it to the original pipeline. We will also discuss the differences between the depth-first and breadth-first approaches, and how we can implement them.

4.11.1 Prerequisites

Before starting the implementation, we set up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = ["single_gpu.py", "data_parallel.py", "pipeline_parallel.py", "utils.py"]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
```

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```
                e,
            )
```

As before, we simulate 8 devices on CPU to demonstrate the parallelism without the need for multiple GPUs or TPUs. If you are running on your local machine and have multiple GPUs available, you can comment out the lines below.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

We now import our standard libraries.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from flax.struct import dataclass
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict

# Helper types
PyTree = Any
Parameter = jax.Array | nn.Partitioned
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We also import the utility functions from the previous notebooks. We also import several functions from the previous notebook Part 3.1, since many utilities like the model and the training step can be reused. It is recommended to have a look at the previous notebook to understand the details of the implementation.

[4]:
```
from pipeline_parallel import (
    PPClassifier,
    get_default_pp_classifier_config,
    train_pipeline_model,
    train_step_pp,
)
from single_gpu import Batch, TrainState, get_num_params, print_metrics
```

4.11.2 Looping Pipelines

With all functions set up, we can now start implementing the looping pipeline. We first discuss the communication overlap in the looping pipeline, and then dive deeper into the implementation.

Importance of Communication Overlap

Looping pipelines reduce the pipeline bubble, but for the cost of increased communication overhead. Consider `num_loops` to be the number of separate layers per stage (a standard pipeline has `num_loops=1`). For a single microbatch, a standard pipeline requires `model_axis_size - 1` communications (i.e. once between each stage pair), while a looping pipeline requires `model_axis_size * num_loops - 1` communications (i.e. multiple loops over each stage pair). Many frameworks like JAX support asynchronous communication, which means that the communication can overlap with the computation. However, this is only possible if the computation does not depend on the communicated values. For instance, if the output of stage 1 is communicated to stage 2, stage 2 may not be able to start its computation before the communication is finished (if there are computations that are independent of the input, e.g. RoPE embeddings, they can be executed in parallel). Meanwhile, if stage 1 may not have to wait for stage 4 to finish its computation if it uses the original input and is not yet in the looping regime. Thus, while the looping pipeline seems always superior over the non-looping version in ideal conditions, we may not be able to ignore the communication cost in practice and need to take them into account. An example comparison of GPU utilization between (a) no communication cost versus (b) common communication cost is shown below (figure credit:Joel Lamy-Poirier, 2023). We will have a closer discussion on this in the next notebook on tensor parallelism.

Pipeline parallelism is usually combined with data parallelism to further increase the global batch size. This adds another layer of communication, since after having calculated the gradients for a stage, we need to communicate them across data devices. From our previous discussion, we know that overlapping communication with computation is crucial for efficient distributed training. In standard pipelines, we can only start communicating the gradients after the last microbatch per stage has finished. Depending on the communication cost, this can lead to a significant idle time of the devices, as shown in the computation diagram below (figure credit:Joel Lamy-Poirier, 2023).

In looping pipelines, we can instead structure our layer execution such that we can start communicating gradients earlier. For instance, the breadth-first strategy (Joel Lamy-Poirier, 2023) follows the setup that each stage first finishes all microbatches of its earlier layer before moving on to the next layer. This way, in the backward pass, we finish calculating all gradients for the later layers before having done the computation of the earlier layers. This allows us to start communicating the gradients of the later layers earlier, and overlap it with the computation of the gradients of the early layers. The final communication of the earlier layers will be cheaper than the non-looped version, since significantly fewer gradients need to be communicated (specifically `1/num_loops`). The computation diagram for the backward pass of the breadth-first strategy is shown above. An alternative strategy is the depth-first strategy, which starts with the next layer as early as possible, but cannot take advantage of the early communication of the gradients as well as the breadth-first strategy. While we will mainly focus on the breadth-first strategy, our implementation is designed to support both strategies.

Note: in the current implementation version, we may not support asynchronous gradient communication on GPU. This is because the current implementation needs to stack the parameters over the looping axis within the pipeline, in order to support the SPMD jitting of the pipeline. Thus, the gradients are only communicated once the gradients for all parameters in the pipeline have been calculated. To keep the implementation simple, we will neglect the asynchronous gradient communication for now, and focus on the forward pass of the pipeline. A future version of the implementation may support asynchronous gradient communication once we find a simple way for it, and we will update the notebook accordingly.

Looping Pipeline Implementation

Let's focus now on the implementation of looping pipelines. Compared to the non-looped pipeline, we need to take care of two additional aspects: (1) the looping communication between the last and first stage, and (2) the execution of different layers on a single device over iterations. We will start with the first aspect, and then discuss the second aspect.

If we had the same number of microbatches as model devices, the communication between the last stage and the first stage would not be any different from the communication between any other stage pair after we processed the original input batches. However, if we have more microbatches than model devices, we will need to buffer the outputs of the last stage until we have processed all microbatches of the earlier layers, since the first stage is not ready to process the output of the last stage yet. Thus, at each iteration, we need to check on device 0 which microbatch the communicated features of the last stage belong to and buffer accordingly. We can do this by simply determining the index of the microbatch by using the iteration index, and overwrite the respectively indexed subarray `inputs` of the first stage with the buffered features. For example, with four devices, the last stage will process the first microbatch at iteration 3 (zero-indexed). At the subsequent communication, we overwrite `inputs[0]` on device 0 with the communicated features from the last stage. We can then continue with the execution of the first stage as usual and continue iterating over the input array. This results in a computation graph similar to the one shown below (we show processing of 6 instead of 4 microbatches to visualize the buffering mechanism).

The second aspect we need to take care of are the different layers we need to execute at different iterations. Note that these layer indices are not the same across stages: in the diagram above, the first stage will have to switch from layer 0 to layer 4 earlier than the last stage from layer 3 to 7. We can handle this by using the iteration index to determine the layer index we need to execute, and pass the sub-indexed parameters of the respective layer to the stage.

To keep our implementation as general as possible, we will explicitly pass these "switching" indices to the pipeline function. For this, we implement a `PipelineState` below, which contains: * `inputs`: The input array, which is the original input array at the first iteration, and is used as buffer for the output of the last stage in subsequent loops. * `outputs`: The output array, which will store the output of the final layer of the last stage. * `input_indices`: The indices indicating which microbatch to process at each iteration on the first stage. * `output_indices`: The indices indicating into which output array to write the output of the last stage at each iteration. If -1, the features will not be stored in the `outputs` array. * `update_indices`: The indices indicating which input array index to buffer the last communicated features in. If -1, the features will not be buffered (e.g. initial iterations where the last stage has not received any viable input yet). * `params_indices`: The index of the layer to execute at each iteration. * `last_state`: The last communicated features between stages. * `rngs`: The random number generator keys for the layers (e.g. dropout).

[5]:
```
@dataclass
class PipelineState:
    inputs: jax.Array
    outputs: jax.Array
    input_indices: jax.Array
    output_indices: jax.Array
    update_indices: jax.Array
    params_indices: jax.Array
    last_state: jax.Array
    rngs: PyTree
```

Using this pipeline state, we can implement a single step of the looped pipeline in an SPMD fashion. We first check if we need to buffer the last communicated features, and if so, we do so. We then determine the input to the current stage, which is the last communicated features for all stages except the first. For the first stage, we use the original input array indexed at the current `input_indices`. We then execute the layer indexed at the current `params_indices`. For easiest selection of the parameters, we will stack the parameters over the first axis and select them before executing the `module.apply_fn`. Note that for easiests handling, we use an explicit `apply_fn` since initializing the right number of parameters within this function is not straightforward. More on it later.

After applying the model, we determine whether the features need to be stored in the `outputs` array. If so, we do so. Finally, we communicate the last state to the next stage, and return the new pipeline state.

[6]:
```
def execute_looping_pipeline_step(
    index: jax.Array | int,
    state: PipelineState,
    *args,
    module: nn.Module,
    params: PyTree,
    model_axis_name: str,
    **kwargs,
) -> PipelineState:
    """Single micro-batch pipeline step with loopback communication.

    Args:
        index: Pipeline step index (between 0 and num_loops * num_microbatches + num_
↪stages - 2).
        state: State of the pipeline, including indices for controlling the execution.
        *args: Additional arguments to the module.
        module: Flax module representing the stage layer to execute.
        params: PyTree of parameters. The params for all layers should be stacked along␣
↪the first axis.
        model_axis_name: Name of the model axis in the mesh/shard_map.
        **kwargs: Additional keyword arguments to the module.

    Returns:
        New state of the pipeline after the execution of the pipeline step, with␣
↪potentially updated
        inputs, outputs, rngs, and last_state arrays.
    """
    num_stages = jax.lax.psum(1, model_axis_name)
    input_index = state.input_indices[index]
    output_index = state.output_indices[index]
    update_index = state.update_indices[index]
    params_index = state.params_indices[index]
    # Update inputs with last state. If update_index is -1, do not update.
    # This is used to buffer the communications back to first stage.
    clipped_update_index = jnp.clip(update_index, 0, state.inputs.shape[0] - 1)
    inputs = jax.lax.dynamic_update_index_in_dim(
        state.inputs,
        jnp.where(update_index >= 0, state.last_state, state.inputs[clipped_update_
↪index]),
        clipped_update_index,
        axis=0,
    )
    # Select input of the current stage. For all stages except the first stage,
    # the input is the last output of the previous stage (i.e. last_state).
    step_input = jnp.where(
        input_index >= 0,
        inputs[input_index],
        state.last_state,
    )
    # Apply the module to the input. Select the right set of parameters based
```

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```
    # on the loop index.
    rngs = jax.tree_map(lambda rng: jax.random.split(rng, 2), state.rngs)
    rngs, step_rngs = jax.tree_map(lambda x: x[0], rngs), jax.tree_map(lambda x: x[1],␣
↪rngs)
    params = jax.tree_map(lambda x: x[params_index], params)
    output = module.apply(params, step_input, *args, **kwargs, rngs=step_rngs)
    # Update outputs with the output of the current stage. If output_index is -1,
    # do not update. This is used to buffer the final outputs of the last stage.
    clipped_output_index = jnp.clip(output_index, 0, state.outputs.shape[0] - 1)
    outputs = jax.lax.dynamic_update_index_in_dim(
        state.outputs,
        jnp.where(output_index >= 0, output, state.outputs[clipped_output_index]),
        clipped_output_index,
        axis=0,
    )
    # Communicate the last output to the next stage.
    last_state = jax.lax.ppermute(
        output,
        model_axis_name,
        perm=[(i, (i + 1) % num_stages) for i in range(num_stages)],
    )
    return state.replace(
        inputs=inputs,
        outputs=outputs,
        last_state=last_state,
        rngs=rngs,
    )
```

With the single step set up, we can now write a small helper function to prepare the `input_indices`, `output_indices`, `update_indices`, and `params_indices` for a respective device. We will use this function to prepare the indices for all devices, and then use them to initialize the pipeline state. The indices follow the breadth-first strategy, as discussed in the previous paragraphs.

[7]:
```
def prepare_looping_pipeline_indices(
    num_loops: int, num_microbatches: int, num_stages: int, stage_index: jax.Array | int
) -> Dict[str, jax.Array]:
    """Prepare indices for controlling the execution of the looping pipeline.

    Args:
        num_loops: Number of loops in the pipeline, or separate stage layers per device.␣
↪num_loops=1 is equivalent to a non-looping pipeline.
        num_microbatches: Number of microbatches to split the batch into.
        num_stages: Number of stages/devices the pipeline is distributed over.
        stage_index: Index of the stage/device in the pipeline.

    Returns:
        Dictionary of indices for controlling the execution of the pipeline.
    """
    num_iterations = num_loops * num_microbatches + num_stages - 1
    index_array = -jnp.ones((num_iterations,), dtype=jnp.int32)
    # Only first stage uses inputs. Looping communications from last
    # stage are buffered in the inputs, so we repeatedly iterate over
```

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```
    # the inputs.
    input_indices = jnp.where(
        stage_index == 0,
        index_array.at[: num_loops * num_microbatches].set(
            jnp.tile(jnp.arange(num_microbatches), reps=(num_loops,))
        ),
        index_array,
    )
    # For the first stage, identify input indices that we use to buffer
    # the communications from the last stage. For all other stages, we
    # use the last state from the previous stage as input.
    update_indices = jnp.where(
        stage_index == 0,
        index_array.at[num_stages : num_stages + (num_loops - 1) * num_microbatches].set(
            jnp.tile(jnp.arange(num_microbatches), reps=(num_loops - 1,))
        ),
        index_array,
    )
    # For the last stage, we use the outputs of the last loop as the
    # final outputs.
    output_indices = jnp.where(
        stage_index == num_stages - 1,
        index_array.at[-num_microbatches:].set(jnp.arange(num_microbatches)),
        index_array,
    )
    # For all stages, we iterate over the parameters of the different loops.
    # We use the 0-index for indices that fall into the pipeline bubble.
    params_indices = jnp.zeros_like(index_array)
    for i in range(num_loops):
        start_index = stage_index + i * num_microbatches
        params_indices = jax.lax.dynamic_update_slice_in_dim(
            params_indices,
            jnp.full(shape=(num_microbatches,), fill_value=i, dtype=params_indices.
↪dtype),
            start_index,
            axis=0,
        )
    return {
        "input": input_indices,
        "output": output_indices,
        "update": update_indices,
        "params": params_indices,
    }
```

The easiest way of understanding these indices is to print them for a simple example. Let's do this for a model with three devices, two loops, and four microbatches. In this setup, we get the following indices for the three devices:

[8]:
```
num_stages = 3
num_loops = 2
num_microbatches = 4
for i in range(num_stages):
    indices = prepare_looping_pipeline_indices(
```

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```
        num_loops=num_loops,
        num_microbatches=num_microbatches,
        num_stages=num_stages,
        stage_index=i,
    )
    s = ["step  : " + " ".join(f"{t:2d}" for t in range(len(indices["input"])))]
    for k, v in indices.items():
        s.append(f"{k:6s}: " + " ".join(f"{t:2d}" for t in v))
    max_len = max(map(len, s))
    s.insert(0, (f" Stage Index {i} ").center(max_len, "="))
    print("\n".join(s) + "\n")
```

```
2024-03-07 10:47:39.006121: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

```
=========== Stage Index 0 ===========
step  :  0  1  2  3  4  5  6  7  8  9
input :  0  1  2  3  0  1  2  3 -1 -1
output: -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
update: -1 -1 -1  0  1  2  3 -1 -1 -1
params:  0  0  0  0  1  1  1  1  0  0

=========== Stage Index 1 ===========
step  :  0  1  2  3  4  5  6  7  8  9
input : -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
output: -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
update: -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
params:  0  0  0  0  0  1  1  1  1  0

=========== Stage Index 2 ===========
step  :  0  1  2  3  4  5  6  7  8  9
input : -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
output: -1 -1 -1 -1 -1 -1  0  1  2  3
update: -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
params:  0  0  0  0  0  0  1  1  1  1
```

The first device iterates over its input array as in a standard pipeline. Once the end is reached, it loops back to the first microbatch. At this point, the array will have been updated (seen by the `update_indices` being 0 at step 3) and contain the output features of the first microbatch after layer 2 on stage 2. In terms of the parameter indices, the first stage executes four times layer 0 (iterates over the four input microbatches), and then switches to layer 3. For the last two steps, we can arbitrarily select the layer since the output is not used anymore.

For the second device, we see that it does not use the input, output or update indices, since it will always process the last communicated features and send them to the next stage. The parameter indices are shifted by one in comparison to the first device, since it needs to wait for the first device to process the microbatches by the first layer.

Finally, the third device has the same `input` and `update` indices as the second device, since it always processes the last communicated features. The `output` indices are set to -1 for the first six steps, since these outputs are from layer 2 and not the final layer. The last four microbatches are processed by the final layer and hence stored in the output array. The parameter indices are shifted by two in comparison to the first device, since it needs to wait for the first and second device to process the microbatches by the first and second layer, respectively.

With the indices prepared, we can now implement the full pipeline execution. In comparison to the previous implementation, we do not use a `nn.scan` operation since we need to handle the parameter indices explicitly. This is because we need multiple parameters for the same module, but fewer than the number of iterations and each device using different parameters at different iterations. Instead, we use a `jax.lax.fori_loop` operation, which allows us to handle the parameter indices explicitly. We also need to handle the RNGs explicitly, since we cannot arbitrarily mix JAX and Flax transformations. After finishing the loop, we reshape the output back to the original shape, and return the reshaped output.

[9]:
```
@jax.named_scope("pipeline")
def execute_looping_pipeline(
    module: nn.Module,
    params: PyTree,
    x: jax.Array,
    rngs: PyTree,
    *args,
    num_loops: int,
    num_microbatches: int,
    model_axis_name: str,
    **kwargs,
):
    """Execute a looping pipeline of stages on a batch of data.

    Uses a breadth-first strategy to execute the pipeline stages in parallel.

    Args:
        module: Flax module representing a single pipeline stage to execute.
        params: PyTree of parameters for the pipeline stages.
        x: Batch of input data, only needed on device of the first stage. Data will be␣
↪split into micro-batches.
        rngs: PyTree of random number generators for the pipeline stages.
        *args: Additional arguments to the module.
        num_loops: Number of loops in the pipeline, or separate stage layers per device.␣
↪num_loops=1 is equivalent to a non-looping pipeline.
        num_microbatches: Number of micro-batches to split the batch into.
        model_axis_name: Name of the model axis in the mesh/shard_map.
        **kwargs: Additional keyword arguments to the module.

    Returns:
        Output of the last stage of the pipeline, with equivalent shape to input x. For␣
↪devices that are not
        the last stage, the output is zeros.
    """
    num_stages = jax.lax.psum(1, model_axis_name)
    assert num_stages > 1, "Pipeline must have at least 2 stages."
    stage_index = jax.lax.axis_index(model_axis_name)
    # Structure the input data into micro-batches.
    batch_size = x.shape[0]
    assert (
        batch_size % num_microbatches == 0
    ), f"Batch size {batch_size} must be divisible by number of microbatches {num_
↪microbatches}"
    microbatch_size = batch_size // num_microbatches
    microbatches = jnp.reshape(x, (num_microbatches, microbatch_size, *x.shape[1:]))
```

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```
    last_state = jnp.zeros_like(microbatches[0])
    outputs = jnp.zeros_like(microbatches)
    # Prepare indices for each stage.
    indices = prepare_looping_pipeline_indices(
        num_loops=num_loops,
        num_microbatches=num_microbatches,
        num_stages=num_stages,
        stage_index=stage_index,
    )
    num_iterations = indices["input"].shape[0]
    pipeline_state = PipelineState(
        inputs=microbatches,
        outputs=outputs,
        input_indices=indices["input"],
        output_indices=indices["output"],
        update_indices=indices["update"],
        params_indices=indices["params"],
        last_state=last_state,
        rngs=rngs,
    )
    # Execute the pipeline via a jax fori_loop. Alternatively, a
    # scan could be used to execute the pipeline.
    pipeline_fn = functools.partial(
        execute_looping_pipeline_step,
        *args,
        module=module,
        params=params,
        model_axis_name=model_axis_name,
        **kwargs,
    )
    pipeline_state = jax.lax.fori_loop(
        0,
        num_iterations,
        body_fun=pipeline_fn,
        init_val=pipeline_state,
    )
    # Return the final outputs, reshaped as original input.
    outputs = pipeline_state.outputs
    return jnp.reshape(outputs, (batch_size, *outputs.shape[2:]))
```

The final piece we need to implement is the `LoopingPipelineModule` as an extension of the `PipelineModule` before. During training, we will create the module of the stage as before, but pass its variables and RNGs explicitly to the looping pipeline function. During initialization, we need to create the parameters for the different layers in the looping pipeline explicitly. We do this by simply using a `nn.scan` during init, which loops over the number of layers and creates the parameters for each layer while stacking them on the first dimension. Since we do not use the output of the initialization, we can ignore the output of the scan and simply return the initialized parameters. This also reduces initialization time, since we do not need to run the whole pipeline function during initialization.

[10]:
```
class LoopingPipelineModule(nn.Module):
    num_loops: int
    model_axis_name: str
    num_microbatches: int
```

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```
    module_fn: Callable[..., nn.Module]

    @nn.compact
    def __call__(self, x: jax.Array, *args, **kwargs):
        if self.is_initializing():
            # During initialization, we want to create a separate set of parameters
            # for each loop. We do this by scanning the module during init. Note that
            # we do not need to execute the pipeline, since we only need to create the
            # parameters.
            sample_microbatch = x[:: self.num_microbatches]
            module = self.module_fn()
            scan_fn = nn.scan(
                lambda module, carry, _: (module(carry, *args, **kwargs), None),
                variable_axes={"params": 0},
                split_rngs={"params": True, "dropout": True},
                length=self.num_loops,
            )
            out, _ = scan_fn(module, sample_microbatch, ())
            return jnp.repeat(out, self.num_microbatches, axis=0)
        else:
            # During the forward pass, we extract the initialized parameters for
            # all loops. In the pipeline, we then sub-index the parameters based on
            # the loop index.
            module = self.module_fn()
            params = module.variables
            # Since we make use of a non-flax transformation, we need to pass the
            # RNGs explicitly to the pipeline.
            rngs = {name: self.make_rng(name) for name in self.scope.rngs}
            return execute_looping_pipeline(
                module=module,
                params=params,
                x=x,
                rngs=rngs,
                *args,
                num_loops=self.num_loops,
                num_microbatches=self.num_microbatches,
                model_axis_name=self.model_axis_name,
                **kwargs,
            )
```

For the full model, we can then simply reuse the `PPClassifier` class, and pass the `LoopingPipelineModule` with the loops equal to the number of layers per device. Each module itself will then contain a single layer, with two modules per stage (with four model devices).

[11]:
```
def get_looping_classifier(config: ConfigDict) -> nn.Module:
    looping_model_config = config.copy_and_resolve_references()
    looping_model_config.num_layers = 1
    looping_module_class = functools.partial(
        LoopingPipelineModule,
        num_loops=config.num_layers,
    )
    return PPClassifier(config=looping_model_config, pipeline_module_class=looping_
↪module_class)
```

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```
config = get_default_pp_classifier_config()
model_lpp = get_looping_classifier(config.model)
optimizer = optax.adamw(
    learning_rate=config.optimizer.learning_rate,
)
```

Initialization

The initialization of the looping pipeline follows the same principles as the non-looped pipeline. We first redefine the initialization function, the mesh and create the example batch, as done in the previous notebook.

[12]:
```
device_array = np.array(jax.devices()).reshape(-1, config.model_axis_size)
mesh = Mesh(device_array, (config.data_axis_name, config.model_axis_name))
```

[13]:
```
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng, data_labels_rng = jax.random.split(rng, 3)
batch = Batch(
    inputs=jax.random.normal(data_inputs_rng, (config.data.batch_size, config.data.input_
↪size)),
    labels=jax.random.randint(
        data_labels_rng, (config.data.batch_size,), 0, config.data.num_classes
    ),
)
```

[14]:
```
def init_fn(rng: jax.random.PRNGKey, x: jax.Array, model: nn.Module) -> TrainState:
    init_rng, rng = jax.random.split(rng)
    variables = model.init({"params": init_rng}, x, train=False)
    params = variables.pop("params")
    state = TrainState.create(
        apply_fn=model.apply,
        params=params,
        tx=optimizer,
        rng=rng,
    )
    return state
```

We then need to identify the partitioning of the parameters, which we do below.

[15]:
```
init_lpp_fn = shard_map(
    functools.partial(init_fn, model=model_lpp),
    mesh,
    in_specs=(P(), P(config.data_axis_name)),
    out_specs=P(),
    check_rep=False,
)
state_lpp_shapes = jax.eval_shape(init_lpp_fn, model_init_rng, batch.inputs)
state_lpp_specs = nn.get_partition_spec(state_lpp_shapes)
pprint(state_lpp_specs.params)
```

```
{'input_dense': {'sharded': {'bias': PartitionSpec('model', None),
                             'kernel': PartitionSpec('model', None, None)}},
 'output_dense': {'sharded': {'bias': PartitionSpec('model', None),
                              'kernel': PartitionSpec('model', None, None)}},
 'output_norm': {'sharded': {'bias': PartitionSpec('model', None),
                             'scale': PartitionSpec('model', None)}},
 'pipeline': {'sharded': {'mlp_layers': {'block': {'input_dense': {'bias': PartitionSpec(
↪'model', None, None, None),
                                                                   'kernel':␣
↪PartitionSpec('model', None, None, None, None)},
                                                   'output_dense': {'bias':␣
↪PartitionSpec('model', None, None, None),
                                                                    'kernel':␣
↪PartitionSpec('model', None, None, None, None)},
                                                   'pre_norm': {'bias': PartitionSpec(
↪'model', None, None, None),
                                                                'scale': PartitionSpec(
↪'model', None, None, None)}}}}}}
```

Since we use the same config for both the non-looped and the looped pipeline, the partitioning is the almost same as before, except that the pipeline parameters each have an additional axis. This is because each parameter in the pipeline has the structure `(model devices, stages per device, layers per stage, ...)` instead of `(model devices, layers per device, ...)`. We can see this by comparing the shapes of the parameters of the non-looped and looped pipeline after the full initialization:

[16]:
```
init_lpp_fn = jax.jit(
    shard_map(
        functools.partial(init_fn, model=model_lpp),
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_lpp_specs,
        check_rep=False,
    ),
)
state_lpp = init_lpp_fn(model_init_rng, batch.inputs)

pprint(
    jax.tree_map(lambda x: x.shape, state_lpp.params["pipeline"]["sharded"]["mlp_layers
↪"]["block"])
)
```

```
{'input_dense': {'bias': Partitioned(value=(4, 2, 1, 512),
                                     names=('model', None, None, None),
                                     mesh=None),
                 'kernel': Partitioned(value=(4, 2, 1, 512, 512),
                                       names=('model', None, None, None, None),
                                       mesh=None)},
 'output_dense': {'bias': Partitioned(value=(4, 2, 1, 512),
                                      names=('model', None, None, None),
                                      mesh=None),
                  'kernel': Partitioned(value=(4, 2, 1, 512, 512),
                                        names=('model', None, None, None, None),
                                        mesh=None)},
```

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```
 'pre_norm': {'bias': Partitioned(value=(4, 2, 1, 512),
                                  names=('model', None, None, None),
                                  mesh=None),
              'scale': Partitioned(value=(4, 2, 1, 512),
                                   names=('model', None, None, None),
                                   mesh=None)}}
```

In the default config, we distribute the pipeline over 4 model devices, each having 2 stages and 1 layer per stage. The axis for the layer per stage is introduced by the scan in `MLPLayers`. This axis could also be removed by directly using `MLPBlock` in the `LoopingPipelineModule`, but we keep it for minimal changes between the non-looped and looped version.

Training

Let's now compile the train step, which is again identical to the non-looped version and simply needs updated sharding specifications.

[17]:
```
train_step_lpp_fn = jax.jit(
    shard_map(
        functools.partial(train_step_pp, config=config),
        mesh,
        in_specs=(state_lpp_specs, P(), P(config.data_axis_name)),
        out_specs=(state_lpp_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
state_shapes, metric_shapes = jax.eval_shape(
    train_step_lpp_fn,
    state_lpp,
    None,
    batch,
)
metrics_lpp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
state_lpp, metrics_lpp = train_step_lpp_fn(state_lpp, metrics_lpp, batch)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[1,512]),
↪ ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]), ShapedArray(float32[1,
↪512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,512]),␣
↪ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512,512]),␣
↪ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512,512]),␣
↪ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512]),␣
↪ShapedArray(float32[1,512]), ShapedArray(float32[1,784,512]), ShapedArray(float32[1,
↪10]), ShapedArray(float32[1,512,10]), ShapedArray(float32[1,512]),␣
↪ShapedArray(float32[1,512]), ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,
↪1,512,512]), ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512,512]),␣
↪ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512]),␣
↪ShapedArray(float32[1,512]), ShapedArray(float32[1,784,512]), ShapedArray(float32[1,
↪10]), ShapedArray(float32[1,512,10]), ShapedArray(float32[1,512]),␣
↪ShapedArray(float32[1,512]), ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,
↪1,512,512]), ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512,512]),␣
↪ShapedArray(float32[1,2,1,512]), ShapedArray(float32[1,2,1,512]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

We print the number of overall parameters to verify that it is the same as in the non-looped version.

[18]:
```
print(f"Number of parameters: {get_num_params(state_lpp):_}")
```

```
Number of parameters: 5_842_984
```

We can also train the model on the random data classification task, and check if the model is training as expected.

[19]:
```
for _ in range(15):
    state_lpp, metrics_lpp = train_step_lpp_fn(state_lpp, metrics_lpp, batch)
final_metrics_lpp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_lpp, final_metrics_lpp = train_step_lpp_fn(state_lpp, final_metrics_lpp, batch)
print_metrics(final_metrics_lpp, title="Final Metrics - Looping Pipeline")
```

```
 Final Metrics - Looping Pipeline
accuracy: 1.000000
loss: 0.000213
```

The accuracy and loss of the model are as expected very similar to the non-looped pipeline, and the model is training as expected.

4.11.3 Testing Pipeline Parallelism

We have now implemented both the non-looped and looped pipeline parallelism, and trained the model on a simple random data classification task. We can now test if the model parallelized across devices works identically to the non-parallelized single-device model. We can do this by comparing the outputs of the non-parallelized and parallelized model for the same input and parameters. We will use the same random input for both models, and compare the outputs of the final layer. If the outputs are the same, we can conclude that the model parallelized across devices works identically to the non-parallelized single-device model.

We start by training a non-looped pipeline model on the random data classification task as the base model.

[20]:
```
state_pp = train_pipeline_model(
    config=config, mesh=mesh, batch=batch, model_init_rng=model_init_rng, num_steps=15
)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[1,512]),
↪ ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]), ShapedArray(float32[1,
↪512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]),␣
↪ShapedArray(float32[1,512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,784,512]), ShapedArray(float32[1,10]),␣
↪ShapedArray(float32[1,512,10]), ShapedArray(float32[1,512]), ShapedArray(float32[1,
↪512]), ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512,512]),␣
↪ShapedArray(float32[1,2,512]), ShapedArray(float32[1,2,512]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

We then create the mesh for a single-device model parallelism.

[21]:
```
single_device_mesh = Mesh(np.array(jax.devices()).reshape(-1, 1), ("data", "model"))
```

We create the respective configuration and models. Since the different strategies may split the RNGs in different ways, we set the dropout to zero to remove the randomness from the model.

[22]:
```
single_device_config = config.model.copy_and_resolve_references()
single_device_config.model_axis_size = 1
single_device_config.num_layers *= config.model.model_axis_size
single_device_config.dropout_rate = 0.0
multi_device_config = config.model.copy_and_resolve_references()
multi_device_config.dropout_rate = 0.0
single_device_model = PPClassifier(config=single_device_config)
multi_device_pp_model = PPClassifier(config=multi_device_config)
multi_device_lpp_model = get_looping_classifier(config=multi_device_config)
```

We now create the parameters for each model. We will use the pretrained model from the pipeline model, and need to reshape them for the other setups.

[23]:
```
plain_pipeline_params = state_pp.params
```

In comparison to the standard pipeline, the looping pipeline needs to reorder the layers. While the standard pipeline has the first two layers on device 0, the looping pipeline has layer 0 and layer 4 on device 0. Hence, we reshape and transpose the parameters accordingly.

[24]:
```
def plain_to_looping_params(p: jax.Array) -> jax.Array:
    p = p.reshape(
        (
            p.shape[1],
```

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```
            p.shape[0],
            1,
        )
        + p.shape[2:]
    )
    p = p.transpose((1, 0) + tuple(range(2, p.ndim)))
    return p


looping_pipeline_params = jax.device_get({k: v for k, v in state_pp.params.items()})
looping_pipeline_params["pipeline"] = jax.tree_map(
    lambda x: nn.Partitioned(value=plain_to_looping_params(x.value), names=x.names),
    looping_pipeline_params["pipeline"],
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
)
```

For the single parameters, we need to set the model axis to 1, and move all layers to the second axis in the pipeline parameters. For the input and output layers, we select the device which has non-zero parameters.

[25]:
```
single_params = jax.device_get({k: v for k, v in state_pp.params.items()})
single_params["input_dense"] = jax.tree_map(
    lambda x: nn.Partitioned(value=x.value[0:1], names=x.names),
    single_params["input_dense"],
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
)
single_params["output_dense"] = jax.tree_map(
    lambda x: nn.Partitioned(value=x.value[-1:], names=x.names),
    single_params["output_dense"],
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
)
single_params["output_norm"] = jax.tree_map(
    lambda x: nn.Partitioned(value=x.value[-1:], names=x.names),
    single_params["output_norm"],
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
)
single_params["pipeline"] = jax.tree_map(
    lambda x: nn.Partitioned(value=x.value.reshape(1, -1, *x.value.shape[2:]), names=x.
↪names),
    single_params["pipeline"],
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
)
```

We can now distribute the parameters on the respective meshes. We simply create the state with the passed parameters, and then use the `shard` function to distribute the parameters over the mesh.

[26]:
```
def create_single_state_pp() -> TrainState:
    return TrainState.create(
        apply_fn=single_device_model.apply,
        params=single_params,
        tx=optimizer,
        rng=jax.random.PRNGKey(0),
    )
```

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```
create_single_state_pp_fn = jax.jit(
    shard_map(
        create_single_state_pp,
        single_device_mesh,
        in_specs=P(),
        out_specs=P(),
        check_rep=False,
    ),
)
single_state_pp_shapes = jax.eval_shape(create_single_state_pp_fn)
single_state_pp_specs = nn.get_partition_spec(single_state_pp_shapes)
single_state_pp = jax.jit(
    shard_map(
        create_single_state_pp,
        single_device_mesh,
        in_specs=P(),
        out_specs=single_state_pp_specs,
        check_rep=False,
    ),
)()
```

[27]:
```
def create_multi_state_pp(state: TrainState) -> TrainState:
    return TrainState.create(
        apply_fn=multi_device_pp_model.apply,
        params=state.params,
        tx=state.tx,
        rng=jax.random.PRNGKey(0),
    )


state_pp_specs = nn.get_partition_spec(state_pp)
create_multi_state_pp_fn = jax.jit(
    shard_map(
        create_multi_state_pp,
        mesh,
        in_specs=(state_pp_specs,),
        out_specs=P(),
        check_rep=False,
    ),
)
multi_state_pp_shapes = jax.eval_shape(create_multi_state_pp_fn, state_pp)
multi_state_pp_specs = nn.get_partition_spec(multi_state_pp_shapes)
multi_state_pp = jax.jit(
    shard_map(
        create_multi_state_pp,
        mesh,
        in_specs=(state_pp_specs,),
        out_specs=multi_state_pp_specs,
        check_rep=False,
    ),
```

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```
)(state_pp)
```

[28]:
```
def create_multi_state_lpp(params: PyTree) -> TrainState:
    return TrainState.create(
        apply_fn=multi_device_lpp_model.apply,
        params=params,
        tx=optimizer,
        rng=jax.random.PRNGKey(0),
    )


input_lpp_specs = nn.get_partition_spec(looping_pipeline_params)
create_multi_state_lpp_fn = jax.jit(
    shard_map(
        create_multi_state_lpp,
        mesh,
        in_specs=(input_lpp_specs,),
        out_specs=P(),
        check_rep=False,
    ),
)
multi_state_lpp_shapes = jax.eval_shape(create_multi_state_lpp_fn, looping_pipeline_
↪params)
multi_state_lpp_specs = nn.get_partition_spec(multi_state_lpp_shapes)
multi_state_lpp = jax.jit(
    shard_map(
        create_multi_state_lpp,
        mesh,
        in_specs=(input_lpp_specs,),
        out_specs=multi_state_lpp_specs,
        check_rep=False,
    ),
)(looping_pipeline_params)
```

Finally, we define the respective training steps.

[29]:
```
train_step_single_pp_fn = jax.jit(
    shard_map(
        functools.partial(train_step_pp, config=config),
        single_device_mesh,
        in_specs=(single_state_pp_specs, P(), P(config.data_axis_name)),
        out_specs=(single_state_pp_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
train_step_multi_pp_fn = jax.jit(
    shard_map(
        functools.partial(train_step_pp, config=config),
        mesh,
        in_specs=(multi_state_pp_specs, P(), P(config.data_axis_name)),
        out_specs=(multi_state_pp_specs, P()),
```

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```
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
train_step_multi_lpp_fn = jax.jit(
    shard_map(
        functools.partial(train_step_pp, config=config),
        mesh,
        in_specs=(multi_state_lpp_specs, P(), P(config.data_axis_name)),
        out_specs=(multi_state_lpp_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)

metrics_single_pp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
metrics_multi_pp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
metrics_multi_lpp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
```

Below, we execute each training step three times, and compare the final metrics. If the metrics are the same, we can conclude that the pipeline versions work identically to the non-parallelized single-device model.

[30]:
```
for _ in range(3):
    single_state_pp, metrics_single_pp = train_step_single_pp_fn(
        single_state_pp, metrics_single_pp, batch
    )
    multi_state_pp, metrics_multi_pp = train_step_multi_pp_fn(
        multi_state_pp, metrics_multi_pp, batch
    )
    multi_state_lpp, metrics_multi_lpp = train_step_multi_lpp_fn(
        multi_state_lpp, metrics_multi_lpp, batch
    )

print_metrics(metrics_single_pp, title="Final Metrics - Single Device Pipeline")
print()
print_metrics(metrics_multi_pp, title="Final Metrics - Multi Device Pipeline")
print()
print_metrics(metrics_multi_lpp, title="Final Metrics - Multi Device Looping Pipeline")
```

```
 Final Metrics - Single Device Pipeline
accuracy: 1.000000
loss: 0.002235

 Final Metrics - Multi Device Pipeline
accuracy: 1.000000
loss: 0.002235

 Final Metrics - Multi Device Looping Pipeline
accuracy: 1.000000
loss: 0.002235
```

All models have the same loss and accuracy, and we can conclude that the pipeline versions work identically to the non-parallelized single-device model. Note that with lower precision like bfloat16, the results may differ slightly due to different reduces happening in the train steps, but the difference should be negligible.

4.11.4 Profiling

We can now profile the model to see if the looping pipeline is more efficient than the non-looped pipeline. For simplicity, we use the MLP classifier in this notebook and scale it up to 16 layers with 2048 hidden size and mlp expansion of 4, and 8 microbatches. We distribute the model over one node with 8 A5000 GPUs, and use a model axis size of 2. Every pair of GPUs in the model axis are connected via 4 NVLink connections with a measured communication speed of 60GB/s in each direction. All other devices are connected via the PCIe bus, such that larger pipeline sizes would lead to a significant increase in communication cost. In general, we use the profiling to verify the working of the pipeline, and not to measure the absolute performance of the pipeline. All traces are uploaded here.

We first show the trace for the non-looped pipeline:

Compared to the previous networks, we see many small operations and scans, which are difficult to see all from the image above. If you want to dive deeper into the trace, you can download the trace and open it in TensorBoard. We find the expected pattern of the forward pass being an outer loop of 9 steps (8 microbatches + 1 pipeline shift slot), and each step containing the execution of the 8 layers per stage with communication. The backward pass is similar with 9 outer steps and 8 inner steps. Although the communication is not overlapped with the computation, the communication between stages only takes $17\mu s$ compared to 5ms of a single stage forward pass. Where a lot of time is lost, though, is in the gradient synchronization after the backward pass. Since the gradients only finish computing in the last microbatch step, we need to wait almost until the end before we can start communicating the gradients. This is a significant bottleneck in the non-looped pipeline, especially on hardware with high communication costs over the data axis. We also note that in Transformer models, we would see a slightly different pattern, since the activations are significantly larger (additional sequence length) and reduce the relative communication cost of the gradients. Further, we find a significant amount of time is spent in the `dynamic_slice_update` operation of the inner `scan` operation over layers, which suggests that we may get a significant speedup by removing the scan as in the single-GPU setup.

We now show the trace for the looped pipeline:

This trace has even more small operations, which we need to zoom in to see. We find the expected pattern of the forward pass being an outer loop of $8 * 8 + 1 = 65$ steps, and each step containing the execution of only 1 layer. The backward pass is similar with 65 outer steps and 1 inner step. The communication again makes up only a small fraction of the total time, and the compiler overlaps the time with the `scan` operation computation. Still, we find a similar bottleneck in the gradient synchronization after the backward pass, which, in theory, the looping pipeline should be able to reduce. This is because the current implementation needs to stack the parameters over the looping axis within the pipeline, in order to support the SPMD jitting of the pipeline. Thus, the gradients are only communicated once the gradients for all parameters in the pipeline have been calculated. To obtain the maximum efficiency of the pipeline, we would need to support asynchronous gradient communication, which is left for future times. Nonetheless, already in its current version, the looping pipeline is 7% faster, taking 190ms for a full forward and backward pass versus 205ms for the non-looped pipeline.

4.11.5 Conclusion

In this notebook, we have discussed and implemented pipeline parallelism with micro-batching and looping pipelines. The main challenge of pipelines remains the pipeline bubble, which can reduce their efficiency. While looping pipelines and other strategies can improve its efficiency, we usually have to trade-off communication cost and computation time. Hence, the best trade-off depends on the specific model and hardware setup. We have also shown how to combine pipeline parallelism with data parallelism, and how to test the pipeline parallelism by comparing the outputs of the non-parallelized and parallelized model. For simplicity, we have not applied full sharding data parallelism, but the same principles apply and can be implemented without changes to the pipeline wrapper. We will show that in the final notebook on 3D parallelism. In the next notebook, we will discuss tensor parallelism, which is another strategy to parallelize the model across multiple devices.

4.11.6 References and Resources

[Huang et al., 2019] Huang, Y., Cheng, Y., Bapna, A., Firat, O., Chen, D., Chen, M., Lee, H., Ngiam, J., Le, Q.V. and Wu, Y., 2019. Gpipe: Efficient training of giant neural networks using pipeline parallelism. Advances in neural information processing systems, 32. Paper link

[Narayanan et al., 2021] Narayanan, D., Shoeybi, M., Casper, J., LeGresley, P., Patwary, M., Korthikanti, V., Vainbrand, D., Kashinkunti, P., Bernauer, J., Catanzaro, B. and Phanishayee, A., 2021, November. Efficient large-scale language model training on gpu clusters using megatron-lm. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (pp. 1-15). Paper link

[Lamy-Poirier, 2023] Lamy-Poirier, J., 2023. Breadth-First Pipeline Parallelism. Proceedings of Machine Learning and Systems, 5. Paper link

[McKinney, 2023] McKinney, A., 2023. A Brief Overview of Parallelism Strategies in Deep Learning. Blog post link

[Huggingface, 2024] Huggingface, 2024. Model Parallelism. Documentation link

[DeepSpeed, 2024] DeepSpeed, 2024. Pipeline Parallelism. Documentation link

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For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.12 Part 4.1: Tensor Parallelism

Filled notebook:

Author: Phillip Lippe

In this tutorial, we will discuss tensor parallelism, another important parallelism strategy for training large-scale deep learning models. Similar to pipeline parallelism, tensor parallelism is a model parallelism strategy, which means that it focuses on parallelizing the model itself, rather than the data. The key difference between pipeline and tensor parallelism is how they split the model over devices. In pipeline parallelism, the model is split over devices along the sequence of layers (i.e. vertically), while in tensor parallelism, the model is split over devices along the feature dimensions (i.e. horizontally). Each device will then process a different subset of features, and the model's forward and backward passes will be split over devices accordingly. A short overview of the parallelism strategies is shown below.

Tensor parallelism can be applied on a per-module/per-layer basis. This gives more flexibility in how to split the model over devices than pipeline parallelism, and can even handle situations where a single layer is too big to fit on a single device. Furthermore, tensor parallelism does not suffer from the pipeline bubble problem, as all devices can work on the same batch of data at the same time. The key behind making tensor parallelism efficient will be, again, to overlap computation with communication, and to minimize the amount of communication required.

Still, tensor parallelism relies on frequent communication between devices, such that it requires devices with high speed interconnects like TPUs or GPUs with NVLink, and is often restricted to devices within a node. For example, Gemini v1 was trained with model parallelism within a node (TPU superpod), but applies only data parallelism across nodes.

In this tutorial, we will discuss the principles of tensor parallelism, and how to implement it in JAX. We will first start with an implementation on a simple MLP model. In Part 4.2, we discuss techniques from models like the ViT-22b to maximize efficiency of tensor parallelism with compute-communication overlaps. Finally, in Part 4.3, we will discuss how to apply tensor parallelism to the transformer model specifically, and how to combine tensor parallelism with fully-sharded data parallelism.

4.12.1 Prerequisites

First, let's start with setting up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
```

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```
# Files to download.
python_files = ["single_gpu.py", "data_parallel.py", "pipeline_parallel.py", "utils.py"]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

As before, we simulate 8 devices on CPU to demonstrate the parallelism without the need for multiple GPUs or TPUs. If you are running on your local machine and have multiple GPUs available, you can comment out the lines below.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

We now import our standard libraries.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Literal, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict

PyTree = Any
Parameter = jax.Array | nn.Partitioned
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We also import the utility functions from the previous notebooks. Our notebook will rely on the `ModelParallelismWrapper` from the pipeline parallelism notebook. If you are not familiar with it, it is recommended to look at the implementation of this module before continuing.

[4]:
```
from data_parallel import fold_rng_over_axis, sync_gradients
from pipeline_parallel import ModelParallelismWrapper
from single_gpu import Batch, TrainState, accumulate_gradients, print_metrics
```

4.12.2 Tensor Parallelism for Linear Layers

The key design principle behind tensor parallelism is to split the model over devices along the feature dimensions. For instance, consider a Transformer model with a hidden size of 1024, and we want to split the model over 4 devices. We would then split the hidden size over the devices, such that device 0 will process features 0-255, device 1 will process features 256-511, and so on. However, as we know from basic deep learning principles, the hidden dimensions are rarely independently processed. Thus, we need to design the model layers such that they communicate features or outputs between devices efficiently, whenever it is needed.

As the most basic neural network operations, let's consider a matrix multiplication as we would do it in an MLP. We can write it as $Ax = y$, with $A \in \mathbb{R}^{d_y \times d_x}$ being the weight matrix, $x \in \mathbb{R}^{d_x \times B}$ the input (batch last for simplicity), and $y \in \mathbb{R}^{d_y \times B}$ the output. In tensor parallelism, each device will carry a subset of the input dimensions, e.g. x is split into x_0, x_1, x_2, x_3 across devices. The goal is to end up with the same output y as if we had computed it on a single device, but again partitioned across devices (y_0, y_1, y_2, y_3). This is visualized below.

The question is now how to split A such that we can compute y in a distributed manner. There are two main strategies we can follow are communicating the input (gather) or the output (scatter).

In the **gather** strategy, we communicate the input x to all devices, such that each device has the full x (this communication type is called all_gather). Then, we can compute the output y_i on each device i independently by: $y_i = \sum_j A_{i,j} x_j$.

In the **scatter** strategy, we compute the sub-result of each input x_i on the output y independently on each device: $y_j^{(i)} = A_{i,j} x_i$. Afterwards, we communicate the results across devices and sum the needed result on each device: $y_i = \sum_j y_i^{(j)}$. This communication type is called (psum) scatter.

In terms of the weight matrix A, the two strategies differ in that the gather strategy splits the rows of A across devices, while the scatter strategy splits the columns of A across devices. We visualize the two strategies below (for simplicity, the communication is not explicitly visualized).

Which of the two strategies is more efficient depends on the size of the input and output dimensions. In general, we want to communicate as little data as possible, and thus the gather strategy is more efficient if the input dimension is much larger than the output dimension, and vice versa. Since the dimensions will be different for each layer, we will need to decide on a per-layer basis which strategy to use. For example, in an MLP block of a Transformer where we expand the hidden dimension by 4x, we will want to use the gather strategy for the first linear layer, and the scatter strategy for the second linear layer. This way, we avoid communicating the large hidden dimensionality.

Let's now implement the two strategies in JAX. In the gather strategy, each device will hold $A_{i,:} \in \mathbb{R}^{d_y/4 \times d_x}$ of the weight matrix, and in the scatter strategy, each device will hold $A_{:,i} \in \mathbb{R}^{d_y \times d_x/4}$ of the weight matrix. This raises a small difficulty during initialization. Many initialization strategies depend on the shape of the full weight matrix, and we need to adjust them to the shape of the split weight matrix. As a simple trick, we will implement a wrapper around the init function that will scale the values by a specified constant. We then leave it up the user to adjust the constant such that the initialization is appropriate for the split weight matrix. For instance, if we use a fan-in initialization (e.g. He initialization), we would scale the initialization by $\sqrt{1/\text{num\_devices}}$ for the scatter strategy to adjust for the $1/\text{num\_devices}$ smaller input dimension. For the gather strategy, we would not need to scale the initialization, since all devices will process the full input dimension. For more details on network initialization, see our initialization tutorial. As an alternative, we could implement our own initializer functions that directly take into account the split weight matrix dimensions (which may be tedious to support all initializations), or initialize the full weight matrix on each device and then split it. However, the latter would be less efficient and would potentially even fail if the weight matrix is too large to fit on a single device.

[5]:
```
def scale_init(init_fn: Callable, scale_factor: float = 1.0):
    """Scales the output of the given init function by the given factor.
```

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```
    Args:
        init_fn: The init function to scale.
        scale_factor: The factor to scale the output of the init function by.

    Returns:
        A new init function that scales the output of the given init function by the␣
↪given factor.
    """

    def _init_fn(rng, *args, **kwargs):
        return scale_factor * init_fn(rng, *args, **kwargs)

    return _init_fn
```

We implement the tensor parallelism for the linear layer below in a wrapper module `TPDense`. It takes as input a constructor `dense_fn` to create the linear layer. The `TPDense` module will then split the weight matrix over the devices, and implement the gather and scatter strategies for the forward and backward passes. For some layers, we may need to implement custom communications. For instance, the very first layer of the model may already have the input gather over devices, since we can prefetch the batch from the host to all devices. Similarly, in the last layer of the module, we may not want to scatter the output, but rather gather it to a single device to compute the loss. We will implement these custom communications in the full model later, and for now support them via the keyword `skip_communication`.

[6]:
```
class TPDense(nn.Module):
    """Dense layer with Tensor Parallelism support.

    This layer can be used to perform a dense layer with Tensor Parallelism support.

    Attributes:
        dense_fn: Constructor function of the dense layer to use. Needs to support the␣
↪keyword argument `kernel_init`.
        model_axis_name: The name of the model axis.
        tp_mode: The Tensor Parallelism mode to use. Can be "scatter", "gather", or "none
↪".
        skip_communication: Whether to skip communication in the Tensor Parallelism␣
↪strategy. Useful for layers with custom communication or where input has been already␣
↪gathered beforehand.
        kernel_init: The initializer to use for the kernel of the dense layer.
        kernel_init_adjustment: The adjustment factor to use for the kernel initializer.
        dense_name: The name of the dense layer module.
    """

    dense_fn: Any
    model_axis_name: str
    tp_mode: Literal["scatter", "gather", "none"] = "none"
    skip_communication: bool = False
    kernel_init: Callable = nn.initializers.lecun_normal()
    kernel_init_adjustment: float = 1.0
    dense_name: str = "module"

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.model_axis_name)
```

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```
        tp_mode = self.tp_mode if tp_size > 1 else "none"
        # Wrap the dense layer in a ModelParallelismWrapper to shard the parameters.
        dense_fn = functools.partial(
            ModelParallelismWrapper,
            model_axis_name=self.model_axis_name,
            module_fn=functools.partial(
                self.dense_fn,
                kernel_init=scale_init(self.kernel_init, self.kernel_init_adjustment),
            ),
            name=self.dense_name,
        )

        if tp_mode == "none":
            # Vanilla dense layer.
            x = self.dense_fn(kernel_init=self.kernel_init)(x)
        elif tp_mode == "gather":
            # Gather strategy: communicate all the inputs to all the devices, then␣
↪perform the dense layer.
            if not self.skip_communication:
                x = jax.lax.all_gather(x, self.model_axis_name, axis=-1, tiled=True)
            x = dense_fn()(x)
        elif tp_mode == "scatter":
            # Scatter strategy: perform the dense layer on each device, then communicate␣
↪the outputs to all the devices.
            x = dense_fn()(x)
            if not self.skip_communication:
                x = jax.lax.psum_scatter(
                    x, axis_name=self.model_axis_name, scatter_dimension=x.ndim - 1,␣
↪tiled=True
                )
        else:
            raise ValueError(f"Unknown Tensor Parallel mode: {tp_mode}")
        return x
```

Note that one small difference we are skipping over for now is the bias term in the scatter strategy. In the current implementation, each device will hold a separate bias term, and we will sum the bias terms across devices in the forward pass. This gives the bias a four times higher learning rate, which may be undesirable. For simplicity, we will ignore this for now since this will not be our final module, but in later modules, we show how this is addressed.

MLP Block

As an example network, we will implement an MLP block of the same form as used in Transformers. It consists of a normalization layer, a linear layer scaling up the hidden dimensionality, a non-linearity, and a linear layer scaling down the hidden dimensionality again. As discussed before, we will use the gather strategy for the first linear layer, and the scatter strategy for the second linear layer. The computation graph per device is visualized below.

Here, h_0 are the intermediate features in the MLP (can be of different dimensions than x), and y^0 the outputs calculated on h_0 alone. The gather and scatter operations are performed at the two ends of the MLP, such that no communication needs to performed within the MLP block, increasing efficiency.

We start with implementing the input layer, which consists of the normalization and the first linear layer. Afterwards,

we want to wrap this module in a TPDense module with the gather strategy. As an example, we use the RMSNorm layer which is used in several recent large models, including ViT-22b and Gemma. Compared to LayerNorm, it does not center the input and does not apply a bias parameter, leading to a small speed gain without degrading model performance. More details are given in the paper. Further, for simplicity and following common practice, we do not apply Dropout within the MLP block.

[7]:
```
class MLPBlockInput(nn.Module):
    config: ConfigDict
    features: int
    kernel_init: Callable = nn.initializers.lecun_normal()
    use_bias: bool = True
    use_norm: bool = True

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        if self.use_norm:
            x = nn.RMSNorm(dtype=self.config.dtype, name="pre_norm")(x)
        x = nn.Dense(
            features=self.features,
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            dtype=self.config.dtype,
            name="dense",
        )(x)
        return x
```

The output layer will consist of the second linear layer and the non-linearity. We will wrap this module in a TPDense module with the scatter strategy. As an example, we use the SiLU non-linearity. Whether we apply the non-linearity in the output layer or input layer is a design choice in this case, since we use the gather strategy for the input layer. However, had we applied the scatter strategy for the input layer, we can only apply the non-linearity in the output layer, since we would have otherwise summed over the outputs of the activation function instead of the raw outputs in the scatter.

[8]:
```
class MLPBlockOutput(nn.Module):
    config: ConfigDict
    features: int
    kernel_init: Callable = nn.initializers.lecun_normal()
    use_bias: bool = True

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        x = nn.silu(x)
        x = nn.Dense(
            features=self.features,
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            dtype=self.config.dtype,
            name="dense",
        )(x)
        return x
```

We can now combine the two modules in a single MLPBlock module. For the parallelism strategies to work correctly, we need to adjust the features count accordingly. Each device has $1/\text{num\_devices}$ of the hidden features, and outputs the full hidden features. As mentioned earlier, we also adjust the initialization of the scatter layer by scaling the initialization

by $\sqrt{1/\text{num\_devices}}$, since we use a fan-in initialization strategy.

[9]:
```
class TPMLPBlock(nn.Module):
    config: ConfigDict
    train: bool

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        input_features = x.shape[-1]
        # Input layer
        x = TPDense(
            dense_fn=functools.partial(
                MLPBlockInput,
                config=self.config,
                features=self.config.hidden_size * self.config.mlp_expansion // tp_size,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="gather",
            name="input",
        )(x)
        # Output layer
        x = TPDense(
            dense_fn=functools.partial(
                MLPBlockOutput,
                config=self.config,
                features=input_features * tp_size,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="scatter",
            kernel_init_adjustment=tp_size**-0.5,  # fan-in with tp_size fewer inputs.
            name="output",
        )(x)
        return x
```

MLP Classifier

Our example model will consists of a stack of MLP blocks. For this, we write below a simple wrapper around the `MLPBlock` to stack multiple blocks. For efficient compilation, we use a `nn.scan` to apply the same MLP block structure in all layers. The carry between the modules is the sharded features over the model axis.

[10]:
```
class TPMLPLayers(nn.Module):
    config: ConfigDict
    train: bool
    block_class: Callable[..., nn.Module] = TPMLPBlock

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        module = self.block_class(config=self.config, train=self.train, name="block")
        x, _ = nn.scan(
            lambda module, carry, _: (module(carry) + carry, None),
            variable_axes={"params": 0},
```

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```
            split_rngs={"params": True, "dropout": True},
            length=self.config.num_layers,
            metadata_params={
                "partition_name": None
            },  # We do not need to partition the parameters over the layer axis.
        )(module, x, ())
        return x
```

Finally, we combine the MLP blocks with an input and output layer. We expect that the input to the model is duplicated over model devices and thus does not need to be gathered anymore. This is likely the best case for the input processing as well, since the batch can already be prefetched to all devices and we may not be able to split the input over model devices equally (e.g. text may be only single integers, so that we cannot split it over feature dimensions). If working with a mesh where the model axis goes across processes, we may want to split the input over model devices on the batch dimension as well, and gather it before applying the model. This ensures all model devices will start with the same input.

The output layer will be a linear layer with the number of classes as output dimensions. We will wrap this layer in a `TPDense` module with the scatter strategy, but we will not scatter the output. Instead, to compute the loss, a device needs to have the full output features. Hence, we apply a `jax.lax.psum` to sum the final output over devices. Note that this gives all model devices the same tensor, and thus the same loss. We may want to then only calculate the loss on a single device, and broadcast it back to all devices via the `psum` operation. For models with large output sizes, this might be inefficient since a single device needs to be able to hold the entire output. For simplicity, we will ignore this for now here, but address it in the transformer model later. Finally, as usual, we convert the output to float32 to avoid numerical issues in the loss computation.

[11]:
```
class TPClassifier(nn.Module):
    config: ConfigDict
    block_class: Callable[..., nn.Module] = TPMLPBlock

    @nn.compact
    def __call__(self, x: jax.Array, train: bool) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        # Input layer
        x = TPDense(
            dense_fn=functools.partial(
                nn.Dense,
                features=self.config.hidden_size // tp_size,
                dtype=self.config.dtype,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="gather",
            skip_communication=True,  # Input already gathered.
            name="input_layer",
        )(x)
        # Backbone MLP blocks
        x = TPMLPLayers(config=self.config, train=train, name="mlp", block_class=self.
↪block_class)(
            x
        )
        # Output layer
        x = TPDense(
            dense_fn=functools.partial(
                nn.Dense,
```

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```
                features=self.config.num_classes,
                dtype=self.config.dtype,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="scatter",
            skip_communication=True,  # Manual communication.
            name="output_layer",
            kernel_init_adjustment=tp_size**-0.5,  # fan-in with tp_size fewer inputs.
        )(x)
        x = jax.lax.psum(x, axis_name=self.config.model_axis_name)
        x = x.astype(jnp.float32)
        return x
```

Initialization

With the model implemented, we can now initialize the model. We start with the config definition, which is similar to previous notebooks. We parallelize the model over 4 devices, and for simplicity, keep the MLP expansion factor at 1. Feel free to experiment with different configurations.

[12]:
```
data_config = ConfigDict(
    dict(
        batch_size=128,
        num_classes=10,
        input_size=784,
    )
)
model_config = ConfigDict(
    dict(
        hidden_size=512,
        dropout_rate=0.1,
        mlp_expansion=1,
        num_layers=3,
        dtype=jnp.bfloat16,
        num_classes=data_config.num_classes,
        data_axis_name="data",
        model_axis_name="model",
        model_axis_size=4,
    )
)
optimizer_config = ConfigDict(
    dict(
        learning_rate=1e-3,
        num_minibatches=1,
    )
)
config = ConfigDict(
    dict(
        model=model_config,
        optimizer=optimizer_config,
        data=data_config,
        data_axis_name=model_config.data_axis_name,
```

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```
        model_axis_name=model_config.model_axis_name,
        model_axis_size=model_config.model_axis_size,
        seed=42,
    )
)
```

The rest of the initialization is identical to the previous notebook on pipeline parallelism. We first create our mesh over data and model.

[13]:
```
device_array = np.array(jax.devices()).reshape(-1, config.model_axis_size)
mesh = Mesh(device_array, (config.data_axis_name, config.model_axis_name))
```

```
2024-03-07 10:48:19.003795: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

We then create the model object and the optimizer. We stick with simple Adam in this example, but feel free to change the optimizer setup.

[14]:
```
model_tp = TPClassifier(config=config.model)
optimizer = optax.adamw(
    learning_rate=config.optimizer.learning_rate,
)
```

For simplicity, we will train the model on a simple random data classification task. This is mainly to demonstrate the pipeline parallelism, and not to achieve state-of-the-art results. In practice, one would instead create a dataset and dataloader at this point, and setup the data prefetching.

[15]:
```
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng, data_labels_rng = jax.random.split(rng, 3)
batch = Batch(
    inputs=jax.random.normal(data_inputs_rng, (config.data.batch_size, config.data.input_
↪size)),
    labels=jax.random.randint(
        data_labels_rng, (config.data.batch_size,), 0, config.data.num_classes
    ),
)
```

The initialization function follows the same principles as in the previous notebook, creating the parameters via `model.init` and the optimizer parameters in the `TrainState.create`.

[16]:
```
def init_tp(rng: jax.random.PRNGKey, x: jax.Array, model: nn.Module) -> TrainState:
    init_rng, rng = jax.random.split(rng)
    variables = model.init({"params": init_rng}, x, train=False)
    params = variables.pop("params")
    state = TrainState.create(
        apply_fn=model.apply,
        params=params,
        tx=optimizer,
        rng=rng,
    )
    return state
```

Before we can run the full initialization, we need to identify the partitioning of the parameters. Since we annotated the partitioning of all parameters via `nn.Partitioned` in the model, we can obtain the partitioning by calling `jax.eval_shape` on the init function. This will return the state shapes, as well as the `nn.Partitioned` parameter leafs. From those, we can read out the partitioning using `nn.get_partition_spec`. For the initial call, we can leave the `out_specs` of the shard map empty, since we do not create the actual parameters during shape evaluation.

[17]:
```
init_tp_fn = shard_map(
    functools.partial(init_tp, model=model_tp),
    mesh,
    in_specs=(P(), P(config.data_axis_name)),
    out_specs=P(),
    check_rep=False,
)
state_tp_shapes = jax.eval_shape(init_tp_fn, model_init_rng, batch.inputs)
state_tp_specs = nn.get_partition_spec(state_tp_shapes)
```

Let's investigate the partitioning of the parameters.

[18]:
```
pprint(state_tp_specs.params)
```

```
{'input_layer': {'module': {'sharded': {'bias': PartitionSpec('model', None),
                                        'kernel': PartitionSpec('model', None, None)}}},
 'mlp': {'block': {'input': {'module': {'sharded': {'dense': {'bias': PartitionSpec(None,
↪ 'model', None),
                                                                'kernel':␣
↪PartitionSpec(None, 'model', None, None)},
                                                     'pre_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)}}}},
                   'output': {'module': {'sharded': {'dense': {'bias':␣
↪PartitionSpec(None, 'model', None),
                                                                 'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}}}}},
 'output_layer': {'module': {'sharded': {'bias': PartitionSpec('model', None),
                                         'kernel': PartitionSpec('model', None, None)}}}}
```

All parameters in the model have a partitioning over the `model` axis. For the input and output layer, this is over the first dimension, while for the MLP blocks, this is over the second dimension. This is because the first dimension of the MLPs are the number of layer (i.e. the scan). This also demonstrates how our implementation works well under function transformations like scan, vmap, etc. Since we do not apply FSDP for now, the parameters are not partitioned over the data axis. The several sub-keys in the parameter PyTree are due to the stacking and wrapping of the modules (e.g. `sharded` introduced by `ModelParallelismWrapper`, `module` introduced by `TPDense`). Alternatively, some of these wrapper could be rewritten into functions to avoid the sub-keys.

We can now continue with the initialization:

[19]:
```
init_tp_fn = jax.jit(
    shard_map(
        functools.partial(init_tp, model=model_tp),
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_tp_specs,
        check_rep=False,
    ),
)
state_tp = init_tp_fn(model_init_rng, batch.inputs)
```

We inspect the shapes of the parameters below.

[20]:
```
print("TP Parameters - Input Layer")
pprint(jax.tree_map(lambda x: x.shape, state_tp.params["input_layer"]["module"]["sharded
↪"]))
```

```
TP Parameters - Input Layer
{'bias': Partitioned(value=(4, 128), names=('model', None), mesh=None),
 'kernel': Partitioned(value=(4, 784, 128),
                       names=('model', None, None),
                       mesh=None)}
```

The input layer uses a gather strategy, such that its input size is the full feature size (784), but its output is split over model devices ($512/4 = 128$).

[21]:
```
print("TP Parameters - MLP Layers Input")
pprint(
    jax.tree_map(lambda x: x.shape, state_tp.params["mlp"]["block"]["input"]["module"][
↪"sharded"])
)
print()
print("TP Parameters - MLP Layers Output")
pprint(
    jax.tree_map(lambda x: x.shape, state_tp.params["mlp"]["block"]["output"]["module"][
↪"sharded"])
)
```

```
TP Parameters - MLP Layers Input
{'dense': {'bias': Partitioned(value=(3, 4, 128),
                               names=(None, 'model', None),
                               mesh=None),
           'kernel': Partitioned(value=(3, 4, 512, 128),
                                 names=(None, 'model', None, None),
                                 mesh=None)},
 'pre_norm': {'scale': Partitioned(value=(3, 4, 512),
                                   names=(None, 'model', None),
                                   mesh=None)}}

TP Parameters - MLP Layers Output
{'dense': {'bias': Partitioned(value=(3, 4, 512),
                               names=(None, 'model', None),
                               mesh=None),
           'kernel': Partitioned(value=(3, 4, 128, 512),
                                 names=(None, 'model', None, None),
                                 mesh=None)}}
```

The MLP input layer uses a gather strategy, such that it also has the full feature size as input, but its output is split over model devices ($512/4 = 128$). Note that the norm layer has different scaling parameters for each device. This is usually not a problem, since the norm layer is usually followed by a linear layer, which allows for scaling of the weights. Still, it's a difference to the single device case, which is important to keep in mind, and could be shared across devices if needed.

The MLP output layer follows the scatter pattern, such that its input is split over model devices ($512/4 = 128$), but its output is the full feature size.

[22]:
```
print("TP Parameters - Output Layer")
pprint(jax.tree_map(lambda x: x.shape, state_tp.params["output_layer"]["module"]["sharded
↪"]))
```

```
TP Parameters - Output Layer
{'bias': Partitioned(value=(4, 10), names=('model', None), mesh=None),
 'kernel': Partitioned(value=(4, 128, 10),
                       names=('model', None, None),
                       mesh=None)}
```

Finally, the final output layer follows the scatter pattern, such that its input is split over model devices ($512/4 = 128$), but its output is the full number of classes. Note that whether we manually implement the communication or use the `TPDense` communication does not have an impact on the feature size.

Another aspect to check is whether the initialization across devices works as expected. Since each device holds a different part of the weight matrix, we expect them to be initialized differently. We can check this by inspecting the parameters.

[23]:
```
state_tp.params["mlp"]["block"]["input"]["module"]["sharded"]["dense"]["kernel"].value[:,
↪ :, 0, 0]
```

[23]:
```
Array([[-0.06087485, -0.04099965,  0.04802493, -0.00385336],
       [ 0.0586801 , -0.01241772, -0.00626128,  0.00607279],
       [-0.05654007,  0.02550504, -0.02855512, -0.08177456]],      dtype=float32)
```

The above cell prints the kernel of the MLP input layer over the layer axis and devices. We can see that the parameters are indeed initialized differently across devices, and thus we can continue to train the model.

Training with Tensor Parallelism

The training loop is identical to the examples in the previous notebooks. The loss function is a simple cross-entropy loss, where we only calculate the loss for the first device.

[24]:
```
def loss_fn_tp(
    params: PyTree,
    apply_fn: Any,
    batch: Batch,
    rng: jax.Array,
) -> Tuple[jax.Array, Dict[str, Any]]:
    # Since dropout masks vary across the batch dimension, we want each device to␣
↪generate a
    # different mask. We can achieve this by folding the rng over the data axis, so that␣
↪each
    # device gets a different rng and thus mask.
    dropout_rng = fold_rng_over_axis(rng, (config.data_axis_name, config.model_axis_
↪name))
    # Remaining computation is the same as before for single device.
    logits = apply_fn(
        {"params": params},
        batch.inputs,
        train=True,
        rngs={"dropout": dropout_rng},
    )
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, batch.labels)
```

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```
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), batch.labels)
    batch_size = np.prod(batch.labels.shape)
    # Mask out loss and accuracy for model devices except first one.
    model_idx = jax.lax.axis_index(config.model_axis_name)
    loss = jnp.where(model_idx != 0, 0.0, loss)
    correct_pred = jnp.where(model_idx != 0, False, correct_pred)
    batch_size = jnp.where(model_idx != 0, 0, batch_size)
    # Collect metrics and return loss.
    step_metrics = {
        "loss": (loss.sum(), batch_size),
        "accuracy": (correct_pred.sum(), batch_size),
    }
    loss = loss.mean()
    return loss, step_metrics
```

In the training, we want to support 2D parallelism with (fully-sharded) data parallelism and tensor parallelism. Thus, after having determined the gradients per device, we need to sync them over the data axis accordingly. For this, we can reuse the `sync_gradients` functions from our fully-sharded data parallelism implementation. We then apply the optimizer update as usual.

Finally, we can summarize all in the training step below. It is identical to the fully-sharded data parallelism training step up to syncing gradients over the data and model axis (which is now 2D). We then apply the optimizer update as usual.

[25]:
```
def train_step_tp(
    state: TrainState,
    metrics: Metrics | None,
    batch: Batch,
    loss_fn: Callable = loss_fn_tp,
) -> Tuple[TrainState, Metrics]:
    rng, step_rng = jax.random.split(state.rng)
    grads, step_metrics = accumulate_gradients(
        state,
        batch,
        step_rng,
        config.optimizer.num_minibatches,
        loss_fn=loss_fn,
    )
    # Update parameters. We need to sync the gradients across devices before updating.
    with jax.named_scope("sync_gradients"):
        grads = sync_gradients(grads, (config.data_axis_name, config.model_axis_name))
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Sum metrics across replicas. Alternatively, we could keep the metrics separate
    # and only synchronize them before logging. For simplicity, we sum them here.
    with jax.named_scope("sync_metrics"):
        step_metrics = jax.tree_map(
            lambda x: jax.lax.psum(x, axis_name=(config.data_axis_name, config.model_
↪axis_name)),
            step_metrics,
        )
    if metrics is None:
        metrics = step_metrics
    else:
```

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```
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

With the training loop implemented, we can now train the model. We will train the model on a simple random data classification task, and expect the model to learn to classify the data with high accuracy. We will use a small batch size to run the model easily on a CPU-only system.

[26]:
```
train_step_tp_fn = jax.jit(
    shard_map(
        train_step_tp,
        mesh,
        in_specs=(state_tp_specs, P(), P(config.data_axis_name)),
        out_specs=(state_tp_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
state_shapes, metric_shapes = jax.eval_shape(
    train_step_tp_fn,
    state_tp,
    None,
    batch,
)
metrics_tp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes)
state_tp, metrics_tp = train_step_tp_fn(state_tp, metrics_tp, batch)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[1,128]),
↪ ShapedArray(float32[1,784,128]), ShapedArray(float32[3,1,128]), ShapedArray(float32[3,
↪1,512,128]), ShapedArray(float32[3,1,512]), ShapedArray(float32[3,1,512]),␣
↪ShapedArray(float32[3,1,128,512]), ShapedArray(float32[1,10]), ShapedArray(float32[1,
↪128,10]), ShapedArray(float32[1,128]), ShapedArray(float32[1,784,128]),␣
↪ShapedArray(float32[3,1,128]), ShapedArray(float32[3,1,512,128]),␣
↪ShapedArray(float32[3,1,512]), ShapedArray(float32[3,1,512]), ShapedArray(float32[3,1,
↪128,512]), ShapedArray(float32[1,10]), ShapedArray(float32[1,128,10]),␣
↪ShapedArray(float32[1,128]), ShapedArray(float32[1,784,128]), ShapedArray(float32[3,1,
↪128]), ShapedArray(float32[3,1,512,128]), ShapedArray(float32[3,1,512]),␣
↪ShapedArray(float32[3,1,512]), ShapedArray(float32[3,1,128,512]),␣
↪ShapedArray(float32[1,10]), ShapedArray(float32[1,128,10]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

We run the model for 15 steps and print the final loss and accuracy.

[27]:
```
for _ in range(15):
    state_tp, metrics_tp = train_step_tp_fn(state_tp, metrics_tp, batch)
final_metrics_tp = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_tp, final_metrics_tp = train_step_tp_fn(state_tp, final_metrics_tp, batch)
print_metrics(final_metrics_tp, title="Final Metrics - Tensor Parallelism")
```

```
 Final Metrics - Tensor Parallelism
accuracy: 1.000000
loss: 0.000030
```

As we expected, the model is able to learn the task with high accuracy. We can now continue to the next part, where we discuss a more efficient implementation exploiting the compute and communication overlap.

Intermediate Summary

In this part, we discussed the principles of tensor parallelism, and how to implement it in JAX. We implemented a simple MLP model with tensor parallelism, and trained it on a simple random data classification task. We also discussed the sharding of the parameters. In the next part, we will discuss how to maximize the efficiency of tensor parallelism with compute-communication overlaps.

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4.13 Part 4.2: Asynchronous Linear Layers with Tensor Parallelism

Filled notebook:

Author: Phillip Lippe

In Part 4.1, we implemented a parallel linear layer using tensor parallelism. However, our implementation has one major inefficiency. In the gather strategy, we first need to communicate the features over all devices before we can compute the output. This means that all devices are idle until we finish the communication, and we do not overlap communication with computation. Similarly, in the scatter strategy, we first need to compute the output on all devices before we can communicate the results and sum them. This means that all devices are busy until we finish the computation, and then need to wait for the communication to finish before continuing with subsequent layers. This is a major inefficiency, and we would like to avoid it if possible.

To tackle this challenge, we will implement asynchronous linear layers in this notebook. Using an asynchronous gather and scatter strategy, we will overlap communication with computation, which will allow us to hide the communication latency and improve the overall performance of our model. The techniques we will use in this notebook are inspired by the ViT-22b model, which used these techniques to scale up Vision Transformers. In Part 4.3, we will apply these techniques to scale up our Transformer-based language model.

4.13.1 Prerequisites

First, let's start with setting up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = ["single_gpu.py", "data_parallel.py", "pipeline_parallel.py", "tensor_
↪parallel.py", "utils.py"]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

As before, we simulate 8 devices on CPU to demonstrate the parallelism without the need for multiple GPUs or TPUs. If you are running on your local machine and have multiple GPUs available, you can comment out the lines below.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

We now import our standard libraries.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, List, Literal, Sequence, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict

PyTree = Any
Parameter = jax.Array | nn.Partitioned
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We also import the utility functions from the previous notebooks. Our notebook will rely on the `ModelParallelismWrapper` from the pipeline parallelism notebook and functions from Part 4.1. If you are not familiar with those modules, it is recommended to look at the implementation of this module before continuing.

[4]:
```
from pipeline_parallel import ModelParallelismWrapper
from single_gpu import Batch, print_metrics
from tensor_parallel import (
    MLPBlockInput,
    MLPBlockOutput,
    TPClassifier,
    get_default_tp_classifier_config,
    init_tp,
    scale_init,
    train_step_tp,
)
```

Additionally, we recreate the config, mesh, and batch from Part 4.1 to use the same task as before.

[5]:
```
# Load the default configuration for the classifier.
config = get_default_tp_classifier_config()
# Initialize multi-device mesh.
device_array = np.array(jax.devices()).reshape(-1, config.model_axis_size)
mesh = Mesh(device_array, (config.data_axis_name, config.model_axis_name))
# Batch for random classification task.
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng, data_labels_rng = jax.random.split(rng, 3)
batch = Batch(
    inputs=jax.random.normal(data_inputs_rng, (config.data.batch_size, config.data.input_
↪size)),
```

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```
    labels=jax.random.randint(
        data_labels_rng, (config.data.batch_size,), 0, config.data.num_classes
    ),
)
```

```
2024-03-07 10:48:41.885331: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

4.13.2 Tensor Parallelism with Compute-Communication Overlap

In the previous notebook on pipeline parallelism, we discussed how one can overlap communication with computation by sending sub-results as soon as they become available. We can apply the same principle to tensor parallelism. At the start of the linear layer, each device has a subset of the input features. We can directly start computing the output with respect to these features, which corresponds to $A_{i,i}x_i$ in our original notation. While we do that, we can already communicate the features to the next device, such that we overlap communication with computation. As soon as the next device receives the features, it can start computing the output with respect to these features, and continue the process. This way, we save the time of waiting for the communication to finish before we can start computing the output, and we improve the efficiency of the model, closer to the theoretical maximum.

Before we can implement this strategy, we need to have a way of performing the communication efficiently and asynchronously with respect to the computation. In JAX, we can do this with `jax.lax.ppermute`, which is a parallel permutation operation and we have seen in previous notebooks before. It allows us to send an array to the next device in a ring topology, and receive an array from the previous device. As long as we do not try to access the array before it has been fully communicated, we can continue with the computation and overlap communication with computation. We will use this operation to implement an asynchronous version of our gather and scatter-sum operations.

Async Gather

We start with the gather strategy. Each device holds a subset of the input features, and we want to communicate the input features asynchronously to all devices. We start by performing a `jax.lax.ppermute` to send the current features to the next device in our ring topology. This means device 0 sends the features to device 1, device 1 sends the features to device 2, and so on, until the last device sends its features to device 0. However, instead of concatenating the communicated features with the current features, as we would get with `jax.lax.all_gather`, we collect the communicated arrays in a list. This way, the features present on the device and the communicated features become two independent arrays, on which we can perform independent operations. For instance, we could already start computing the output with respect to the current features, while waiting for the communication to finish.

At this point, each device has its own features and those of its neighbor. However, we want all features to be gathered on all devices. We achieve this by communicating the newly communicated features to the next device as soon as they become available. For example, device 0 sends the communicated features from device 3 to device 1, device 1 sends the communicated features from device 0 to device 2, and so on. By continuining this pattern, we can ensure that all devices have all features by using the minimal amount of communication (each device only sends and receives $N-1$ features, where N is the number of devices).

The communication pattern is visualized below. The first column shows the initial features on each device, and each block represents the list of features per device. The second column shows the communicated features after a single `jax.lax.ppermute`, and so on. The arrows indicate the communication pattern.

We note that in contrast to the all-gather operation, each device ends up with a different order of the features. This is not a problem for our purposes, since our final operation of performing a matrix multiplication with the weight matrix

is independent of the order of the features. We will sum the outputs of each feature and learn the weight matrix from scratch, thus being able to handle the different order of the features. Still, one should keep in mind that this might lead to a different weight matrix order than in the all-gather operation, and converting between the two operations requires a permutation of the weight matrix.

Let's now implement the async gather strategy below. In implementation, we can decide which direction of the ring we communicate along (device 0 to device 1, or device 1 to device 0). More on this later. We further write the implementation general enough such that it also supports PyTree's that we need to communicate across devices. This becomes helpful when we have a more complex model, and the module's input or output is a PyTree.

[6]:
```
def async_gather(x: PyTree, axis_name: str, shift_up: bool = True) -> List[PyTree]:
    """All gather using ring permutation.

    Args:
        x: The input to gather.
        axis_name: The axis name to gather along.
        shift_up: Whether to shift up (device 0 send to device 1) or down (device 1 send␣
↪to device 0).

    Returns:
        List of gathered inputs.
    """
    tp_size = jax.lax.psum(1, axis_name)
    # Determine communication permutation.
    if shift_up:
        shift_perm = [(j, (j + 1) % tp_size) for j in range(tp_size)]
    else:
        shift_perm = [(j, (j - 1) % tp_size) for j in range(tp_size)]
    ps = [x]
    p = x
    # Perform all-gather using ring permutation.
    for _ in range(1, tp_size):
        p = jax.lax.ppermute(p, axis_name, perm=shift_perm)
        ps.append(p)
    return ps
```

The output is now a list of arrays, on which we can perform independent, asynchronous operations. We can schedule each operation as the features become available, and are only blocked once we want to access an array that has not finished communicating yet. As long as the individual operations are sufficiently making use of the device, we can overlap communication with computation.

Example

Let's make a small example to illustrate the async gather strategy. We will use a simple feature array of shape `(2, 4, 1)` (data axis, model axis, feature axis), and split it over our 8 devices.

[7]:
```
x = np.arange(jax.local_device_count(), dtype=jnp.float32)
x = np.reshape(x, (-1, config.model_axis_size, 1))
x
```

[7]:
```
array([[[0.],
        [1.],
        [2.],
        [3.]],
```

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```
       [[4.],
        [5.],
        [6.],
        [7.]]], dtype=float32)
```

We now call the async gather function with the feature array over the model axis. We will use the default communication direction, which is from device 0 to device 1.

[8]:
```
gather_model_fn = shard_map(
    functools.partial(async_gather, axis_name=config.model_axis_name),
    mesh=mesh,
    in_specs=P(config.data_axis_name, config.model_axis_name),
    out_specs=P(config.data_axis_name, config.model_axis_name),
)
x_gather_model = gather_model_fn(x)
x_gather_model = jax.device_get(x_gather_model)
for idx in range(jax.local_device_count()):
    print(
        f"Device {idx}: {[feat.reshape(-1, feat.shape[-1])[idx].item() for feat in x_
↪gather_model]}"
    )
```

```
Device 0: [0.0, 3.0, 2.0, 1.0]
Device 1: [1.0, 0.0, 3.0, 2.0]
Device 2: [2.0, 1.0, 0.0, 3.0]
Device 3: [3.0, 2.0, 1.0, 0.0]
Device 4: [4.0, 7.0, 6.0, 5.0]
Device 5: [5.0, 4.0, 7.0, 6.0]
Device 6: [6.0, 5.0, 4.0, 7.0]
Device 7: [7.0, 6.0, 5.0, 4.0]
```

The output is a list of arrays, where each array is the communicated features from the previous device. Device 0 to device 3 show the same communication pattern as we have visualized above. Device 0 sends its first features to device 1, and receives the first features from device 3. If we had flipped the direction, device 0 would have `1.0` as its first feature. Meanwhile, device 4 to device 7 are an independent model group, since they are stacked over the data axis. Thus, device 4 communicates its first features to device 5, and receives the first features from device 7.

Bidirectional Communication

Our implementation of the async gather strategy allows us to communicate the features in both directions, which we can exploit further. For instance, in TPU superpods, TPUs are connected in a 2D/3D torus mesh, such that each TPU has an interconnect to all its neighbors. Therefore, we can communicate the features in both directions at the same time to maximize our usage of bandwidth (more details here). Similarly, NVLink connections between GPUs allow for bidirectional communication, which we can exploit.

At each step, we perform a `jax.lax.ppermute` in both directions, and collect the communicated features. Note that we need to keep track of the features we send in both directions separately, since in the second step, device 1 will send device 0's features to device 2 and not accidentally back to device 0. Further, we can ensure the same order in the list as the non-bidirectional version by keeping two separate lists and merge them afterwards. The communication pattern is visualized below.

We can now implement the bidirectional async gather strategy below, with the same principles as the non-bidirectional version.

[9]:
```
def async_gather_bidirectional(
    x: jax.Array, axis_name: str, shift_up: bool = True
) -> List[jax.Array]:
    """All gather using ring permutation with bidirectional communication.

    Args:
        x: The input to gather.
        axis_name: The axis name to gather along.
        shift_up: Whether to return the order of tensors that complies with the␣
↪unidirectional version of shift up (device 0 send to device 1) or down (device 1 send␣
↪to device 0).

    Returns:
        List of gathered inputs.
    """
    tp_size = jax.lax.psum(1, axis_name)
    shift_up_perm = [(j, (j + 1) % tp_size) for j in range(tp_size)]
    shift_down_perm = [(j, (j - 1) % tp_size) for j in range(tp_size)]
    ps_up = []
    ps_down = []
    p_up = x
    p_down = x
    for i in range(1, tp_size):
        if i % 2 == 0:
            p_down = jax.lax.ppermute(p_down, axis_name=axis_name, perm=shift_down_perm)
            ps_down.append(p_down)
        else:
            p_up = jax.lax.ppermute(p_up, axis_name=axis_name, perm=shift_up_perm)
            ps_up.append(p_up)
    # Combine communication in both directions.
    # This list will have the same order as the unidirectional up version.
    if shift_up:
        ps = [x] + ps_up + ps_down[::-1]
    else:
        ps = [x] + ps_down + ps_up[::-1]
    return ps
```

As before, we can make a small example to illustrate the bidirectional async gather strategy. We will use the same feature array as before.

[10]:
```
gather_bidir_model_fn = shard_map(
    functools.partial(async_gather_bidirectional, axis_name=config.model_axis_name),
    mesh=mesh,
    in_specs=P(config.data_axis_name, config.model_axis_name),
    out_specs=P(config.data_axis_name, config.model_axis_name),
)
x_gather_model = gather_bidir_model_fn(x)
x_gather_model = jax.device_get(x_gather_model)
for idx in range(jax.local_device_count()):
    print(
        f"Device {idx}: {[feat.reshape(-1, feat.shape[-1])[idx].item() for feat in x_
↪gather_model]}"
```

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```
    )
```

```
Device 0: [0.0, 3.0, 2.0, 1.0]
Device 1: [1.0, 0.0, 3.0, 2.0]
Device 2: [2.0, 1.0, 0.0, 3.0]
Device 3: [3.0, 2.0, 1.0, 0.0]
Device 4: [4.0, 7.0, 6.0, 5.0]
Device 5: [5.0, 4.0, 7.0, 6.0]
Device 6: [6.0, 5.0, 4.0, 7.0]
Device 7: [7.0, 6.0, 5.0, 4.0]
```

The result is identical to the unidirectional version, but we have communicated the features in both directions at the same time. This can be useful to maximize the usage of the interconnect bandwidth, and is especially useful in TPU nodes.

If you look carefully at the diagram, you spot another minor inefficiency. If we have an even number of devices, the last communication cycle will be unidirectional again since we require an uneven amount of communication cycles. An alternative bidirectional communication strategy that overcomes this inefficiency is to split the features over the hidden dimension, and communicate half in one direction and half in the other direction. This way, we can ensure that we always communicate in both directions, and may speed up the latency of the first feature to be communicated, since the features are smaller. However, this strategy requires more communication cycles and may require operations on smaller arrays, which may have a lower utilization of the devices depending on the feature and operation size. Additionally, it gives a strictly different list structure of the features than the unidirectional version. We implement this strategy below.

[11]:
```
def async_gather_split(x: jax.Array, axis_name: str) -> List[jax.Array]:
    """All gather using ring permutation with features split for bidirectional␣
↪communication.

    Args:
        x: The input to gather.
        axis_name: The axis name to gather along.

    Returns:
        List of gathered inputs. Length is 2 * axis size - 1.
    """
    x1, x2 = jax.tree_map(lambda x: jnp.split(x, 2, axis=-1), x)
    return async_gather(x1, axis_name, shift_up=True) + async_gather(x2, axis_name,␣
↪shift_up=False)
```

We can make a small example again, where we double the feature dimension of `x` to allow for splitting over the hidden dimension.

[12]:
```
gather_split_model_fn = shard_map(
    functools.partial(async_gather_split, axis_name=config.model_axis_name),
    mesh=mesh,
    in_specs=P(config.data_axis_name, config.model_axis_name),
    out_specs=P(config.data_axis_name, config.model_axis_name),
)
x_double = np.concatenate([x, x + 0.5], axis=-1)
x_gather_model = gather_split_model_fn(x_double)
x_gather_model = jax.device_get(x_gather_model)
for idx in range(jax.local_device_count()):
    print(
```

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```
        f"Device {idx}: {[feat.reshape(-1, feat.shape[-1])[idx].item() for feat in x_
↪gather_model]}"
    )
```

```
Device 0: [0.0, 3.0, 2.0, 1.0, 0.5, 1.5, 2.5, 3.5]
Device 1: [1.0, 0.0, 3.0, 2.0, 1.5, 2.5, 3.5, 0.5]
Device 2: [2.0, 1.0, 0.0, 3.0, 2.5, 3.5, 0.5, 1.5]
Device 3: [3.0, 2.0, 1.0, 0.0, 3.5, 0.5, 1.5, 2.5]
Device 4: [4.0, 7.0, 6.0, 5.0, 4.5, 5.5, 6.5, 7.5]
Device 5: [5.0, 4.0, 7.0, 6.0, 5.5, 6.5, 7.5, 4.5]
Device 6: [6.0, 5.0, 4.0, 7.0, 6.5, 7.5, 4.5, 5.5]
Device 7: [7.0, 6.0, 5.0, 4.0, 7.5, 4.5, 5.5, 6.5]
```

As one can see, the communication pattern is different than the unidirectional version, and we have communicated the features in both directions at the same time. Due to the different setup and need for more operations, we will focus on the other bidirectional communication strategy in the following.

Async Scatter

We now turn to the scatter implementation. In scatter, we have the opposite situation than in gather: all inputs are already available at the start of the operation, and instead, we want to communicate the output to all devices. Thus, we want to start communicating as soon as we have computed a part of the output needed on another device. The asynchronous scatter strategy is visualized below.

As input, we have the full output features on each device. For clarity, we denote the arrays as $a_0, ..., a_3$ for device 0 and so on, where a_i corresponds to $y_i^{(0)}$ in our earlier notation. Note that not all arrays need to be ready at this point, and mainly start with a list of arrays to indicate the computation graph to the compiler. In eager mode, this can correspond to the setup where the CPU offloaded the computation of the array to the GPU, but can already continue with the next operation until the values of the array are needed.

In the first step, we communicate the first outputs of all devices in a round robin fashion. This communication can be performed as soon as a_0, b_0, c_0, and d_0 are available (highlighted in red), and will be overlapped with the computation of a_1, b_1, c_1, and d_1. The communicated arrays will then be added to the output arrays a_1, b_1, c_1, and d_1 as soon as they become available, and we start the next round of communication. This round overlaps with the computation of a_2, b_2, c_2, and d_2, and so on. This way, we can overlap communication with computation and improve the efficiency of the model. The final output on each device will be the sum of some output part of all devices, which follows the scatter pattern. However, in comparison to the non-async scatter, the order of the output parts will be different: device 0 has the sum $a_3 + b_0 + c_1 + d_2$, while in the non-async scatter, it would have been $a_0 + b_0 + c_0 + d_0$. As for the async gather operation, this is usually not a problem, since the order of the output parts is not important for the learned linear layer.

We can now implement the async scatter strategy below. Given a list of arrays, we will communicate the arrays in a round robin fashion, and add the communicated arrays to the output arrays as soon as they become available. The output is the sum of all communicated arrays and the last output array.

[13]:
```
def async_scatter(xs: Sequence[PyTree], axis_name: str, shift_up: bool = True) -> PyTree:
    """Scatter sum using ring permutation.

    Args:
        xs: The inputs to scatter sum. The length of the list should match the size of␣
↪the axis.
        axis_name: The axis name to scatter sum along.
        shift_up: Whether to shift up (device 0 send to device 1) or down (device 1 send␣
↪to device 0).
```

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```
    Returns:
        The scatter summed output.
    """
    tp_size = jax.lax.psum(1, axis_name)
    assert (
        len(xs) == tp_size
    ), f"Number of shards needs to match axis size, but got {len(xs)} with {axis_name}␣
↪axis size {tp_size}."
    if shift_up:
        shift_perm = [(j, (j + 1) % tp_size) for j in range(tp_size)]
    else:
        shift_perm = [(j, (j - 1) % tp_size) for j in range(tp_size)]
    y = xs[0]
    for x in xs[1:]:
        y = jax.lax.ppermute(y, axis_name, perm=shift_perm)
        y = jax.tree_map(jnp.add, y, x)
    return y
```

Example

Let's make a small example to illustrate the async scatter strategy. We will use a simple feature array of shape `(2, 4, 4)` (data axis, model axis, feature axis), and split it over our 8 devices.

[14]:
```
np_rng = np.random.default_rng(42)
x = np_rng.integers(
    low=0,
    high=10,
    size=(
        jax.local_device_count() // config.model_axis_size,
        config.model_axis_size,
        config.model_axis_size,
    ),
)
pprint(x)
```

```
array([[[0, 7, 6, 4],
        [4, 8, 0, 6],
        [2, 0, 5, 9],
        [7, 7, 7, 7]],

       [[5, 1, 8, 4],
        [5, 3, 1, 9],
        [7, 6, 4, 8],
        [5, 4, 4, 2]]])
```

In this example, we have device 0 with $a_0 = 0, a_1 = 0, a_2 = 2, a_3 = 7$, and so on. We call the async scatter function with the feature array over the model axis.

[15]:
```
scatter_model_fn = shard_map(
    lambda x: async_scatter(x, axis_name=config.model_axis_name),
```

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```
    mesh=mesh,
    in_specs=P(config.data_axis_name, config.model_axis_name),
    out_specs=P(config.data_axis_name, config.model_axis_name),
)
xs = np.split(x, x.shape[-1], axis=-1)
y_scatter_model = scatter_model_fn(xs)
for idx in range(jax.local_device_count()):
    print(f"Device {idx}: {y_scatter_model.reshape(-1, y_scatter_model.shape[-1])[idx]}")
```

```
Device 0: [15]
Device 1: [21]
Device 2: [23]
Device 3: [20]
Device 4: [19]
Device 5: [28]
Device 6: [15]
Device 7: [14]
```

To check the result, we can do the operation by hand using the figure above, and get:

- Output on device 0: $a_3 + b_0 + c_1 + d_2 = 4 + 4 + 0 + 7 = 15$
- Output on device 1: $a_2 + b_3 + c_0 + d_1 = 6 + 6 + 2 + 7 = 21$
- Output on device 2: $a_1 + b_2 + c_3 + d_0 = 7 + 0 + 9 + 7 = 23$
- Output on device 3: $a_0 + b_1 + c_2 + d_3 = 0 + 8 + 5 + 7 = 20$

The result is identical to the expected output, suggesting we have successfully implemented the async scatter strategy.

Bidirectional Communication

Similar to the async gather strategy, we can also communicate the features in both directions at the same time by splitting the features over the hidden dimension. This way, we can ensure that we always communicate in both directions, and may improve efficiency. We implement this strategy below.

[16]:
```
def async_scatter_split(xs: Sequence[PyTree], axis_name: str) -> PyTree:
    """Scatter sum using ring permutation with features split for bidirectional␣
↪communication.

    Args:
        xs: The inputs to scatter sum. The length of the list should match the size of␣
↪the axis.
        axis_name: The axis name to scatter sum along.

    Returns:
        The scatter summed output.
    """

    def _split(x: PyTree) -> Tuple[PyTree, PyTree]:
        return (
            jax.tree_map(lambda x: x[..., : x.shape[-1] // 2], x),
            jax.tree_map(lambda x: x[..., x.shape[-1] // 2 :], x),
        )
```

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```
    tp_size = jax.lax.psum(1, axis_name)
    assert (
        len(xs) == tp_size
    ), f"Number of shards needs to match axis size, but got {len(xs)} with {axis_name}␣
↪axis size {tp_size}."
    shift_perm_up = [(j, (j + 1) % tp_size) for j in range(tp_size)]
    shift_perm_down = [(j, (j - 1) % tp_size) for j in range(tp_size)]
    y_up, y_down = _split(xs[0])
    for x in xs[1:]:
        y_up = jax.lax.ppermute(y_up, axis_name, perm=shift_perm_up)
        y_down = jax.lax.ppermute(y_down, axis_name, perm=shift_perm_down)
        x_up, x_down = _split(x)
        y_up = jax.tree_map(jnp.add, y_up, x_up)
        y_down = jax.tree_map(jnp.add, y_down, x_down)
    return jax.tree_map(lambda y1, y2: jnp.concatenate([y1, y2], axis=-1), y_up, y_down)
```

The first half of the features are processed in the same way as in the unidirectional version with `shift_up=True`, and the second half of the features are processed in the same way as in the unidirectional version with `shift_up=False`. We can verify this by repeating our example array over the last axis and check the output.

[17]:
```
scatter_model_fn = shard_map(
    lambda x: async_scatter_split(x, axis_name=config.model_axis_name),
    mesh=mesh,
    in_specs=P(config.data_axis_name, config.model_axis_name),
    out_specs=P(config.data_axis_name, config.model_axis_name),
)
x_double = np.repeat(x, 2, axis=-1)
xs = np.split(x_double, x.shape[-1], axis=-1)
y_scatter_model = scatter_model_fn(xs)
for idx in range(jax.local_device_count()):
    print(f"Device {idx}: {y_scatter_model.reshape(-1, y_scatter_model.shape[-1])[idx]}")
```

```
Device 0: [15 11]
Device 1: [21 18]
Device 2: [23 27]
Device 3: [20 23]
Device 4: [19 16]
Device 5: [28 22]
Device 6: [15 18]
Device 7: [14 20]
```

The first feature dimension is indeed the same as in the unidirectional version above. We can verify the second feature dimension by hand or running the previous example with `shift_up=False`. The result is identical to the expected output, suggesting we have successfully implemented the bidirectional async scatter strategy. Due to the different setup and need for more operations, we will focus on the unidirectional scatter version in the following, but the bidirectional version can be more efficient in some cases.

Asynchronous Linear Layer

We can now implement the async gather and scatter strategies in a linear layer, as for example used in the ViT-22b model. Both follow very closely the asynchronous communication functions we implemented above, just with added computation.

In the gather strategy, we start with computing the output with respect to the current features (i.e. $A_{i,i}x_i$ on device i), since they are already available on each device. At the same time, we communicate the features to the next device. Once the features are communicated and we finished the computation, we can start computing the output with respect to the communicated features, and continue the process. All outputs are summed to obtain the final output. This process is visualized below (figure credit: Dehghani et al., 2023).

In the scatter strategy, we start with computing the output that will require the longest path of communication. Once computed, we send the output to the next device, and calculate the next output. We then sum the output with the communicated features, and continue the process. As the final output, we compute the features for the current device. This process is visualized below (figure credit: Dehghani et al., 2023).

We extend our previous `TPDense` class to implement the asynchronous version. Instead of applying the dense layer only once, we apply it in a loop over the sub-features in the two strategies. We let the compiler figure out when to optimally schedule the individual communication and computation operations, which is expected to be close to our computation diagrams above. By splitting the dense layer into multiple smaller layers, each weight matrix will be of size $d_y/\text{num\_devices} \times d_x/\text{num\_devices}$, such that we may need to adjust the kernel differently (e.g. fan-in adjustment in both scatter and gather). Further, we ensure that for each final output feature, we only use a single bias parameter to remain consistent with the non-parallelised models.

[18]:
```
class TPAsyncDense(nn.Module):
    """Tensor-Parallel Dense Layer with Asynchronous Communication.

    This layer can be used to perform a dense layer with Tensor Parallelism support, and␣
↪overlaps communication with computation whenever possible.

    Attributes:
        dense_fn: Constructor function of the dense layer to use. Needs to support the␣
↪keyword argument `kernel_init`.
        model_axis_name: The name of the model axis.
        tp_mode: The Tensor Parallelism mode to use. Can be "scatter", "gather", or "none
↪".
        kernel_init: The initializer to use for the kernel of the dense layer.
        kernel_init_adjustment: The adjustment factor to use for the kernel initializer.
        dense_name: The name of the dense layer module.
        use_bidirectional_gather: Whether to use bidirectional or unidirectional gather␣
↪over the device ring for communication.
    """

    dense_fn: Any
    model_axis_name: str
    tp_mode: Literal["scatter", "gather", "none"] = "none"
    kernel_init: Callable = nn.initializers.lecun_normal()
    kernel_init_adjustment: float = 1.0
    dense_name: str = "module"
    use_bidirectional_gather: bool = True
```

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```
    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.model_axis_name)
        tp_mode = self.tp_mode if tp_size > 1 else "none"

        dense_fn = functools.partial(
            ModelParallelismWrapper,
            model_axis_name=self.model_axis_name,
            module_fn=functools.partial(
                self.dense_fn,
                kernel_init=scale_init(self.kernel_init, self.kernel_init_adjustment),
            ),
            name=self.dense_name,
        )

        if tp_mode == "none":
            y = self.dense_fn(kernel_init=self.kernel_init, name="shard_0")(x)
        elif tp_mode == "gather":
            # Async gathering of all inputs.
            async_op = (
                async_gather_bidirectional if self.use_bidirectional_gather else async_
↪gather
            )
            xs = async_op(x, axis_name=self.model_axis_name)
            # Compute output per input (scheduled as communication makes inputs␣
↪available).
            ys = [
                dense_fn(
                    module_kwargs={
                        "use_bias": (i == 0)
                    },  # Only need a single per final output feature.
                    name=f"shard_{i}",
                )(x)
                for i, x in enumerate(xs)
            ]
            # Final sum of all outputs.
            y = jax.tree_map(lambda *args: sum(args), *ys)
        elif tp_mode == "scatter":
            # Calculate all outputs per device.
            ys = [
                dense_fn(
                    module_kwargs={
                        "use_bias": (i == 0)
                    },  # Only need a single per final output feature.
                    name=f"shard_{i}",
                )(x)
                for i in range(tp_size)
            ]
            # Async scatter sum of all outputs (communication already starts after first␣
↪output is ready).
            y = async_scatter(ys, axis_name=self.model_axis_name)
        else:
```

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```
            raise ValueError(f"Unknown Tensor Parallel mode: {tp_mode}")
        return y
```

Now, let's use these asynchronous linear layers to improve the efficiency of our MLP blocks. We will implement the same MLP block as before, but replace the `TPDense` layers with `TPAsyncDense` layers. We will use the gather strategy for the first linear layer, and the scatter strategy for the second linear layer. For the input layer, we also need to adjust the initialization by scaling the values by $\sqrt{1/\text{num\_devices}}$, since the input to each layer will be $1/\text{num\_devices}$ of the full feature size.

While the splitting of the dense layer into multiple smaller layers works without problems, we also need to apply other layers in the same way. For instance, the activation function can be applied independently on each input, such that we do not need to adjust for it. However, the normalization layer commonly contains statistics that are computed over the full feature size, and we cannot do it anymore within the input layer (in the non-async implementation, the gather strategy allowed for it). Instead, we first apply the normalization layer and compute the statistics across devices. Luckily, in Flax, this is already supported by passing an `axis_name` to the normalization layer (see e.g. the docs for RMSNorm). We only need to wrap it in a model parallelism wrapper since each device will have scaling parameters for its respective features. This gives us the same result as if we had computed the statistics over the full feature size on a single device, and we can continue with the rest of the operations. Let's implement this norm class below.

[19]:
```
class TPNorm(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        x = ModelParallelismWrapper(
            model_axis_name=self.config.model_axis_name,
            module_fn=functools.partial(
                nn.RMSNorm,
                dtype=self.config.dtype,
                axis_name=self.config.model_axis_name,
            ),
            name="norm",
        )(x)
        return x
```

We use this normalization layer in the `TPAsyncMLPBlock` class below to define the whole block.

[20]:
```
class TPAsyncMLPBlock(nn.Module):
    config: ConfigDict
    train: bool

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        input_features = x.shape[-1]
        # Normalize across devices before the input layer.
        x = TPNorm(config=self.config, name="pre_norm")(x)
        # Input dense layer with async gather.
        x = TPAsyncDense(
            dense_fn=functools.partial(
                MLPBlockInput,
                config=self.config,
                features=self.config.hidden_size * self.config.mlp_expansion // tp_size,
```

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```
                use_norm=False,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="gather",
            kernel_init_adjustment=tp_size**-0.5,
            name="input",
        )(x)
        # Output dense layer with async scatter.
        x = TPAsyncDense(
            dense_fn=functools.partial(
                MLPBlockOutput,
                config=self.config,
                features=input_features,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="scatter",
            kernel_init_adjustment=tp_size**-0.5,
            name="output",
        )(x)
        return x
```

Initialization

The rest of the model is identical to the non-async version. Let's first create the classifier model with the new async MLP block. Note that the input and output layer do not require the async strategy. The input layer has already features gathered, such that no communication is needed. For the output, we require all outputs to be available on all devices (or at least device), which we ensure via `jax.lax.psum` and requires blocking communications.

[21]:
```
model_tp_async = TPClassifier(config.model, block_class=TPAsyncMLPBlock)
optimizer = optax.adamw(learning_rate=config.optimizer.learning_rate)
```

We reuse the same initialization function with the new model.

[22]:
```
init_tp_async_fn = shard_map(
    functools.partial(init_tp, model=model_tp_async, optimizer=optimizer),
    mesh,
    in_specs=(P(), P(config.data_axis_name)),
    out_specs=P(),
    check_rep=False,
)
state_tp_async_shapes = jax.eval_shape(init_tp_async_fn, model_init_rng, batch.inputs)
state_tp_async_specs = nn.get_partition_spec(state_tp_async_shapes)
```

Let's inspect how the async layers have impacted the parameter sharding in the MLP block.

[23]:
```
pprint(state_tp_async_specs.params)
```

```
{'input_layer': {'module': {'sharded': {'bias': PartitionSpec('model', None),
                                        'kernel': PartitionSpec('model', None, None)}}},
 'mlp': {'block': {'input': {'shard_0': {'sharded': {'dense': {'bias':␣
↪PartitionSpec(None, 'model', None),
                                                               'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}},
```

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```
                              'shard_1': {'sharded': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}},
                              'shard_2': {'sharded': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}},
                              'shard_3': {'sharded': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}}},
                    'output': {'shard_0': {'sharded': {'dense': {'bias':␣
↪PartitionSpec(None, 'model', None),
                                                                 'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}},
                               'shard_1': {'sharded': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}},
                               'shard_2': {'sharded': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}},
                               'shard_3': {'sharded': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, None)}}}},
                    'pre_norm': {'norm': {'sharded': {'scale': PartitionSpec(None, 'model
↪', None)}}}}},
 'output_layer': {'module': {'sharded': {'bias': PartitionSpec('model', None),
                                         'kernel': PartitionSpec('model', None, None)}}}}
```

Each input and output layer of the MLP block contains several sub-modules now, one per smaller dense layer (equivalent to number of devices). Each has a kernel with the same sharding as before, but only the first layer has a bias term. The normalization layer is now outside of the input layer, with the same sharding as before. The input and output layers of the whole model did not change.

We can now continue with the initialization.

[24]:
```
init_tp_async_fn = jax.jit(
    shard_map(
        functools.partial(init_tp, model=model_tp_async, optimizer=optimizer),
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_tp_async_specs,
        check_rep=False,
    ),
)
state_tp_async = init_tp_async_fn(model_init_rng, batch.inputs)
```

Let's also inspect the parameter shapes to ensure the initialization worked as expected.

[25]:
```
print("TP Parameters - MLP Layers Pre-Norm")
pprint(
    jax.tree_map(
        lambda x: x.shape, state_tp_async.params["mlp"]["block"]["pre_norm"]["norm"][
↪"sharded"]
    )
)
print()
print("TP Parameters - MLP Layers Input")
pprint(
    jax.tree_map(
        lambda x: x.shape, state_tp_async.params["mlp"]["block"]["input"]["shard_0"][
↪"sharded"]
```

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```
    )
)
print()
print("TP Parameters - MLP Layers Output")
pprint(
    jax.tree_map(
        lambda x: x.shape, state_tp_async.params["mlp"]["block"]["output"]["shard_0"][
↪"sharded"]
    )
)
```

```
TP Parameters - MLP Layers Pre-Norm
{'scale': Partitioned(value=(3, 4, 128),
                      names=(None, 'model', None),
                      mesh=None)}

TP Parameters - MLP Layers Input
{'dense': {'bias': Partitioned(value=(3, 4, 128),
                               names=(None, 'model', None),
                               mesh=None),
           'kernel': Partitioned(value=(3, 4, 128, 128),
                                 names=(None, 'model', None, None),
                                 mesh=None)}}

TP Parameters - MLP Layers Output
{'dense': {'bias': Partitioned(value=(3, 4, 128),
                               names=(None, 'model', None),
                               mesh=None),
           'kernel': Partitioned(value=(3, 4, 128, 128),
                                 names=(None, 'model', None, None),
                                 mesh=None)}}
```

Each dense layer has now a smaller kernel ($512/4 = 128$), which is why we needed the adjusted initialization schemes. The scale parameter of the pre-norm also has the same sharding, such that the parameters are consistent with the expected shapes.

Training

We can now train the model with the async MLP block. The training loop is identical to the non-async version, and we expect the model to learn the task with high accuracy.

[26]:
```
train_step_tp_async_fn = jax.jit(
    shard_map(
        functools.partial(train_step_tp, config=config),
        mesh,
        in_specs=(state_tp_async_specs, P(), P(config.data_axis_name)),
        out_specs=(state_tp_async_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
state_shapes, metric_shapes = jax.eval_shape(
```

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```
    train_step_tp_async_fn,
    state_tp_async,
    None,
    batch,
)
metrics_tp_async = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_tp_async, metrics_tp_async = train_step_tp_async_fn(state_tp_async, metrics_tp_
↪async, batch)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[1,128]),
↪ ShapedArray(float32[1,784,128]), ShapedArray(float32[3,1,128]), ShapedArray(float32[3,
↪1,128,128]), ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128]), ShapedArray(float32[1,10]), ShapedArray(float32[1,128,
↪10]), ShapedArray(float32[1,128]), ShapedArray(float32[1,784,128]),␣
↪ShapedArray(float32[3,1,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128]), ShapedArray(float32[1,10]), ShapedArray(float32[1,128,
↪10]), ShapedArray(float32[1,128]), ShapedArray(float32[1,784,128]),␣
↪ShapedArray(float32[3,1,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128,128]), ShapedArray(float32[3,1,128,128]),␣
↪ShapedArray(float32[3,1,128]), ShapedArray(float32[1,10]), ShapedArray(float32[1,128,
↪10]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

We train the model again for 15 steps and print the final loss and accuracy.

[27]:
```
for _ in range(15):
    state_tp_async, metrics_tp_async = train_step_tp_async_fn(
        state_tp_async, metrics_tp_async, batch
    )
final_metrics_tp_async = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype),␣
↪metric_shapes)
state_tp_async, final_metrics_tp_async = train_step_tp_async_fn(
    state_tp_async, final_metrics_tp_async, batch
)
print_metrics(final_metrics_tp_async, title="Final Metrics - Tensor Parallelism Async")
```

```
 Final Metrics - Tensor Parallelism Async
accuracy: 1.000000
loss: 0.000022
```

As we expected, the model is able to learn the task with high accuracy. We have successfully implemented the async

gather and scatter strategies in our linear layer, and improved the efficiency of our model. We can now continue to the next section, where we discuss the implementation of a full transformer model with tensor parallelism and fully-sharded data parallelism.

4.13.3 Intermediate Summary

In this notebook, we discussed the principles of tensor parallelism with compute-communication overlap. We implemented the asynchronous communication patterns of gather and scatter, and applied them to a linear layer distributed over multiple devices. We then used these layers to implement an asynchronous MLP block, and trained a model with it. In the next notebook, we will discuss how to implement tensor parallelism in a transformer model. Furthermore, we will profile the model to show the efficiency of the async communication patterns in such models.

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4.14 Part 4.3: Transformers with Tensor Parallelism

Filled notebook:

Author: Phillip Lippe

In the previous two parts on tensor parallelism, we have seen how to parallelize simple models across multiple GPUs. In this part, we will see how to parallelize a transformer model across multiple GPUs. Transformer models are a common use case for tensor parallelism, as they are widely used in large-scale models for natural language processing and computer vision. For instance, it is the key architecture in GPT-4, Gemini, PALM, and ViT-22b. Hence, we will review the specific challenges of parallelizing transformers, how to address them, and how to maximize the efficiency of the parallelization. In the end, we will profile a 1-billion parameter model on 8 GPUs and discuss potential bottlenecks remaining.

4.14.1 Prerequisites

First, let's start with setting up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = [
    "single_gpu.py",
    "data_parallel.py",
    "pipeline_parallel.py",
    "tensor_parallel.py",
    "tensor_parallel_async.py",
    "utils.py",
]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

As before, we simulate 8 devices on CPU to demonstrate the parallelism without the need for multiple GPUs or TPUs. If you are running on your local machine and have multiple GPUs available, you can comment out the lines below.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

We now import our standard libraries.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
import numpy as np
import optax
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict
from tqdm.auto import tqdm

PyTree = Any
Parameter = jax.Array | nn.Partitioned
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We also import the utility functions from the previous notebooks. Our notebook will rely on the `ModelParallelismWrapper` from the pipeline parallelism notebook. If you are not familiar with it, it is recommended to look at the implementation of this module before continuing.

[4]:
```
from data_parallel import fold_rng_over_axis, shard_module_params
from pipeline_parallel import ModelParallelismWrapper
from single_gpu import Batch, TrainState, get_num_params, print_metrics
from tensor_parallel import MLPBlockInput, MLPBlockOutput, train_step_tp
from tensor_parallel_async import TPAsyncDense, TPAsyncMLPBlock, TPNorm
```

4.14.2 Tensor Parallelism in Transformer Models

In this section, we will implement a transformer model with tensor parallelism and fully-sharded data parallelism. We will use the same async linear layer as before, but extend it to the full transformer model, including the attention layers. In that, we show common implementation strategies in tensor parallelism for transformers specifically.

Attention Layer

The attention layer is the key component of the transformer model, and is used to model the interactions between different input tokens. It consists of a query, key, and value projection, followed by a scaled dot-product attention, and a final linear layer. The computation graph of the attention layer is visualized below (figure credit - Vaswani et al., 2017).

Splitting the query, key and value over hidden dimension would require several communications between devices, since all hidden dimensions are needed for calculating the attention scores. This would be inefficient, and we would like to avoid it if possible. Instead, we can exploit another key aspect of the attention layers in transformer models: multi-head attention. In multi-head attention, we project the input features into multiple heads, and perform the attention computation independently on each head. We then concatenate the outputs of each head, and project the concatenated output back to the original feature size. To reduce communication, we therefore split the attention calculation over the heads across devices, and only need to communicate the original input and the output of the individual heads. This becomes very similar to the MLP block we implemented earlier, and we can use the same async linear layers to implement the attention layer.

Let's start with implementing the input layer. We first need to project the input features into the query, key, and value space, which we do with individual linear layer. The `DenseGeneral` layer allows us to directly output the reshaped array of `[..., num_heads, head_dim]` instead of a manual reshape. Following PALM and ViT-22b, we do not apply a bias term to the projection layers. Further, the ViT-22b model normalizes the query and key features before the attention computation. This prevents instability at large scale where the attention logits can become very large and cause a close-to one-hot attention distribution very early in the training. We adopt this normalization in our implementation below.

[5]:
```
class QKVDense(nn.Module):
    config: ConfigDict
    num_heads: int
    head_dim: int
    kernel_init: Callable
    use_bias: bool = False

    @nn.compact
    def __call__(self, x: jax.Array) -> Tuple[jax.Array, jax.Array, jax.Array]:
        q = nn.DenseGeneral(
            (self.num_heads, self.head_dim),
            kernel_init=self.kernel_init,
            use_bias=False,
            dtype=self.config.dtype,
            name="query",
        )(x)
        k = nn.DenseGeneral(
            (self.num_heads, self.head_dim),
            kernel_init=self.kernel_init,
            use_bias=False,
            dtype=self.config.dtype,
            name="key",
        )(x)
        v = nn.DenseGeneral(
            (self.num_heads, self.head_dim),
            kernel_init=self.kernel_init,
            use_bias=False,
            dtype=self.config.dtype,
```

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```
            name="value",
        )(x)

        if self.config.normalize_qk:
            q = nn.RMSNorm(
                dtype=self.config.dtype,
                name="query_norm",
            )(q)
            k = nn.RMSNorm(
                dtype=self.config.dtype,
                name="key_norm",
            )(k)
        return q, k, v
```

Since each device will calculate an independent set of heads, the dot product attention does not need to parallelized. Instead, we can simply reuse our implementation from the first notebook for single-GPU usage, where we adjusted the attention calculation to higher precision for numerical stability of the attention softmax.

[6]:
```
def dot_product_attention(
    query: jax.Array,
    key: jax.Array,
    value: jax.Array,
    mask: jax.Array | None,
    softmax_dtype: jnp.dtype = jnp.float32,
):
    """Dot-product attention.

    Follows the setup of https://flax.readthedocs.io/en/latest/api_reference/flax.linen/
↪layers.html#flax.linen.dot_product_attention,
    but supports switch to float32 for numerical stability during softmax.

    Args:
        query: The query array, shape [..., num queries, num heads, hidden size].
        key: The key array, shape [..., num keys, num heads, hidden size].
        value: The value array, shape [..., num keys, num heads, hidden size].
        mask: The boolean mask array (0 for masked values, 1 for non-masked). If None,␣
↪no masking is applied.
        softmax_dtype: The dtype to use for the softmax operation.

    Returns:
        The attention output array, shape [..., num queries, num heads, hidden size].
    """
    num_features = query.shape[-1]
    dtype = query.dtype
    scale = num_features**-0.5
    query = query * scale
    # Switch dtype right before the dot-product for numerical stability.
    query = query.astype(softmax_dtype)
    key = key.astype(softmax_dtype)
    weights = jnp.einsum("...qhd,...khd->...hqk", query, key)
    if mask is not None:
        weights = jnp.where(mask, weights, jnp.finfo(softmax_dtype).min)
```

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```
    weights = nn.softmax(weights, axis=-1)
    # After softmax, switch back to the original dtype
    weights = weights.astype(dtype)
    new_vals = jnp.einsum("...hqk,...khd->...qhd", weights, value)
    new_vals = new_vals.astype(dtype)
    return new_vals
```

Finally, we apply the output layer, which is a linear layer with the same feature size as the input. Since the input will be a tensor of shape `[..., num_heads, head_dim]`, we apply the dense layer to the last two axis. This is equivalent to flattening the array over the last two dimensions before applying the dense layer.

[7]:
```
class AttnOut(nn.Module):
    config: ConfigDict
    features: int
    kernel_init: Callable = nn.initializers.lecun_normal()
    use_bias: bool = True

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        x = nn.DenseGeneral(
            features=self.features,
            axis=(-2, -1),
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            dtype=self.config.dtype,
            name="out",
        )(x)
        return x
```

With these submodules in place, we can combine them to a full tensor-parallel attention layer. We first apply a normalization layer to the input, and then wrap the qkv input layer in an async dense layer. Each module application calculates all three q, k, and v arrays while only requiring a single communication of the input features, which is more efficient than using three separate async dense layers for the three outputs. Each device will calculate an independent set of heads, such that we split the dense layers over heads. We then apply the dot-product attention, which is done independently on each device. Finally, we apply the output layer, which is an async dense layer with the scatter strategy, as in the MLP block.

[8]:
```
class TPMultiHeadAttn(nn.Module):
    config: ConfigDict
    train: bool
    mask: jax.Array | None = None

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        input_features = x.shape[-1]
        head_dim = self.config.head_dim
        num_heads = self.config.num_heads
        # Normalize across devices before the input layer.
        x = TPNorm(config=self.config, name="pre_norm")(x)
        # Calculate Q, K, V using async dense layers.
        q, k, v = TPAsyncDense(
```

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```
            dense_fn=functools.partial(
                QKVDense,
                config=self.config,
                num_heads=num_heads // tp_size,
                head_dim=head_dim,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="gather",
            kernel_init_adjustment=tp_size**-0.5,
            name="qkv",
        )(x)
        # Attention calculation.
        x = dot_product_attention(q, k, v, self.mask)
        # Output layer with async scatter.
        x = TPAsyncDense(
            dense_fn=functools.partial(
                AttnOut,
                config=self.config,
                features=input_features,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="scatter",
            kernel_init_adjustment=tp_size**-0.5,
            name="out",
        )(x)
        return x
```

Transformer Block

With both the attention and MLP block implemented, we can now combine them to a full transformer block. As seen in our earlier notebooks, we may want to remat individual blocks to reduce the memory footprint, as well as shard the parameters across the data axis. We can do this by wrapping the attention and MLP block in a `remat` and `shard_module_params` function, respectively. We do this below, and will specify our intended strategy in the config.

[9]:
```
def prepare_module(
    layer: Callable[..., nn.Module], layer_name: str, config: ConfigDict
) -> Callable[..., nn.Module]:
    """Remats and shards layer if needed.

    This function wraps the layer function in a remat and/or sharding function if its␣
↪layer name is present in the remat and fsdp configuration, respectively.

    Args:
        layer: The layer to prepare.
        layer_name: The name of the layer.
        config: The configuration to use.

    Returns:
        The layer with remat and sharding applied if needed.
    """
    # Shard parameters over model axis. Performed before remat, such that the gathered␣
↪parameters would not be kept under remat.
```

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```
    if config.get("fsdp", None) is not None and layer_name in config.fsdp.modules:
        layer = shard_module_params(
            layer, axis_name=config.data_axis_name, min_weight_size=config.fsdp.min_
↪weight_size
        )
    if config.get("remat", None) is not None and layer_name in config.remat:
        layer = nn.remat(layer, prevent_cse=False)
    return layer
```

We use this wrapper to define the full transformer block below. On an input `x`, we first apply an attention layer, and then apply a feed-forward layer. The implementation is the same as for the single device case, just that we use tensor-parallel block versions for the attention and MLP block.

[10]:
```
class TPTransformerBlock(nn.Module):
    config: ConfigDict
    train: bool
    mask: jax.Array | None = None

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        # Attention layer
        attn_layer = prepare_module(TPMultiHeadAttn, "Attn", self.config)
        attn_out = attn_layer(
            config=self.config,
            train=self.train,
            mask=self.mask,
            name="attn",
        )(x)
        attn_out = nn.Dropout(rate=self.config.dropout_rate, deterministic=not self.
↪train)(
            attn_out
        )
        x = x + attn_out
        # MLP layer
        mlp_layer = prepare_module(TPAsyncMLPBlock, "MLP", self.config)
        mlp_out = mlp_layer(
            config=self.config,
            train=self.train,
            name="mlp",
        )(x)
        mlp_out = nn.Dropout(rate=self.config.dropout_rate, deterministic=not self.
↪train)(mlp_out)
        x = x + mlp_out
        return x
```

Parallel Blocks

To optimize the efficiency of our model on a large device mesh, we may also consider changing the architecture to further increase the overlap of communication and computation. For instance, a common efficiency trick introduced in Wang and Komatsuzaki, 2021 is to parallelize the attention and MLP block, as shown below in the ViT-22b (figure credit: Dehghani et al., 2023).

The attention and the MLP work on the same input, and we follow them on two separate computation paths before combining them in the end. The main benefit of this parallelization is that we only need to communicate the input x once and can then perform the attention and the MLP block independently. Furthermore, only one normalization layer with blocking communication is needed, and we can reuse the same normalized values for both paths.

One should note though, by changing the architecture, we may also influence the expressiveness of the model. For instance, the attention and the MLP block may not be able to interact with each other as closely as in the sequential version. For small models, this can have a significant impact on the model's performance. However, for large models, the impact is usually much less significant since we have a lot of sequential layers (often well more than 20), and the parallelized version can be more efficient.

Implementing the parallel block only requires minor changes to our current implementation and combine the two paths in the individual blocks. We start with implementing the input layer, which simply calls the `MLPBlockInput` and the `QKVDense` on the same input.

[11]:
```
class QKVMLPDense(nn.Module):
    config: ConfigDict
    num_heads: int
    head_dim: int
    mlp_dim: int
    kernel_init: Callable
    use_bias: bool = False

    @nn.compact
    def __call__(self, x: jax.Array) -> Tuple[jax.Array, Tuple[jax.Array, jax.Array, jax.
↪Array]]:
        h = MLPBlockInput(
            config=self.config,
            features=self.mlp_dim,
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            use_norm=False,
            name="mlp",
        )(x)
        q, k, v = QKVDense(
            config=self.config,
            num_heads=self.num_heads,
            head_dim=self.head_dim,
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            name="qkv",
        )(x)
        return h, (q, k, v)
```

In the output layer, we perform the same combination of layers. Taking two inputs, we apply the `MLPBlockOutput` and the `OutputDense` on their respective inputs. Since both share the same communication pattern, we can use the same async scatter strategy for both and make better use of the communication bandwidth.

[12]:
```python
class AttnMLPOut(nn.Module):
    config: ConfigDict
    features: int
    kernel_init: Callable = nn.initializers.lecun_normal()
    use_bias: bool = True

    @nn.compact
    def __call__(self, x: Tuple[jax.Array, jax.Array]) -> jax.Array:
        mlp_h, attn_v = x
        mlp_out = MLPBlockOutput(
            config=self.config,
            features=self.features,
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            name="mlp",
        )(mlp_h)
        attn_out = AttnOut(
            config=self.config,
            features=self.features,
            kernel_init=self.kernel_init,
            use_bias=self.use_bias,
            name="attn",
        )(attn_v)
        out = mlp_out + attn_out
        return out
```

Let's combine the input and output layer to the full parallel block below. We start with normalizing the input x, which only has to be done once for the whole block. We then apply the input layer with an async gather strategy, and the attention layer on the qkv outputs. Then, we apply the output layer with an async scatter strategy, apply dropout to the two outputs. Finally, we combine all outputs, leading to the final output of the parallel block.

[13]:
```python
class TPTransformerParallelBlock(nn.Module):
    config: ConfigDict
    train: bool
    mask: jax.Array | None = None

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        input_features = x.shape[-1]
        residual = x
        # Normalize across devices before the input layer.
        x = TPNorm(config=self.config, name="pre_norm")(x)
        # Calculate MLP hidden and q, k, v using async dense layers.
        h, (q, k, v) = TPAsyncDense(
            dense_fn=functools.partial(
                QKVMLPDense,
                config=self.config,
                num_heads=self.config.num_heads // tp_size,
                head_dim=self.config.head_dim,
                mlp_dim=self.config.hidden_size * self.config.mlp_expansion // tp_size,
            ),
            model_axis_name=self.config.model_axis_name,
```

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```
            tp_mode="gather",
            kernel_init_adjustment=tp_size**-0.5,
            name="hqkv",
        )(x)
        # Attention calculation.
        v = dot_product_attention(q, k, v, self.mask)
        # MLP and attention layer with async scatter.
        block_out = TPAsyncDense(
            dense_fn=functools.partial(
                AttnMLPOut,
                config=self.config,
                features=input_features,
            ),
            model_axis_name=self.config.model_axis_name,
            tp_mode="scatter",
            kernel_init_adjustment=tp_size**-0.5,
            name="out",
        )((h, v))
        # Apply dropout and add residual.
        block_out = nn.Dropout(rate=self.config.dropout_rate, deterministic=not self.
↪train)(
            block_out
        )
        out = residual + block_out
        return out
```

Both blocks can be used in the transformer model, and we may select the block type based on the size of the model, computation cost, expressiveness, and other factors. For the example in this notebook, we will use the parallel block.

Full Model

We can now combine the parallel block to a full transformer model. We will use the same config as before, and allow for wrapping the whole block in a `remat` and `shard_module_params` function to optimize the memory footprint and parameter sharding. Note that we usually only want to remat and shard parameters in either the internal modules or the full model, but not both (especially the module sharding only works once). For the parallel version, since both internal modules are applied at the same time, we would remat and shard the whole block. For a more aggressive remat strategy, we could also apply a `nn.remat_scan` and keep the output of only every second block, which would reduce the memory footprint further, but considerably increases computation time. Hence, we stick with the per-module remat strategy in this notebook.

[14]:
```
class TransformerBackbone(nn.Module):
    config: ConfigDict
    train: bool
    mask: jax.Array | None = None
    block_fn: Any = TPTransformerBlock

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        block_fn = prepare_module(
            self.block_fn,
            "Block",
```

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```
            self.config,
        )
        block = block_fn(config=self.config, train=self.train, mask=self.mask, name=
↪"block")
        # Scan version
        x, _ = nn.scan(
            lambda module, carry, _: (module(carry), None),
            variable_axes={"params": 0},
            split_rngs={"params": True, "dropout": True},
            length=self.config.num_layers,
            metadata_params={
                "partition_name": None
            },  # We do not need to partition over the layer axis.
        )(block, x, ())
        return x
```

Besides the transformer blocks, we also need to implement the input and output layers. In this example, we focus on a transformer for natural language processing, such that the input layer consists of an embedding layer and a positional encoding layer. For efficiency, we will also want to parallelize them across model devices.

For the positional encoding, we consider the two common variants of learned embeddings and fixed sinusoidal embeddings. For the learned embeddings, we do not require any adjustment to support tensor parallelism, since the model parallelism wrapper will split the parameters accordingly across devices. For the fixed sinusoidal embeddings, we need to determine the device index we are on, and calculate the corresponding part of the positional encodings. We adapt our previous single-GPU implementation to support tensor parallelism below.

[15]:
```
class PositionalEncoding(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        tp_index = jax.lax.axis_index(self.config.model_axis_name)
        seq_len, num_feats = x.shape[-2:]
        if self.config.positional_encoding_type == "learned":
            pos_emb = self.param(
                "pos_emb",
                nn.initializers.normal(stddev=0.02),
                (seq_len, num_feats),
            )
        elif self.config.positional_encoding_type == "sinusoidal":
            # Adjusted to multi-device setting.
            position = jnp.arange(0, seq_len, dtype=jnp.float32)[:, None]
            div_term = jnp.exp(
                jnp.arange(tp_index * num_feats, (tp_index + 1) * num_feats, 2)
                * (-np.log(10000.0) / (tp_size * num_feats))
            )
            pos_emb = jnp.stack(
                [jnp.sin(position * div_term), jnp.cos(position * div_term)], axis=-1
            )
            pos_emb = jnp.reshape(pos_emb, (seq_len, num_feats))
        else:
            raise ValueError(
```

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```
                f"Unknown positional encoding type: {self.config.positional_encoding_
↪type}"
            )
        pos_emb = pos_emb.astype(
            x.dtype
        )  # Cast to the same dtype as the input, e.g. support bfloat16.
        pos_emb = jnp.expand_dims(pos_emb, axis=range(x.ndim - 2))
        x = x + pos_emb
        return x
```

For the embedding layer, we simply split the features of the embedding matrix across the model axis, and apply the embedding layer on the input tokens. Each device will have the same input indices, such that we end up with the partitioned features over model devices as intended. We then apply our previous positional encoding layer to add the positional information to the embeddings.

[16]:
```
class InputEmbedding(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        tp_size = jax.lax.psum(1, self.config.model_axis_name)
        x = nn.Embed(
            num_embeddings=self.config.vocab_size,
            features=self.config.hidden_size // tp_size,
            embedding_init=nn.initializers.normal(stddev=1.0),
            dtype=self.config.dtype,
            name="token_emb",
        )(x)
        x = PositionalEncoding(config=self.config, name="pos_enc")(x)
        return x
```

We can now wrap the input layer in a model parallelism wrapper to parallelize it and initialize different parameters across model devices.

[17]:
```
class TPInputEmbedding(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        return ModelParallelismWrapper(
            model_axis_name=self.config.model_axis_name,
            module_fn=functools.partial(InputEmbedding, config=self.config),
            name="module",
        )(x)
```

The output layer consists of a normalization layer with subsequent linear layer. In our previous simple model, we decided to give all devices the same outputs by summing the outputs with `jax.lax.psum` instead of scattering. We could do the same here, but it may not be the most efficient way to handle the output. For instance, consider a Transformer with a vocabulary size of 32k, and a batch with size 64 per data device and sequence length 1024. The output per model device would be of shape `(64, 1024, 32k)`, which would be already 4GB per device with bfloat16. However, due to the numerical instability of the softmax operation, we may want to use float32 for the output, which would double the memory footprint. This requires a lot of memory on a single device. Instead, we can switch our strategy in the output layer to sequence parallelism. Before the layer, we gather the input over the feature axis, but split them over

the sequence length. Since each token is independently processed by the output layer over the sequence length, we can parallelize the output layer over the sequence length. This way, we can reduce the memory footprint since each device will only need to process a part of the sequence length, reducing it by a factor of the number of devices. With this strategy, all model devices need to share the same parameters. To again reduce memory footprint, we shard the parameters across the model axis as we do in fully-sharded data parallelism.

We start with an operation that splits the input over the sequence length. Note that we use a slightly inefficient way of switching between the two parallelism strategies, since we need to gather the input over the feature axis and then scatter it over the sequence length. While there are more efficient ways to do this, especially for a large model axis, we use this approach to keep the implementation simple and easy to understand.

[18]:
```
def split_array_over_mesh(x: jax.Array, axis_name: str, split_axis: int) -> jax.Array:
    axis_size = jax.lax.psum(1, axis_name)
    axis_index = jax.lax.axis_index(axis_name)
    slice_size = x.shape[split_axis] // axis_size
    x = jax.lax.dynamic_slice_in_dim(
        x,
        axis_index * slice_size,
        slice_size,
        axis=split_axis,
    )
    return x
```

Now we can implement the output layer module. We first gather over the feature axis, split over the sequence length, and then apply the output layer.Both normalization and dense layer are wrapped in a `shard_module_params` function to shard the parameters across the model axis.

[19]:
```
class TPOutputLayer(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        # Gather outputs over feature dimension and split over sequence length.
        x = jax.lax.all_gather(x, axis_name=self.config.model_axis_name, axis=-1,␣
↪tiled=True)
        x = split_array_over_mesh(x, axis_name=self.config.model_axis_name, split_axis=1)
        # Shard parameters over model axis.
        norm_fn = shard_module_params(
            nn.RMSNorm,
            axis_name=self.config.model_axis_name,
            min_weight_size=self.config.fsdp.min_weight_size,
        )
        dense_fn = shard_module_params(
            nn.Dense,
            axis_name=self.config.model_axis_name,
            min_weight_size=self.config.fsdp.min_weight_size,
        )
        # Apply normalization and output layer.
        x = norm_fn(dtype=self.config.dtype, name="out_norm")(x)
        x = dense_fn(
            features=self.config.num_outputs,
            dtype=jnp.float32,
            name="output_layer",
        )(x)
```

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```
        return x
```

Let's now combine all parts to the full transformer model below. We apply the input layer, the transformer blocks, and the output layer, and return the final output. If the mask is None, we further support the model to be used for autoregressive tasks, such as language modeling, by applying a causal mask to the attention layers.

[20]:
```
class Transformer(nn.Module):
    config: ConfigDict
    block_fn: Any = TPTransformerBlock

    @nn.compact
    def __call__(self, x: jax.Array, train: bool, mask: jax.Array | None = None) -> jax.
↪Array:
        if mask is None and self.config.causal_mask:
            mask = nn.make_causal_mask(x, dtype=jnp.bool_)
        x = TPInputEmbedding(
            config=self.config,
            name="input_embedding",
        )(x)
        x = TransformerBackbone(
            config=self.config,
            train=train,
            mask=mask,
            block_fn=self.block_fn,
            name="backbone",
        )(x)
        x = TPOutputLayer(
            config=self.config,
            name="output_layer",
        )(x)
        return x
```

Initialization

We can now initialize the model with the new transformer implementation. We start with defining a new config below. Feel free to adjust the config to experiment with different parallelization strategies and model sizes. By default, we shard the model parameters over the whole data axis on the outer module. This forces the optimizer states to be sharded, but each device needs the memory for storing the whole parameters. For larger models, we may want to change it to a per-module basis. We also remat the model on a per-module basis to reduce the memory footprint, and apply the parallel block to the transformer blocks. Since this notebook runs on CPU, we keep the model size small to avoid running out of memory and long computation times.

[21]:
```
data_config = ConfigDict(
    dict(
        batch_size=8,
        vocab_size=100,
        seq_len=32,
    )
)
fsdp = ConfigDict(
    dict(
```

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```
        modules=("Transformer",),
        axis_name="data",
        min_weight_size=2**8,
    )
)
model_config = ConfigDict(
    dict(
        hidden_size=256,
        dropout_rate=0.1,
        mlp_expansion=4,
        num_layers=6,
        head_dim=32,
        normalize_qk=True,
        positional_encoding_type="learned",
        parallel_block=True,
        causal_mask=True,
        vocab_size=data_config.vocab_size,
        num_outputs=data_config.vocab_size,
        dtype=jnp.bfloat16,
        data_axis_name="data",
        model_axis_name="model",
        model_axis_size=4,
        remat=("Block",),
        fsdp=fsdp,
    )
)
model_config.num_heads = model_config.hidden_size // model_config.head_dim
optimizer_config = ConfigDict(
    dict(
        learning_rate=1e-3,
        num_minibatches=1,
    )
)
config = ConfigDict(
    dict(
        model=model_config,
        optimizer=optimizer_config,
        data=data_config,
        data_axis_name=model_config.data_axis_name,
        model_axis_name=model_config.model_axis_name,
        model_axis_size=model_config.model_axis_size,
        seed=42,
    )
)
```

[22]:
```
device_array = np.array(jax.devices()).reshape(-1, config.model_axis_size)
mesh = Mesh(device_array, (config.data_axis_name, config.model_axis_name))
```

```
2024-03-07 10:49:03.334086: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

We create the model below and wrap the whole model in a `prepare_module` function to support parameter sharding.

[23]:
```
def get_transformer_module(config: ConfigDict):
    module_class = Transformer
    module_class = prepare_module(
        module_class,
        "Transformer",
        config,
    )
    block_fn = TPTransformerParallelBlock if config.parallel_block else␣
↪TPTransformerBlock
    return module_class(config=config, block_fn=block_fn)
```

Let's finally create the model.

[24]:
```
model_transformer = get_transformer_module(config=config.model)
```

We also create the optimizer below. As common in Transformer language models, we design it to be Adam with an exponential learning rate decay and a linear warmup.

[25]:
```
optimizer_transformer = optax.adam(
    learning_rate=optax.warmup_exponential_decay_schedule(
        init_value=0,
        peak_value=config.optimizer.learning_rate,
        warmup_steps=10,
        transition_steps=1,
        decay_rate=0.99,
    )
)
```

Since we have implemented the transformer for natural language processing, we need to adjust our example task below. We will follow the autoregressive language modeling task, where we predict the next token given a sequence of tokens. We will use a small vocabulary size to run the model easily on a CPU-only system. The first token is a start-of-sentence token, and the labels are the input tokens shifted by one.

[26]:
```
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng = jax.random.split(rng)

tokens = jax.random.randint(
    data_inputs_rng,
    (config.data.batch_size, config.data.seq_len),
    1,
    config.data.vocab_size,
)
batch_transformer = Batch(
    inputs=jnp.pad(tokens[:, :-1], ((0, 0), (1, 0)), constant_values=0),
    labels=tokens,
)
```

[27]:
```
def init_transformer(rng: jax.random.PRNGKey, x: jax.Array) -> TrainState:
    init_rng, rng = jax.random.split(rng)
    variables = model_transformer.init({"params": init_rng}, x, train=False)
    params = variables.pop("params")
    state = TrainState.create(
```

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```
        apply_fn=model_transformer.apply,
        params=params,
        tx=optimizer_transformer,
        rng=rng,
    )
    return state
```

As usual, we first determine the partitioning of the model parameters in the init function.

[28]:
```
init_transformer_fn = jax.jit(
    shard_map(
        init_transformer,
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=P(),
        check_rep=False,
    ),
)
state_transformer_shapes = jax.eval_shape(
    init_transformer_fn, model_init_rng, batch_transformer.inputs
)
state_transformer_specs = nn.get_partition_spec(state_transformer_shapes)
```

We can inspect them below.

[29]:
```
print("Input Embedding")
pprint(state_transformer_specs.params["input_embedding"])
```

```
Input Embedding
{'module': {'sharded': {'pos_enc': {'pos_emb': PartitionSpec('model', None, 'data')},
                        'token_emb': {'embedding': PartitionSpec('model', 'data', None)}}
↪}}
```

The input embedding is sharded over both model and data axis. The data sharding is done over the feature dimensions for the positional encoding and over the vocabulary size for the embedding layer. The axes are selected based on which is the largest one that is divisible by the number of devices. For the default config, the vocabulary size is larger than the per-model-device feature dimension (100 vs 64). For other setups, where the vocabulary size is non-divisible by the number of devices, the sharding would likely happen over the feature dimension as well.

[30]:
```
print("Output Layer")
pprint(state_transformer_specs.params["output_layer"])
```

```
Output Layer
{'out_norm': {'scale': PartitionSpec()},
 'output_layer': {'bias': PartitionSpec(),
                  'kernel': PartitionSpec('model', 'data')}}
```

The parameters in the output layer can be partitioned over the data and model axis. However, due to the small size of the model, only the kernel is sharded over the both axis. The bias and the scale parameter of the normalization are duplicated over all devices.

[31]:
```
print("Transformer Block")
pprint(state_transformer_specs.params["backbone"])
```

```
Transformer Block
{'block': {'hqkv': {'shard_0': {'sharded': {'mlp': {'dense': {'bias': PartitionSpec(None,
↪ 'model', 'data'),
                                                              'kernel':␣
↪PartitionSpec(None, 'model', None, 'data')}},
                                           'qkv': {'key': {'kernel': PartitionSpec(None,
↪ 'model', 'data', None, None)},
                                                   'key_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'query': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)},
                                                   'query_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'value': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)}}}},
                    'shard_1': {'sharded': {'mlp': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, 'data')}},
                                           'qkv': {'key': {'kernel': PartitionSpec(None,
↪ 'model', 'data', None, None)},
                                                   'key_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'query': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)},
                                                   'query_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'value': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)}}}},
                    'shard_2': {'sharded': {'mlp': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, 'data')}},
                                           'qkv': {'key': {'kernel': PartitionSpec(None,
↪ 'model', 'data', None, None)},
                                                   'key_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'query': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)},
                                                   'query_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'value': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)}}}},
                    'shard_3': {'sharded': {'mlp': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', None, 'data')}},
                                           'qkv': {'key': {'kernel': PartitionSpec(None,
↪ 'model', 'data', None, None)},
                                                   'key_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'query': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)},
                                                   'query_norm': {'scale':␣
↪PartitionSpec(None, 'model', None)},
                                                   'value': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None, None)}}}}},
          'out': {'shard_0': {'sharded': {'attn': {'out': {'bias': PartitionSpec(None,
↪'model', 'data'),
```

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```
                                                                    'kernel': PartitionSpec(None,
↪ 'model', None, None, 'data')}},
                                                'mlp': {'dense': {'bias': PartitionSpec(None,
↪'model', 'data'),
                                                                     'kernel':␣
↪PartitionSpec(None, 'model', 'data', None)}}}},
                    'shard_1': {'sharded': {'attn': {'out': {'kernel': PartitionSpec(None,
↪ 'model', None, None, 'data')}},
                                                'mlp': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None)}}}},
                    'shard_2': {'sharded': {'attn': {'out': {'kernel': PartitionSpec(None,
↪ 'model', None, None, 'data')}},
                                                'mlp': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None)}}}},
                    'shard_3': {'sharded': {'attn': {'out': {'kernel': PartitionSpec(None,
↪ 'model', None, None, 'data')}},
                                                'mlp': {'dense': {'kernel':␣
↪PartitionSpec(None, 'model', 'data', None)}}}}},
           'pre_norm': {'norm': {'sharded': {'scale': PartitionSpec(None, 'model', 'data
↪')}}}}}
```

For the transformer backbone, we see that the input layer `hqkv` is distributed over 4 shards, and each containing an MLP input layer and a QKV layer. The first axis is again the layer index, the second the model axis, and the remaining ones the parameter-specific axes. The output layer `out` shows a similar pattern, with only using biases in the first shard. Finally, the norm parameters in `pre_norm` are sharded over both the model and data axis.

With this in mind, we can now initialize the model.

[32]:
```
init_transformer_fn = jax.jit(
    shard_map(
        init_transformer,
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_transformer_specs,
        check_rep=False,
    ),
)
state_transformer = init_transformer_fn(model_init_rng, batch_transformer.inputs)
```

Feel free to inspect the parameter shapes below. As an example, we will only inspect the parameters of the shard 0 of the output layer in the transformer block.

[33]:
```
print("Transformer Block - Output Layer, Shard 0")
if config.model.parallel_block:
    shard_0_params = state_transformer.params["backbone"]["block"]["out"]["shard_0"][
↪"sharded"]
else:
    shard_0_params = {
        "attn": state_transformer.params["backbone"]["block"]["attn"]["out"]["shard_0"][
↪"sharded"],
        "mlp": state_transformer.params["backbone"]["block"]["mlp"]["output"]["shard_0"][
            "sharded"
        ],
```

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```
    }
pprint(
    jax.tree_map(
        lambda x: x.shape,
        shard_0_params,
    )
)
```

```
Transformer Block - Output Layer, Shard 0
{'attn': {'out': {'bias': Partitioned(value=(6, 4, 64),
                                      names=(None, 'model', 'data'),
                                      mesh=None),
                  'kernel': Partitioned(value=(6, 4, 2, 32, 64),
                                        names=(None,
                                               'model',
                                               None,
                                               None,
                                               'data'),
                                        mesh=None)}},
 'mlp': {'dense': {'bias': Partitioned(value=(6, 4, 64),
                                       names=(None, 'model', 'data'),
                                       mesh=None),
                   'kernel': Partitioned(value=(6, 4, 256, 64),
                                         names=(None, 'model', 'data', None),
                                         mesh=None)}}}
```

In the attention output layer, the kernel has 5 dimensions: number of layers, number of model devices, number of heads per device, head dimension, and feature dimension per device/shard. The full transformer has 8 heads, such that each device processes 2 heads. For the MLP, the kernel has 4 dimensions: number of layers, number of model devices, hidden dimensions of the MLP per device, and feature dimension per device/shard. Since we expand our MLP dimension by 4, the hidden dimension per MLP is 256, with the full MLP having 1024 hidden dimensions. Overall, the parameters have the expected shapes and are sharded as intended.

As one more small check which can be very helpful during development, let's print the number of parameters.

[34]:
```
print(f"Number of parameters: {get_num_params(state_transformer):_}")
```

```
Number of parameters: 4_795_236
```

With 5 million parameters, the model at hand is of course very small due to running on CPU, but on a TPU superpod or GPU cluster, the model can be scaled up to billions of parameters. We can now continue with training the model.

Training

For training, we can reuse our previous loss function since it is a classical cross-entropy prediction task. However, since we split the output layer over the sequence length, we need to evaluate the loss on each device and select the right subset of labels per device. We do this below.

[35]:
```
def loss_fn_transformer(
    params: PyTree,
    apply_fn: Any,
    batch: Batch,
    rng: jax.Array,
```

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```
    config: ConfigDict,
) -> Tuple[jax.Array, Dict[str, Any]]:
    # Since dropout masks vary across the batch dimension, we want each device to␣
↪generate a
    # different mask. We can achieve this by folding the rng over the data axis, so that␣
↪each
    # device gets a different rng and thus mask.
    dropout_rng = fold_rng_over_axis(rng, (config.data_axis_name, config.model_axis_
↪name))
    # Remaining computation is the same as before for single device.
    logits = apply_fn(
        {"params": params},
        batch.inputs,
        train=True,
        rngs={"dropout": dropout_rng},
    )
    labels = split_array_over_mesh(batch.labels, axis_name=config.model_axis_name, split_
↪axis=1)
    assert (
        logits.shape[:-1] == labels.shape
    ), f"Logits and labels shapes do not match: {logits.shape} vs {labels.shape}"
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels)
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), labels)
    batch_size = np.prod(labels.shape)
    # Collect metrics and return loss.
    step_metrics = {
        "loss": (loss.sum(), batch_size),
        "accuracy": (correct_pred.sum(), batch_size),
    }
    loss = loss.mean()
    return loss, step_metrics
```

With this new loss function, we can now train the model. We will use the same training loop as before, and shard it with our previously determined partitioning specs.

[36]:
```
train_step_transformer_fn = jax.jit(
    shard_map(
        functools.partial(train_step_tp, loss_fn=loss_fn_transformer, config=config),
        mesh,
        in_specs=(state_transformer_specs, P(), P(config.data_axis_name)),
        out_specs=(state_transformer_specs, P()),
        check_rep=False,
    ),
    donate_argnames=("state", "metrics"),
)
state_shapes, metric_shapes = jax.eval_shape(
    train_step_transformer_fn,
    state_transformer,
    None,
    batch_transformer,
)
metrics_transformer = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
```

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```
state_transformer, metrics_transformer = train_step_transformer_fn(
    state_transformer, metrics_transformer, batch_transformer
)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[6,1,
↪128]), ShapedArray(float32[6,1,64,128]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,
↪1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,64,128]),␣
↪ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,
↪1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,64,128]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,
↪1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,64,128]),␣
↪ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,
↪1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,2,32,32]), ShapedArray(float32[6,
↪1,32]), ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,2,32,32]),␣
↪ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,2,32,32]),␣
↪ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,2,32,32]),␣
↪ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,32]), ShapedArray(float32[1,
↪32,32]), ShapedArray(float32[1,50,64]), ShapedArray(float32[64,50]),␣
↪ShapedArray(float32[6,1,128]), ShapedArray(float32[6,1,64,128]), ShapedArray(float32[6,
↪1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,
↪1,64,128]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,32]),␣
↪ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,
↪1,32,2,32]), ShapedArray(float32[6,1,64,128]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,
↪1,32]), ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,64,128]),␣
↪ShapedArray(float32[6,1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,
↪1,32,2,32]), ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,32,2,32]),␣
↪ShapedArray(float32[6,1,32]), ShapedArray(float32[6,1,2,32,32]), ShapedArray(float32[6,
↪1,32]), ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,2,32,32]),␣
↪ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,2,32,32]),␣
↪ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,2,32,32]),␣
↪ShapedArray(float32[6,1,128,64]), ShapedArray(float32[6,1,32]), ShapedArray(float32[1,
↪32,32]), ShapedArray(float32[1,50,64]), ShapedArray(float32[64,50]).
```

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```
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

Let's train the model for 50 steps and print the final loss and accuracy.

[37]:
```
for _ in tqdm(range(50)):
    state_transformer, metrics_transformer = train_step_transformer_fn(
        state_transformer, metrics_transformer, batch_transformer
    )
final_metrics_transformer = jax.tree_map(
    lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes
)
state_transformer, final_metrics_transformer = train_step_transformer_fn(
    state_transformer, final_metrics_transformer, batch_transformer
)
print_metrics(final_metrics_transformer, title="Final Metrics - Transformer")
```

```
  0%|          | 0/50 [00:00<?, ?it/s]
```

```
 Final Metrics - Transformer
accuracy: 0.976562
loss: 0.087221
```

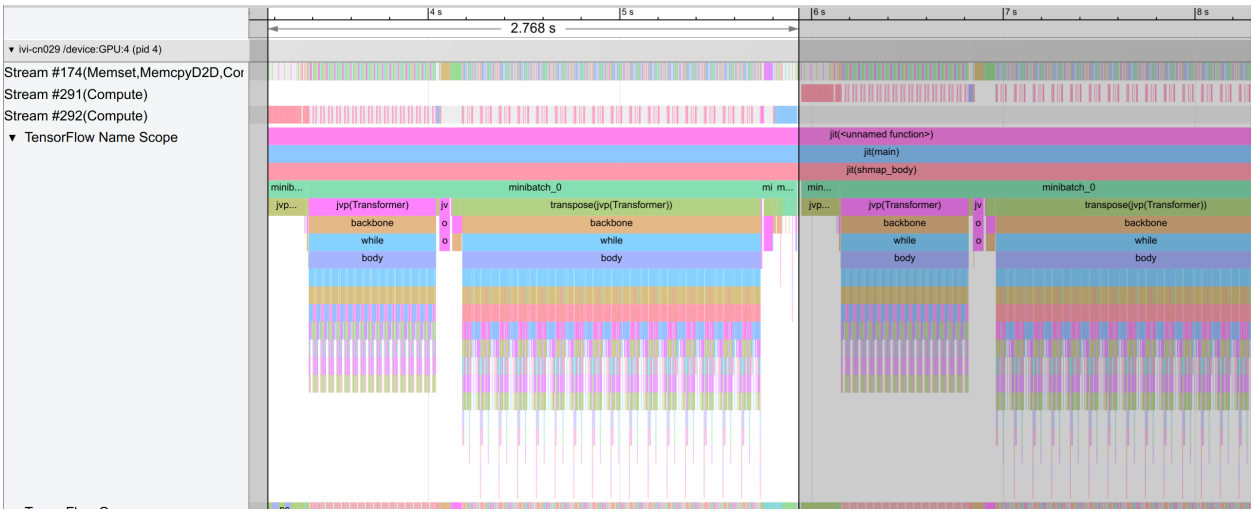
The transformer model is able to learn the task with high accuracy. However, note that in contrast to the previous tasks, the model not be able to reach 100% accuracy, even if we train it for much longer. This is because the first input token is by definition a start-of-sentence token, and the model cannot identify which token comes next. For subsequent tokens, we can use the previous tokens to identify the sequence we are on, such that the model on this single batch can likely achieve accuracies close to 96%. We have successfully implemented a transformer model with tensor parallelism and fully-sharded data parallelism, and trained it on a simple language modeling task.

4.14.3 Profiling Large Model

We can now profile the model to identify potential bottlenecks. We will use the same profiling functions as in our single GPU tutorial, and profile the model for 3 steps. The profiles are uploaded here.

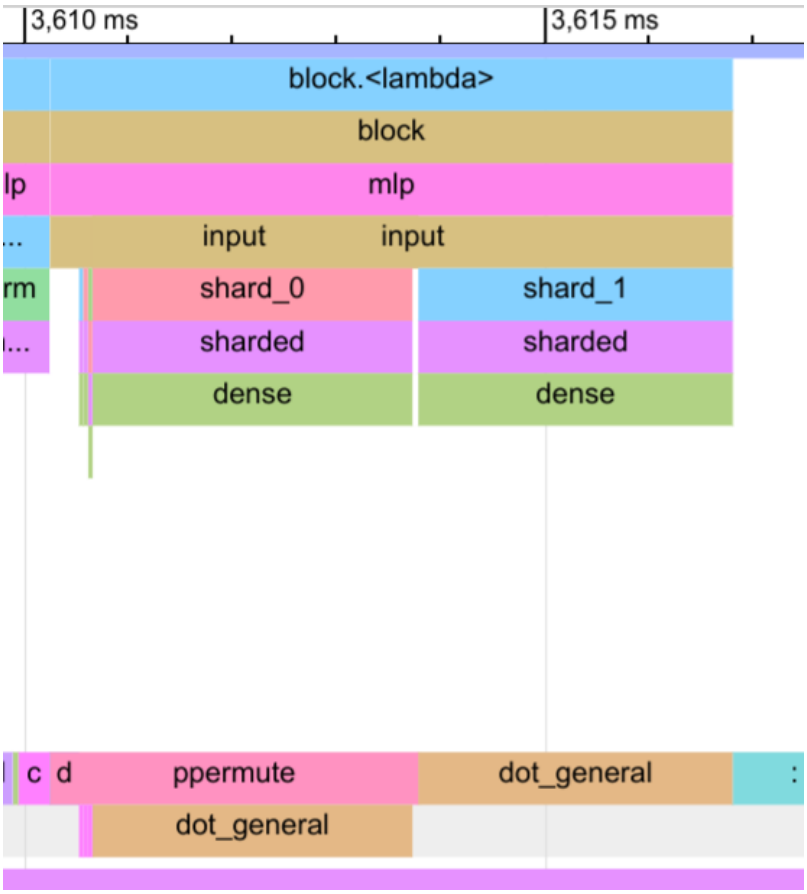
We scale the model up to a hidden size of 2048, 16 layers, vocabulary size of 32k, sequence length 1k, and batch size 128. This results in a model with almost 1 billion parameters. We distribute the model over one node with 8 A5000 GPUs, and use a model axis size of 2. Every pair of GPUs in the model axis are connected via 4 NVLink connections with a measured communication speed of 60GB/s in each direction. The GPUs across the data axis are only connected via the PCIe bus, with significant lower communication speed. Since we require significantly more in-time communication across the model axis, we organize the mesh such that the GPUs in the model axis use the NVLinks.

We start with showing the full trace for a model with a sequential Transformer block below.

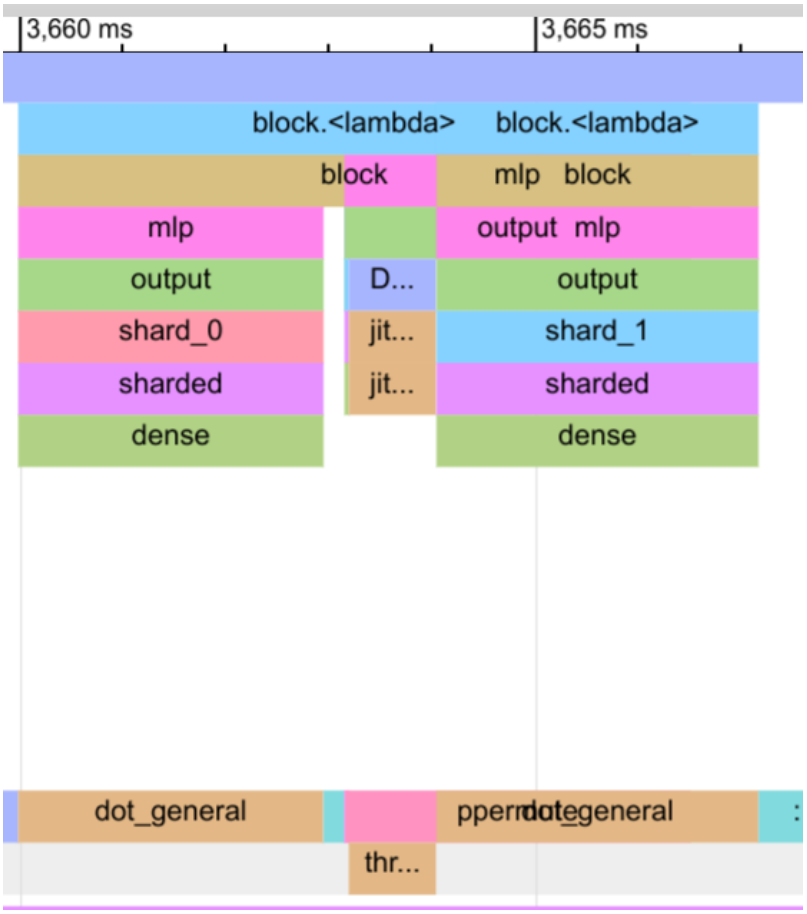


One difference to the single-GPU case is that we have a trace per GPU. In the figure above, we show the trace for GPU-4. A single step takes around 2.8 seconds, and consists of an initial weight gathering across the data axis, the forward pass, and finally the backward pass with remats. Each step in the forward and backward pass iterates over the 16 layers.

Let's take a closer look at the forward pass below. Specifically, we look at the trace of the MLP block:

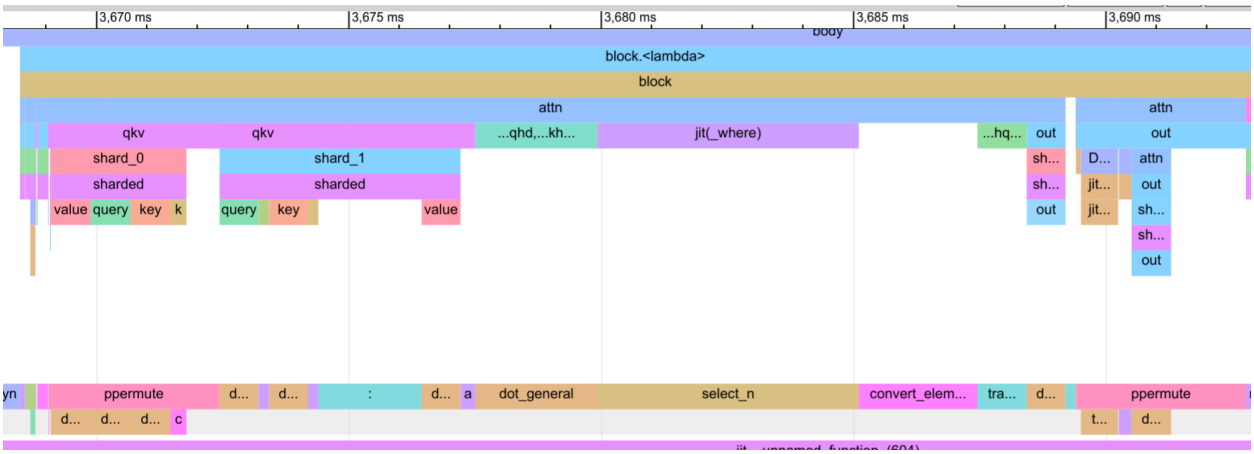


In the input dense layer, we can clearly see how well the communication (`ppermute`) and computation of `shard_0` overlaps. There is only a gap of a few microseconds in which the device is idle.



For the output dense layer, the communication fully overlaps with the computation of the `shard_1` output and the dropout. In the trace, the block for `ppermute` is overlapped with the `dot_general` operation of `shard_1`, which makes it a bit more tricky to read.

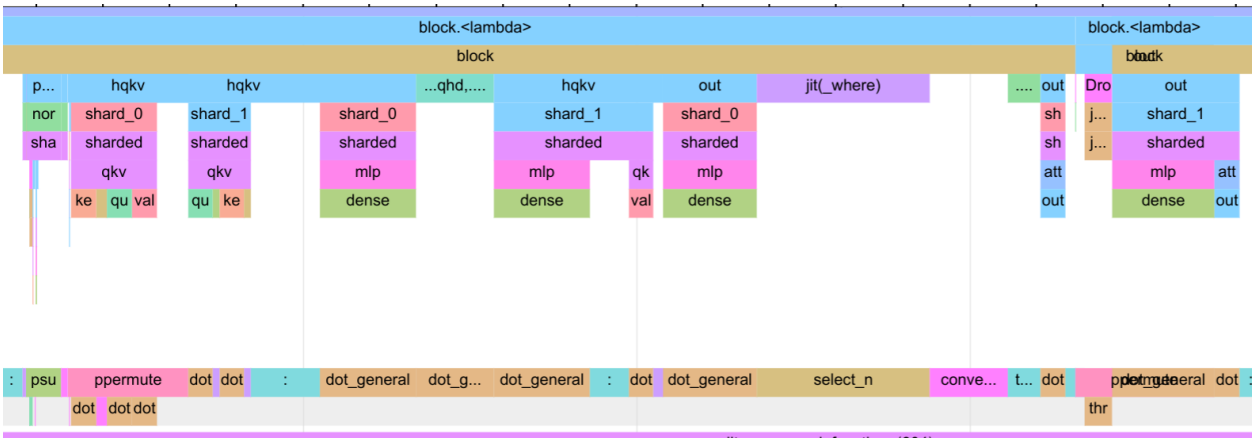
Now let's take a look at the attention block below.



We see that the communication overlap is not as good as for the MLP, and there are some idle gaps in the input and output layer. This is due to the fact that the attention layer has lower computationally complexity in its input and output. For instance, in the input layer, we calculate 3/4-th of the hidden size of the MLP block, and in the output layer, we calculate 1/4-th of the hidden size. This means that the communication would need to be much faster for the attention layer, but our NVLink connections cannot keep up with the speed of the computation (our communication speed in the

trace reach close to the 60GB/s limit).

While we could improve it with better communication hardware or larger scale of the model, we can also reduce the communication by parallelizing the attention and the MLP block, as we have done in the parallel block. The trace for the parallel block is shown below.



In the input layer, the compiler schedules the query, key and value computations to overlap with the communication. This leads to a small idle gap again in the block, but is overall small compared to the execution time of the block. On the output, however, the communication fully overlaps with the output dense layer of the MLP block. This way, we mitigate the communication gap in the previous version of the attention block, and can reduce the overall execution time of the block. We obtain a step time of 2.6 seconds, which is a 7% improvement over the sequential block.

Still, in our execution, there are a few minor inefficiency in terms of communication, like the gathering and sharding of the model weights over the data axis. We could try to further optimize the model by overlapping communication and computation, and by optimizing the communication pattern. However, we have already reached a very good efficiency with the parallel block, and the remaining inefficiencies are minor compared to the overall execution time. Further, better hardware such as a TPU pod may significantly reduce the inefficiency. In summary, we have successfully profiled a large transformer model with tensor parallelism and fully-sharded data parallelism, and identified potential bottlenecks.

4.14.4 Conclusion

In this notebook, we did a deep-dive into tensor parallelism and how to implement it in JAX. Tensor parallelism is a powerful tool to scale up models to billions of parameters, and is widely used in state-of-the-art models. However, it requires careful consideration of the communication patterns and strategies, and may require adjustments to the model architecture to maximize the efficiency. We started our implementation with parallelizing a simple linear layer over multiple devices, and discussed the communication patterns and strategies to improve the efficiency of the model. In particular, we showed how asynchronous communication can help to overlap communication with compute. We then extended the async gather and scatter strategies to the full transformer model, and discussed the parallelization of the attention and MLP block. We implemented the transformer model with tensor parallelism and fully-sharded data parallelism, and trained it on a simple language modeling task. In the next notebook, we will combine all parallelization strategies we have learned so far to implement a full-scale model with tensor parallelism, pipeline parallelism, and data parallelism.

4.14.5 References and Resources

[Shoeybi et al., 2019] Shoeybi, M., Patwary, M., Puri, R., LeGresley, P., Casper, J. and Catanzaro, B., 2019. Megatron-lm: Training multi-billion parameter language models using model parallelism. arXiv preprint arXiv:1909.08053. Paper link

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[Xu et al., 2021] Xu, Y., Lee, H., Chen, D., Hechtman, B., Huang, Y., Joshi, R., Krikun, M., Lepikhin, D., Ly, A., Maggioni, M. and Pang, R., 2021. GSPMD: general and scalable parallelization for ML computation graphs. arXiv preprint arXiv:2105.04663. Paper link

[Dehghani et al., 2022] Dehghani, M., Gritsenko, A., Arnab, A., Minderer, M. and Tay, Y., 2022. Scenic: A JAX library for computer vision research and beyond. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (pp. 21393-21398). Paper link

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[Anil et al., 2023] Anil, R., Dai, A.M., Firat, O., Johnson, M., Lepikhin, D., Passos, A., Shakeri, S., Taropa, E., Bailey, P., Chen, Z. and Chu, E., 2023. Palm 2 technical report. arXiv preprint arXiv:2305.10403. Paper link

[Dehghani et al., 2023] Dehghani, M., Djolonga, J., Mustafa, B., Padlewski, P., Heek, J., Gilmer, J., Steiner, A.P., Caron, M., Geirhos, R., Alabdulmohsin, I., Jenatton, R., et al., 2023. Scaling vision transformers to 22 billion parameters. In International Conference on Machine Learning (pp. 7480-7512). PMLR. Paper link

[McKinney, 2023] McKinney, A., 2023. A Brief Overview of Parallelism Strategies in Deep Learning. Blog post link

[Huggingface, 2024] Huggingface, 2024. Model Parallelism. Documentation link

[Google, 2024] JAX Team Google, 2024. SPMD multi-device parallelism with shard_map. Notebook link

[OpenAI, 2024] OpenAI, 2024. GPT-4. Technical Report

[Google, 2024] Gemini Team Google Deepmind, 2024. Gemini. Technical Report

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.15 Part 5: Language Modeling with 3D Parallelism

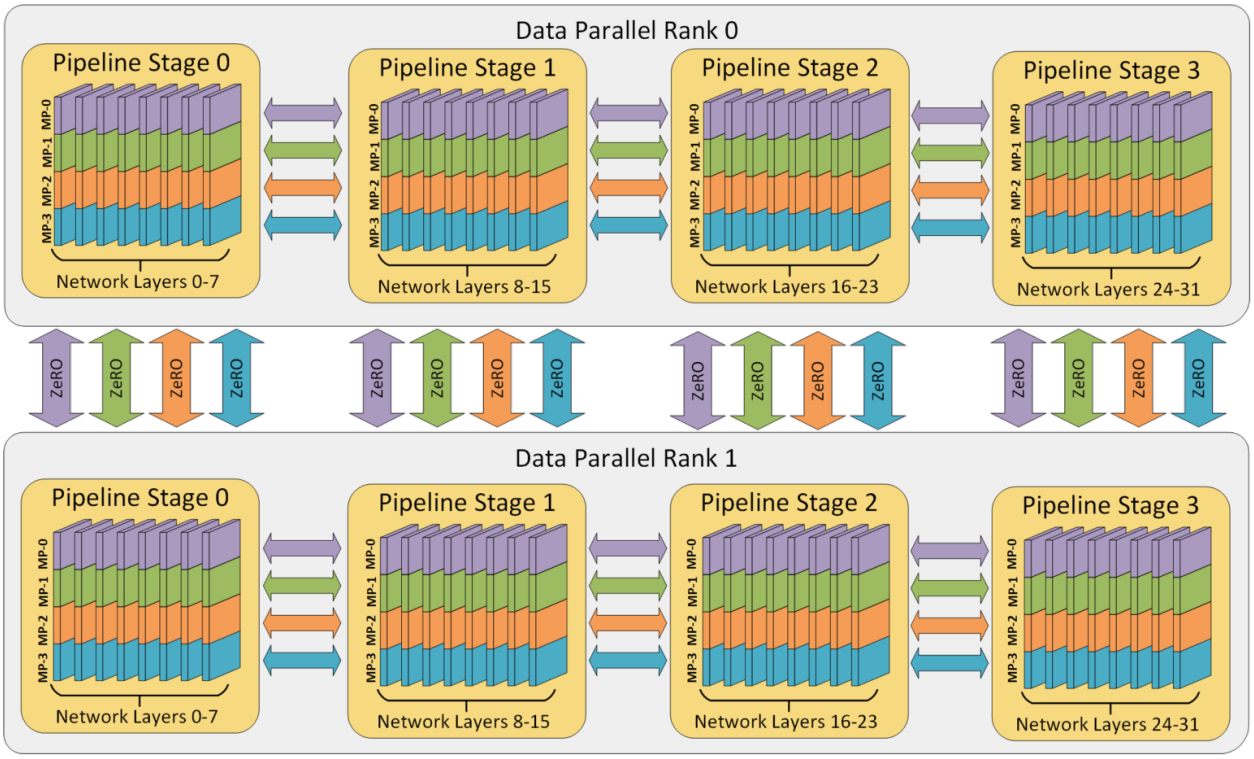
Filled notebook:

Author: Phillip Lippe

In the previous tutorials, we have explored the concept of parallelism in the context of training large language models. We have seen how data parallelism can be used to distribute the training data across multiple devices, and how pipeline and tensor parallelism can be used to distribute the model across multiple devices. For training models with up to trillion parameters, one parallelism strategy alone will not be sufficient. Hence, in this tutorial, we will explore the

concept of **3D parallelism**, which combines data, pipeline, and tensor parallelism to train models like large language models (LLM).

To combine all parallelism strategies, we need to create a three-dimensional mesh of devices. Each axis will correspond to one of our parallelism strategies. The data parallelism axis will be responsible for distributing the training data across devices, the pipeline parallelism axis will be responsible for distributing the model's layers across devices, and the tensor parallelism axis will be responsible for parallelizing the individual layers across devices. Thereby, tensor parallelism requires the highest communication bandwidth, while data parallelism requires the lowest communication bandwidth. We need to take this communication bandwidth into account when designing the 3D parallelism mesh. For instance, GPUs that are within the same node and have a strong NVLink connection should be placed on the same tensor parallelism axis, while GPUs that are in different nodes should be placed on different tensor parallelism axes. Cross-node communication is much slower than the communication within a node, such that we may want to use data parallelism across nodes. Still, for nodes with a high communication bandwidth, we can use pipeline parallelism across nodes. This gives us the flexibility to design the 3D parallelism mesh according to the hardware we have available. An overview of the 3D parallelism mesh is shown in the figure below (figure credit: DeepSpeed, 2024).



In this notebook, we will combine the techniques we have implemented for data, pipeline and tensor parallelism to enable 3D parallelism. We demonstrate how easy it is in JAX to combine the different parallelism strategies, and experiment with different 3D parallelism configurations.

4.15.1 Prerequisites

First, let's start with setting up the basic environment and utility functions we have seen from previous notebooks. We download the python scripts of the previous notebooks below. This is only needed when running on Google Colab, and local execution will skip this step automatically.

[1]:
```
import os
import urllib.request
from urllib.error import HTTPError

# Github URL where python scripts are stored.
base_url = "https://raw.githubusercontent.com/phlippe/uvadlc_notebooks/master/docs/
↪tutorial_notebooks/scaling/JAX/"
# Files to download.
python_files = [
    "single_gpu.py",
    "data_parallel.py",
    "pipeline_parallel.py",
    "tensor_parallel.py",
    "tensor_parallel_async.py",
    "tensor_parallel_transformer.py",
    "utils.py",
]
# For each file, check whether it already exists. If not, try downloading it.
for file_name in python_files:
    if not os.path.isfile(file_name):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_name)
        except HTTPError as e:
            print(
                "Something went wrong. Please try to download the file directly from the␣
↪GitHub repository, or contact the author with the full output including the following␣
↪error:\n",
                e,
            )
```

As before, we simulate 8 devices on CPU to demonstrate the parallelism without the need for multiple GPUs or TPUs. If you are running on your local machine and have multiple GPUs available, you can comment out the lines below.

[2]:
```
from utils import simulate_CPU_devices

simulate_CPU_devices()
```

We now import our standard libraries.

[3]:
```
import functools
from pprint import pprint
from typing import Any, Callable, Dict, Tuple

import flax.linen as nn
import jax
import jax.numpy as jnp
```

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```
import numpy as np
import optax
from jax.experimental.shard_map import shard_map
from jax.sharding import Mesh
from jax.sharding import PartitionSpec as P
from ml_collections import ConfigDict
from tqdm.auto import tqdm

PyTree = Any
Parameter = jax.Array | nn.Partitioned
Metrics = Dict[str, Tuple[jax.Array, ...]]
```

We also import the utility functions from the previous notebooks. Our notebook will rely on many concepts of previous tutorials, such as `shard_module_params` and `sync_gradients` for handling fully-sharded data parallelism, `ModelParallelismWrapper` and `PipelineModule` for handling pipeline parallelism, and the transformer blocks from the tensor parallelism notebook. If you are not familiar with these functions and modules, we recommend to go through the previous tutorials first.

[4]:
```
from data_parallel import fold_rng_over_axis, shard_module_params, sync_gradients
from pipeline_parallel import ModelParallelismWrapper, PipelineModule
from single_gpu import (
    Batch,
    TrainState,
    accumulate_gradients,
    get_num_params,
    print_metrics,
)
from tensor_parallel_transformer import (
    TPInputEmbedding,
    TPTransformerBlock,
    TPTransformerParallelBlock,
    TransformerBackbone,
    split_array_over_mesh,
)
```

4.15.2 3D Parallelism

We will now combine the techniques we have implemented for data, pipeline and tensor parallelism to enable 3D parallelism. Most parallelization implementations we have done over the past tutorials have been designed with the idea that we may want to combine them in the future. For instance, the `ModelParallelismWrapper` supports nested model parallelism, where the module passed to the wrapper might also be partitioned over a different axis. Similarly, the `PipelineModule` operates independently of how the stages in the pipeline may be sharded. Moreover, our parameter sharding implementation in `shard_module_params` supports sharding over multiple axes at once, as we will see later on. All this together allows us to easily combine the different parallelism strategies.

Transformer Model

We start by implementing the transformer model that we will use for our 3D parallelism experiments. We will use the same transformer model as in the tensor parallelism tutorial, but slightly adjust it to also support pipeline parallelism. For this, we first write a wrapper around the transformer backbone, i.e. the scan over layers, such that we can pass it to the `PipelineModule`. It is the same technique as we have seen in the pipeline parallelism notebook. Note that for simplicity, we will not use looping pipelines here, but only a single pipeline stage. However, the implementation would easily allow for looping pipelines as well.

[5]:
```
class PipelineTransformerBackbone(nn.Module):
    """Transformer backbone with pipeline and tensor parallelism.

    This module is a combination of the `TransformerBackbone` from the tensor parallelism tutorial
    and the `PipelineModule` from the pipeline parallelism tutorial.
    """

    config: ConfigDict
    train: bool
    mask: jax.Array | None = None
    block_fn: Any = TPTransformerBlock
    pipeline_module_class: Callable[..., nn.Module] = PipelineModule

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        axis_size = jax.lax.psum(1, self.config.pipeline_axis_name)
        # Define module per pipeline stage.
        stage_module_fn = functools.partial(
            TransformerBackbone,
            config=self.config,
            train=self.train,
            mask=self.mask,
            block_fn=self.block_fn,
            name="layers",
        )
        if axis_size == 1:
            # If pipeline axis size is 1, we don't need to define a pipeline module.
            module = stage_module_fn()
        else:
            # Define pipeline module.
            pipeline_module_fn = functools.partial(
                self.pipeline_module_class,
                model_axis_name=self.config.pipeline_axis_name,
                num_microbatches=self.config.num_microbatches,
                module_fn=stage_module_fn,
            )
            # Wrap pipeline module in parallelism wrapper over pipeline axis.
            # The tensor parallelism is handled within the TPTransformerBlock.
            module = ModelParallelismWrapper(
                module_fn=pipeline_module_fn,
                model_axis_name=self.config.pipeline_axis_name,
                name="pipeline",
            )
```

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```
        x = module(x)
        return x
```

Another component we want to adjust is the output layer. In the tensor parallelism tutorial, we have changed our parallelization strategy from tensor to sequence parallelism, since the output requires the full softmax, i.e. full output size, and this may lead unnecessary replication of large tensors. In the 3d parallelism, we follow the same setup, but also add the pipeline parallel axis to the sequence parallelism. Essentially, from a mesh of `(data, pipeline, tensor)`, we switch to `(data, sequence)` parallelism by combining the pipeline and tensor parallelism.

We first reorganize the input tensors by summing over the pipeline axis and splitting the output. We sum instead of gathering, since in pipeline parallelism, all devices except the last one will have zero's in the output. Hence, summing across the pipeline axis is the equivalent to gathering and selecting only the output of the last stage. We then gather and split the data over the tensor axis as before. With that, each device across the joint pipeline and model axis will have a different subset of the input sequence.

To reduce the parameters per device, we apply parameter sharding as in Zero over the two axis. JAX supports axis names which are tuples of other axis names, such that we can shard over multiple axes at once. We will shard over the pipeline and tensor axis, such that each device will only have a subset of the parameters. We implement this below:

[6]:
```
class TPPPOutputLayer(nn.Module):
    config: ConfigDict

    @nn.compact
    def __call__(self, x: jax.Array) -> jax.Array:
        # Pipeline outputs are zero's for all non-last stages.
        # Summing results results in all stages having the same, correct output.
        x = jax.lax.psum(x, axis_name=self.config.pipeline_axis_name)
        x = split_array_over_mesh(x, axis_name=self.config.pipeline_axis_name, split_
↪axis=1)
        # Gather outputs over feature dimension and split over sequence length.
        x = jax.lax.all_gather(x, axis_name=self.config.model_axis_name, axis=-1,␣
↪tiled=True)
        x = split_array_over_mesh(x, axis_name=self.config.model_axis_name, split_axis=1)
        # Shard parameters over model axis.
        norm_fn = shard_module_params(
            nn.RMSNorm,
            axis_name=(self.config.pipeline_axis_name, self.config.model_axis_name),
            min_weight_size=self.config.fsdp.min_weight_size,
        )
        dense_fn = shard_module_params(
            nn.Dense,
            axis_name=(self.config.pipeline_axis_name, self.config.model_axis_name),
            min_weight_size=self.config.fsdp.min_weight_size,
        )
        # Apply normalization and output layer.
        x = norm_fn(dtype=self.config.dtype, name="out_norm")(x)
        x = dense_fn(
            features=self.config.num_outputs,
            dtype=jnp.float32,
            name="output_layer",
        )(x)
        return x
```

Finally, we can combine everything together to create a Transformer model for 3D parallelism. Since every module

requires different shardings in FSDP, we wrap each module below in its respective sharding. For instance, the input layer will receive the same input across the pipeline and tensor axis. We have already sharded the feature dimension over the tensor axis, such that the remaining parameter axes can be sharded over the data and pipeline axis jointly. We perform the same computation over the pipeline axis in the input layer, but since it only consists of an embedding lookup and adding of positional encoding, its computation is negligible.

The transformer backbone will then process via a pipeline process, with each stage additionally sharded over the tensor axis. In FSDP, we can shard the parameters additionally over the data axis.

Finally, the output layer already shards its parameters over the pipeline and tensor axis. Thus, we only need to shard them additionally over the data axis in FSDP.

A small note on our FSDP implementation: for simplicity, we enforce each application of `shard_module_params` to look for parameter axis that have been unsharded before. This is not strictly necessary, as we already support `shard_module_params` to shard over multiple axes at once. For large arrays with few axes, like the input embeddings, it may be beneficial to support the double sharding in some cases. However, it simplifies the implementation and is sufficient for our purposes here.

[7]:
```
class Transformer(nn.Module):
    config: ConfigDict
    block_fn: Any = TPTransformerBlock

    @nn.compact
    def __call__(self, x: jax.Array, train: bool, mask: jax.Array | None = None) -> jax.
↪Array:
        if mask is None and self.config.causal_mask:
            mask = nn.make_causal_mask(x[0:1], dtype=jnp.bool_)
        # Input embedding. Replicated across pipeline axis.
        input_layer = TPInputEmbedding
        if "Embed" in self.config.fsdp.modules:
            input_layer = shard_module_params(
                input_layer,
                axis_name=(self.config.data_axis_name, self.config.pipeline_axis_name),
                min_weight_size=self.config.fsdp.min_weight_size,
            )
        x = input_layer(
            config=self.config,
            name="input_embedding",
        )(x)
        # Backbone.
        backbone_layer = PipelineTransformerBackbone
        if "Backbone" in self.config.fsdp.modules:
            backbone_layer = shard_module_params(
                backbone_layer,
                axis_name=self.config.data_axis_name,
                min_weight_size=self.config.fsdp.min_weight_size,
            )
        x = backbone_layer(
            config=self.config,
            train=train,
            mask=mask,
            block_fn=self.block_fn,
            name="backbone",
        )(x)
        # Output layer.
```

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```
        output_layer = TPPPOutputLayer
        if "Output" in self.config.fsdp.modules:
            output_layer = shard_module_params(
                output_layer,
                axis_name=self.config.data_axis_name,
                min_weight_size=self.config.fsdp.min_weight_size,
            )
        x = output_layer(
            config=self.config,
            name="output_layer",
        )(x)
        return x
```

And that's it. We have now implemented a transformer model that supports 3D parallelism with few adjustments from the original tensor-parallel model. We can set up the training of the model.

Initialization

We start by defining the config for our model. Since the notebook is supposed to also run on CPU, we choose a very small model here. However, on actual multi-accelerator hardware, we would scale up the model considerably. Feel free to test out different configurations.

[8]:
```
data_config = ConfigDict(
    dict(
        batch_size=32,
        vocab_size=100,
        seq_len=8,
    )
)
fsdp = ConfigDict(
    dict(
        modules=("Embed", "Backbone", "Output"),
        axis_name="data",
        min_weight_size=2**8,
    )
)
model_config = ConfigDict(
    dict(
        hidden_size=256,
        dropout_rate=0.1,
        mlp_expansion=4,
        num_layers=6,
        head_dim=32,
        normalize_qk=True,
        positional_encoding_type="learned",
        parallel_block=True,
        causal_mask=True,
        vocab_size=data_config.vocab_size,
        num_outputs=data_config.vocab_size,
        dtype=jnp.bfloat16,
        data_axis_name="data",
```

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```
        model_axis_name="tensor",
        model_axis_size=2,
        pipeline_axis_name="pipe",
        pipeline_axis_size=2,
        num_microbatches=8,
        remat=("Block",),
        fsdp=fsdp,
    )
)
model_config.num_heads = model_config.hidden_size // model_config.head_dim
model_config.num_layers //= model_config.pipeline_axis_size
optimizer_config = ConfigDict(
    dict(
        learning_rate=2e-4,
        num_minibatches=1,
    )
)
config = ConfigDict(
    dict(
        model=model_config,
        optimizer=optimizer_config,
        data=data_config,
        data_axis_name=model_config.data_axis_name,
        model_axis_name=model_config.model_axis_name,
        model_axis_size=model_config.model_axis_size,
        pipeline_axis_name=model_config.pipeline_axis_name,
        pipeline_axis_size=model_config.pipeline_axis_size,
        seed=42,
    )
)
```

We start by creating our device mesh. We will have three axis this time, which split the devices into a 2x2x2 grid (for 8 devices). The closest devices are on the same tensor axis (e.g. 0 and 1), the next closest devices are on the same pipeline axis (e.g. 0 and 2), and the last axis is the data parallel axis (e.g. 0 and 4). For your actual hardware, you should adjust the device order/mesh to optimally fit your communication hardware. On GPUs, you can find your NVLink connections with `nvidia-smi topo -m`.

[9]:
```
device_array = np.array(jax.devices()).reshape(
    -1, config.pipeline_axis_size, config.model_axis_size
)
mesh = Mesh(
    device_array, (config.data_axis_name, config.pipeline_axis_name, config.model_axis_
↪name)
)
mesh
```

```
2024-03-07 10:49:34.624870: E external/xla/xla/stream_executor/cuda/cuda_driver.cc:273]␣
↪failed call to cuInit: CUDA_ERROR_NO_DEVICE: no CUDA-capable device is detected
CUDA backend failed to initialize: FAILED_PRECONDITION: No visible GPU devices. (Set TF_
↪CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

[9]:
```
Mesh(device_ids=array([[[0, 1],
        [2, 3]],
```

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```
       [[4, 5],
        [6, 7]]]), axis_names=('data', 'pipe', 'tensor'))
```

We next create the transformer module. There is nothing special about it, besides that we do not need to wrap it in a `shard_module_wrapper` since we already shard parameters within the model.

[10]:
```
def get_transformer_module(config: ConfigDict):
    block_fn = TPTransformerParallelBlock if config.parallel_block else␣
↪TPTransformerBlock
    return Transformer(config=config, block_fn=block_fn)


model_transformer = get_transformer_module(config=config.model)
```

We then create the optimizer. Again, we use the same exponential decay schedule with warmup as for the other tutorials, although for an actual training, you may want to consider other alternatives as well, like LAMB or AdamW.

[11]:
```
optimizer_transformer = optax.adam(
    learning_rate=optax.warmup_exponential_decay_schedule(
        init_value=0,
        peak_value=config.optimizer.learning_rate,
        warmup_steps=10,
        transition_steps=1,
        decay_rate=0.99,
    )
)
```

For this notebook, we still with our random token dataset, but you can replace it with any other dataset you like.

[12]:
```
rng = jax.random.PRNGKey(config.seed)
model_init_rng, data_inputs_rng = jax.random.split(rng)

tokens = jax.random.randint(
    data_inputs_rng,
    (config.data.batch_size, config.data.seq_len),
    1,
    config.data.vocab_size,
)
batch_transformer = Batch(
    inputs=jnp.pad(tokens[:, :-1], ((0, 0), (1, 0)), constant_values=0),
    labels=tokens,
)
```

The initialization function is again the same as in the previous tutorials, and all parameter shardings are handled automatically.

[13]:
```
def init_transformer(rng: jax.random.PRNGKey, x: jax.Array) -> TrainState:
    init_rng, rng = jax.random.split(rng)
    variables = model_transformer.init({"params": init_rng}, x, train=False)
    params = variables.pop("params")
    state = TrainState.create(
        apply_fn=model_transformer.apply,
```

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```
        params=params,
        tx=optimizer_transformer,
        rng=rng,
    )
    return state
```

We first infer the partitioning for each parameter below.

[14]:
```
init_transformer_fn = jax.jit(
    shard_map(
        init_transformer,
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=P(),
        check_rep=False,
    ),
)
state_transformer_shapes = jax.eval_shape(
    init_transformer_fn, model_init_rng, batch_transformer.inputs
)
state_transformer_specs = nn.get_partition_spec(state_transformer_shapes)
```

Let's check the partitioning and shapes of the parameters, to see if the sharding has been done correctly and understand the setup. We first extract the shapes, which are per-device since the out-specification is `P()` for now.

[15]:
```
param_shapes = jax.tree_map(
    lambda x: x.value.shape if hasattr(x, "value") else x.shape,
    state_transformer_shapes.params,
    is_leaf=lambda x: isinstance(x, nn.Partitioned),
)
```

For the input layer, we find the following shapes:

[16]:
```
print("Input Embedding")
pprint(state_transformer_specs.params["input_embedding"])
print("Per-device shapes")
pprint(param_shapes["input_embedding"])
```

```
Input Embedding
{'module': {'sharded': {'pos_enc': {'pos_emb': PartitionSpec('tensor', None, ('data',
↪'pipe'))},
                        'token_emb': {'embedding': PartitionSpec('tensor', None, ('data',
↪ 'pipe'))}}}}
Per-device shapes
{'module': {'sharded': {'pos_enc': {'pos_emb': (1, 8, 32)},
                        'token_emb': {'embedding': (1, 100, 32)}}}}
```

Both the positional encoding and embedding are split over the tensor axis, which results in the first axis being 1 per device and partitioned over `tensor`. The last axis is the feature dimension, which is 256 globally, but 128 after the split over the tensor axis. This axis is sharded over `data` and `pipe`, which results in 32 per device (4 devices over the joint axis).

[17]:
```
print("Output Layer")
pprint(state_transformer_specs.params["output_layer"])
print("Per-device shapes")
pprint(param_shapes["output_layer"])
```

```
Output Layer
{'out_norm': {'scale': PartitionSpec()},
 'output_layer': {'bias': PartitionSpec(),
                  'kernel': PartitionSpec(('pipe', 'tensor'), 'data')}}
Per-device shapes
{'out_norm': {'scale': (256,)},
 'output_layer': {'bias': (100,), 'kernel': (64, 50)}}
```

The output layer has the norm and bias replicated over all devices, since in our configuration for the CPU, both of the tensors are very small and below the sharding threshold. The kernel weights are sharded over `pipe` and `tensor` on the first axis, which is the largest and originally 256, which results in 32 per device (4 devices over the joint axis). We additionally shard the last axis over `data`, which results in 50 per device (2 devices over the axis with 100 outputs).

For the transformer backbone, we first look at the input layer of the parallel block. Since the tensor parallelism introduces multiple identical sublayers (shards), we only look at `shard_0` for simplicity. Note that if you are using the sequential block, the lines below need to be adjusted accordingly.

[18]:
```
print("Transformer Backbone - HQKV")
pprint(
    state_transformer_specs.params["backbone"]["pipeline"]["sharded"]["layers"]["block"][
↪"hqkv"][
        "shard_0"
    ]["sharded"]
)
print("Per-device shapes")
pprint(
    param_shapes["backbone"]["pipeline"]["sharded"]["layers"]["block"]["hqkv"]["shard_0
↪"][
        "sharded"
    ]
)
```

```
Transformer Backbone - HQKV
{'mlp': {'dense': {'bias': PartitionSpec('pipe', None, 'tensor', 'data'),
                   'kernel': PartitionSpec('pipe', None, 'tensor', None, 'data')}},
 'qkv': {'key': {'kernel': PartitionSpec('pipe', None, 'tensor', 'data', None, None)},
         'key_norm': {'scale': PartitionSpec('pipe', None, 'tensor', None)},
         'query': {'kernel': PartitionSpec('pipe', None, 'tensor', 'data', None, None)},
         'query_norm': {'scale': PartitionSpec('pipe', None, 'tensor', None)},
         'value': {'kernel': PartitionSpec('pipe', None, 'tensor', 'data', None, None)}}}
Per-device shapes
{'mlp': {'dense': {'bias': (1, 3, 1, 256), 'kernel': (1, 3, 1, 128, 256)}},
 'qkv': {'key': {'kernel': (1, 3, 1, 64, 4, 32)},
         'key_norm': {'scale': (1, 3, 1, 32)},
         'query': {'kernel': (1, 3, 1, 64, 4, 32)},
         'query_norm': {'scale': (1, 3, 1, 32)},
         'value': {'kernel': (1, 3, 1, 64, 4, 32)}}}
```

All parameters share the first three axes: pipeline device stacking (sharded over `pipe`), number of layer per pipeline stage (3 per device), and tensor device stacking (sharded over `tensor`). After that, we have the individual parameter

shapes. For the MLP, the bias and kernel increase the feature size to 1024. This is split over the tensor axis, and sharded over the data axis (hence 1/4 of the feature size per device). The input axis of the kernel is split over different tensor shards, hence 1/2 of the original 256 feature dimension.

For the key, query and value layers, we have the input size of 256, which is split over the tensor axis and sharded over the data axis. The output size is `(4, 32)` per device, since the head dimension is 32 and the number of heads is 8, split over the tensor axis (hence 1/2 of the head count per device).

[19]:
```
print("Transformer Backbone - Output")
pprint(
    state_transformer_specs.params["backbone"]["pipeline"]["sharded"]["layers"]["block"]["out"]["shard_0"]["sharded"]
)
print("Per-device shapes")
pprint(
    param_shapes["backbone"]["pipeline"]["sharded"]["layers"]["block"]["out"]["shard_0"]["sharded"]
)
```

```
Transformer Backbone - Output
{'attn': {'out': {'bias': PartitionSpec('pipe', None, 'tensor', 'data'),
                  'kernel': PartitionSpec('pipe', None, 'tensor', None, None, 'data')}},
 'mlp': {'dense': {'bias': PartitionSpec('pipe', None, 'tensor', 'data'),
                   'kernel': PartitionSpec('pipe', None, 'tensor', 'data', None)}}}
Per-device shapes
{'attn': {'out': {'bias': (1, 3, 1, 64), 'kernel': (1, 3, 1, 4, 32, 64)}},
 'mlp': {'dense': {'bias': (1, 3, 1, 64), 'kernel': (1, 3, 1, 256, 128)}}}
```

On the output side of the transformer backbone, we have the same first three axes. The output kernel of the MLP model is the mirror image of the input size. The attention output kernel is of size `(4, 32, 64)`, where the first is again the number of heads per device, 32 the head dimension, and 64 the feature dimension split over both the tensor and data axis.

With that, the sharding of the parameters appears to be correct. We can now proceed to fully initialize the model.

[20]:
```
init_transformer_fn = jax.jit(
    shard_map(
        init_transformer,
        mesh,
        in_specs=(P(), P(config.data_axis_name)),
        out_specs=state_transformer_specs,
        check_rep=False,
    ),
)
state_transformer = init_transformer_fn(model_init_rng, batch_transformer.inputs)
print(f"Number of parameters: {get_num_params(state_transformer):_}")
```

```
Number of parameters: 4_784_484
```

The model is now fully initialized and ready for training. We can now proceed to the training loop.

Training

The loss function will be the same as in the previous tensor parallelism tutorial, with small modifications to introduce the pipeline parallelism. On the input side, we split the dropout RNG also over the pipeline axis. This gives us a different RNG per device. On the output side, we need to find the labels that correspond to the correct output slice per device. We use again the `split_array_over_mesh` function to subselect the array over the sequence length axis. We then compute the loss as before.

[21]:
```
def loss_fn(
    params: PyTree,
    apply_fn: Any,
    batch: Batch,
    rng: jax.Array,
) -> Tuple[jax.Array, Dict[str, Any]]:
    # Since dropout masks vary across the batch dimension, we want each device to␣
↪generate a
    # different mask. We can achieve this by folding the rng over the data axis, so that␣
↪each
    # device gets a different rng and thus mask.
    dropout_rng = fold_rng_over_axis(
        rng, (config.data_axis_name, config.pipeline_axis_name, config.model_axis_name)
    )
    # Remaining computation is the same as before for single device.
    logits = apply_fn(
        {"params": params},
        batch.inputs,
        train=True,
        rngs={"dropout": dropout_rng},
    )
    # Select the labels per device.
    labels = batch.labels
    labels = split_array_over_mesh(labels, axis_name=config.pipeline_axis_name, split_
↪axis=1)
    labels = split_array_over_mesh(labels, axis_name=config.model_axis_name, split_
↪axis=1)
    assert (
        logits.shape[:-1] == labels.shape
    ), f"Logits and labels shapes do not match: {logits.shape} vs {labels.shape}"
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels)
    correct_pred = jnp.equal(jnp.argmax(logits, axis=-1), labels)
    batch_size = np.prod(labels.shape)
    # Collect metrics and return loss.
    step_metrics = {
        "loss": (loss.sum(), batch_size),
        "accuracy": (correct_pred.sum(), batch_size),
    }
    loss = loss.mean()
    return loss, step_metrics
```

The training step is similarly adjusted. The gradients and the metrics are synced over all three axes. The rest of the training loop is the same as in the previous tutorials.

[22]:
```
def train_step(
    state: TrainState,
```

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```
    metrics: Metrics | None,
    batch: Batch,
) -> Tuple[TrainState, Metrics]:
    rng, step_rng = jax.random.split(state.rng)
    grads, step_metrics = accumulate_gradients(
        state,
        batch,
        step_rng,
        config.optimizer.num_minibatches,
        loss_fn=loss_fn,
    )
    # Update parameters. We need to sync the gradients across devices before updating.
    with jax.named_scope("sync_gradients"):
        grads = sync_gradients(
            grads, (config.data_axis_name, config.pipeline_axis_name, config.model_axis_
↪name)
        )
    new_state = state.apply_gradients(grads=grads, rng=rng)
    # Sum metrics across replicas. Alternatively, we could keep the metrics separate
    # and only synchronize them before logging. For simplicity, we sum them here.
    with jax.named_scope("sync_metrics"):
        step_metrics = jax.tree_map(
            lambda x: jax.lax.psum(
                x,
                axis_name=(
                    config.data_axis_name,
                    config.pipeline_axis_name,
                    config.model_axis_name,
                ),
            ),
            step_metrics,
        )
    if metrics is None:
        metrics = step_metrics
    else:
        metrics = jax.tree_map(jnp.add, metrics, step_metrics)
    return new_state, metrics
```

We are now ready to train our model. We shard the input batch over the data axis, and set the sharding specification as we have inferred during the initialization. Note that if we would run over multiple nodes/hosts and devices across the tensor or pipeline axis have different hosts, we may have difficulties to synchronize the hosts to input the same batch over the two parallelization axes. Alternatively, we can adjust the data input sharding to shard over all axes, and gather the input batch over the tensor and pipeline axis before starting our training step. However, for simplicity, we assume that all devices are on the same host in this notebook.

[23]:
```
train_step_fn = jax.jit(
    shard_map(
        train_step,
        mesh,
        in_specs=(state_transformer_specs, P(), P(config.data_axis_name)),
        out_specs=(state_transformer_specs, P()),
        check_rep=False,
```

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```
    ),
    donate_argnames=("state", "metrics"),
)
_, metric_shapes = jax.eval_shape(
    train_step_fn,
    state_transformer,
    None,
    batch_transformer,
)
metrics_transformer = jax.tree_map(lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_
↪shapes)
state_transformer, metrics_transformer = train_step_fn(
    state_transformer, metrics_transformer, batch_transformer
)
```

```
/home/plippe/anaconda3/envs/jax/lib/python3.10/site-packages/jax/_src/interpreters/mlir.
↪py:761: UserWarning: Some donated buffers were not usable: ShapedArray(float32[1,3,1,
↪256]), ShapedArray(float32[1,3,1,128,256]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,128,256]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,64]), ShapedArray(float32[1,3,1,4,32,64]),␣
↪ShapedArray(float32[1,3,1,64]), ShapedArray(float32[1,3,1,256,128]),␣
↪ShapedArray(float32[1,3,1,4,32,64]), ShapedArray(float32[1,3,1,256,128]),␣
↪ShapedArray(float32[1,3,1,64]), ShapedArray(float32[1,8,32]), ShapedArray(float32[1,
↪100,32]), ShapedArray(float32[64,50]), ShapedArray(float32[1,3,1,256]),␣
↪ShapedArray(float32[1,3,1,128,256]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,128,256]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,32]), ShapedArray(float32[1,3,1,64,4,32]),␣
↪ShapedArray(float32[1,3,1,64]), ShapedArray(float32[1,3,1,4,32,64]),␣
↪ShapedArray(float32[1,3,1,64]), ShapedArray(float32[1,3,1,256,128]),␣
↪ShapedArray(float32[1,3,1,4,32,64]), ShapedArray(float32[1,3,1,256,128]),␣
↪ShapedArray(float32[1,3,1,64]), ShapedArray(float32[1,8,32]), ShapedArray(float32[1,
↪100,32]), ShapedArray(float32[64,50]).
See an explanation at https://jax.readthedocs.io/en/latest/faq.html#buffer-donation.
  warnings.warn("Some donated buffers were not usable:"
```

Finally, we run the model for a few steps. Feel free to adjust the number of steps. We will not run the model for a long time, since we are running on CPU and the model is very small. However, on actual multi-accelerator hardware, you can scale up the model and run for a longer time.

[24]:
```
for _ in tqdm(range(20)):
    state_transformer, metrics_transformer = train_step_fn(
        state_transformer, metrics_transformer, batch_transformer
    )
final_metrics_transformer = jax.tree_map(
    lambda x: jnp.zeros(x.shape, dtype=x.dtype), metric_shapes
)
state_transformer, final_metrics_transformer = train_step_fn(
    state_transformer, final_metrics_transformer, batch_transformer
)
print_metrics(final_metrics_transformer, title="Final Metrics - Transformer")
```

```
  0%|          | 0/20 [00:00<?, ?it/s]
```

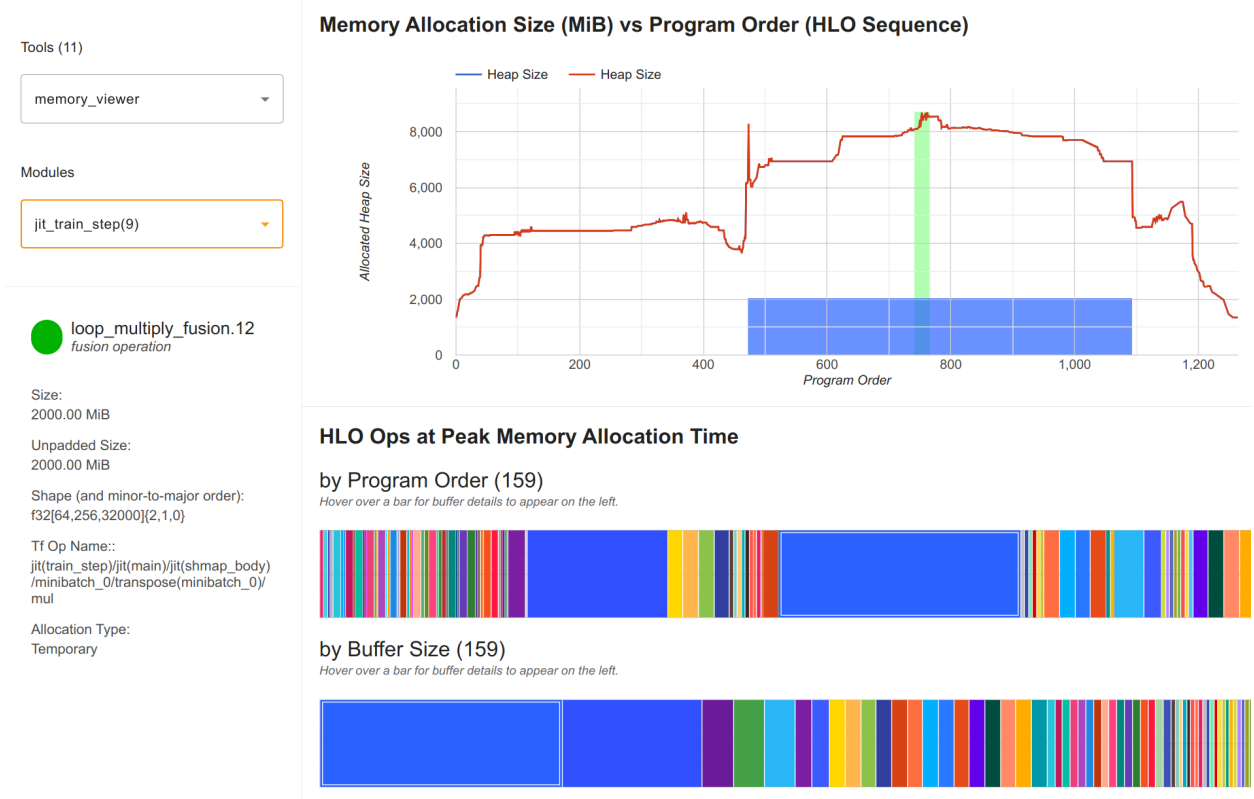
```
 Final Metrics - Transformer
accuracy: 0.855469
loss: 1.063429
```

The model achieves similar results as in the previous tutorials, but may be slightly lower due to the small sequence length (by default 8). You can increase the sequence length to get better results, but keep in mind that the memory requirements will increase as well.

4.15.3 Profiling

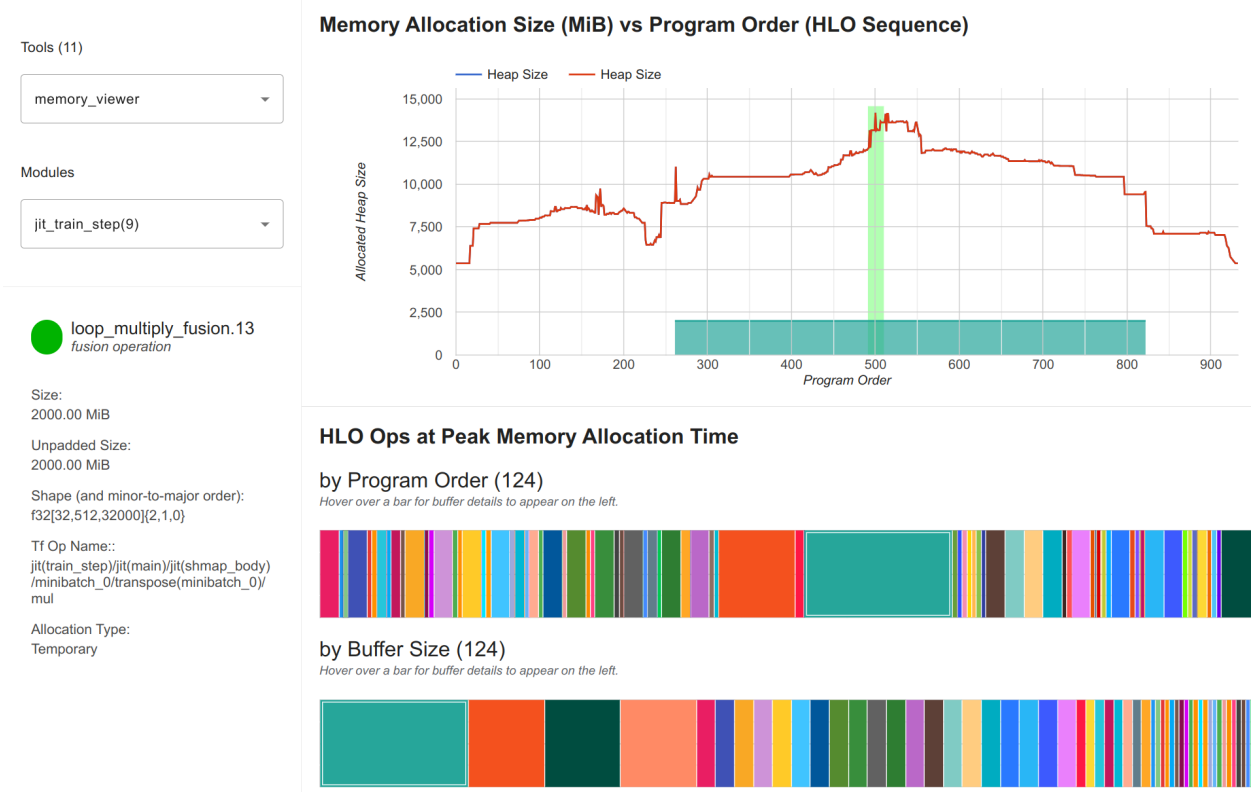
As a final step, we can profile a larger model to see the performance of the 3D parallelism and compare different configurations. We recreate the model from the tensor parallelism tutorial with around 1 billion parameters. We use the same input batch size of 128, sequence length 1024, and vocabulary size 32k. We run the experiments on a single node with 8 A5000 GPUs, each having 24GB memory and having an NVLink between pairs of GPUs with 60GB/s communication bandwidth.

We first use the same 3D parallelism configuration as in the config up, using a 2x2x2 grid. We then profile the model and find a step time of 2.9 seconds. This is slower than the pure tensor parallelism model at 2.6 seconds. This is because the pipeline axis adds additional communication between devices, which are not well connected in our system and requires an additional microbatch of compute. In terms of memory, we only use 8.5GB per device, which is well within the 24GB memory of the A5000:



The largest array are the output logits of size `(64, 256, 32000)` (batch size 128 split over 2 data devices, sequence length 1024 split over 4 tensor and pipeline devices). Further, it is in `float32` precision for numerical stability, which results in 2GB per device for this single array. The other arrays are much smaller and well within the memory limits. This highlights the importance of switching the parallelism strategies in the output to reduce the memory requirements.

Nonetheless, using only 1/3 of our available GPU memory indicates that we can either scale up the model, or use techniques that speed up the training for larger memory usage. For instance, we can disable parameter sharding over the data axis, which increases the per-device memory usage since all parameters are replicated now. If we use a 4x1x2 grid (4 data, 1 pipeline, 2 tensor devices), we have 500 million parameters per device (1 billion parameters in total over the two tensor devices), which requires roughly 6GB extra memory per device. We profile the memory usage below:



Each device now uses 14.5GB, which is still within the 24GB memory of the A5000. The largest array is still the output logits, but more parameter and optimizer state arrays are on each device, as seen by the higher initial memory usage. Without FSDP, we reduce the communication needed over devices, and we have a step time of 2.5 seconds now. This is slightly faster than the 3D parallelism with FSDP, but we may want to use the memory for increased batch sizes or rematting fewer layers. In the end, the best configuration depends on the specific hardware at hand, and the requirements we have from the training (e.g. minimum batch size, sequence length, etc.).

4.15.4 Conclusion

In this tutorial, we have combined the techniques we have implemented for data, pipeline and tensor parallelism to enable 3D parallelism. We have seen how easy it is in JAX to combine the different parallelism strategies using our previous implementations, and experiment with different 3D parallelism configurations. We have also seen how to profile the performance of the 3D parallelism and compare different configurations.

With that, we conclude our tutorial series on parallelism in JAX. We hope you have gained a good understanding of the different parallelism strategies and how to implement them in JAX. We hope you have enjoyed the tutorials and learned something new. If you have any questions or feedback, feel free to reach out or create an issue on our GitHub repository. Happy scaling!

4.15.5 References and Resources

[Shoeybi et al., 2019] Shoeybi, M., Patwary, M., Puri, R., LeGresley, P., Casper, J. and Catanzaro, B., 2019. Megatron-lm: Training multi-billion parameter language models using model parallelism. arXiv preprint arXiv:1909.08053. Paper link

[Hagemann et al., 2023] Hagemann, J., Weinbach, S., Dobler, K., Schall, M. and de Melo, G., 2023, October. Efficient Parallelization Layouts for Large-Scale Distributed Model Training. In Workshop on Advancing Neural Network Training: Computational Efficiency, Scalability, and Resource Optimization (WANT@ NeurIPS 2023). Paper link

[Huggingface, 2024] Huggingface, 2024. Model Parallelism. Documentation link

[DeepSpeed, 2024] DeepSpeed, 2024. Pipeline Parallelism. Tutorial link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.16 Tutorial 2: Introduction to PyTorch

Filled notebook:
Recordings:
Author: Phillip Lippe

Welcome to our PyTorch tutorial for the Deep Learning course 2023 at the University of Amsterdam! The following notebook is meant to give a short introduction to PyTorch basics, and get you setup for writing your own neural networks. PyTorch is an open source machine learning framework that allows you to write your own neural networks and optimize them efficiently. However, PyTorch is not the only framework of its kind. Alternatives to PyTorch include TensorFlow, JAX and Caffe. We choose to teach PyTorch at the University of Amsterdam because it is well established, has a huge developer community (originally developed by Facebook), is very flexible and especially used in research. Many current papers publish their code in PyTorch, and thus it is good to be familiar with PyTorch as well. Meanwhile, TensorFlow (developed by Google) is usually known for being a production-grade deep learning library. Still, if you know one machine learning framework in depth, it is very easy to learn another one because many of them use the same concepts and ideas. For instance, TensorFlow's version 2 was heavily inspired by the most popular features of PyTorch, making the frameworks even more similar. If you are already familiar with PyTorch and have created your own neural network projects, feel free to just skim this notebook.

We are of course not the first ones to create a PyTorch tutorial. There are many great tutorials online, including the "60-min blitz" on the official PyTorch website. Yet, we choose to create our own tutorial which is designed to give you the basics particularly necessary for the practicals, but still understand how PyTorch works under the hood. Over the next few weeks, we will also keep exploring new PyTorch features in the series of Jupyter notebook tutorials about deep learning.

We will use a set of standard libraries that are often used in machine learning projects. If you are running this notebook on Google Colab, all libraries should be pre-installed. If you are running this notebook locally, make sure you have installed our `dl2023` environment and have activated it.

[1]:
```
## Standard libraries
import os
import math
import numpy as np
import time

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgba
import seaborn as sns
sns.set()

## Progress bar
from tqdm.notebook import tqdm
```

```
/tmp/ipykernel_875535/3937499902.py:11: DeprecationWarning: `set_matplotlib_formats` is␣
↪deprecated since IPython 7.23, directly use `matplotlib_inline.backend_inline.set_
↪matplotlib_formats()`
  set_matplotlib_formats('svg', 'pdf') # For export
```

4.16.1 The Basics of PyTorch

We will start with reviewing the very basic concepts of PyTorch. As a prerequisite, we recommend to be familiar with the `numpy` package as most machine learning frameworks are based on very similar concepts. If you are not familiar with numpy yet, don't worry: here is a tutorial to go through.

So, let's start with importing PyTorch. The package is called `torch`, based on its original framework Torch. As a first step, we can check its version:

[2]:
```
import torch
print("Using torch", torch.__version__)
```

```
Using torch 2.1.0
```

At the time of writing this tutorial (end of October 2023), the current stable version is 2.1. You should therefore see the output `Using torch 2.1.0` or `Using torch 2.0.0`, eventually with some extension for the CUDA version on Colab. In case you use the `dl2023` environment, you should see `Using torch 2.1.0`. In general, it is recommended to keep the PyTorch version updated to the newest one. If you see a lower version number than 2.0, make sure you have installed the correct environment, or ask one of your TAs. In case PyTorch 2.2 or newer will be published during the time of the course, don't worry. The interface between PyTorch versions doesn't change too much, and hence all code should also be runnable with newer versions.

As in every machine learning framework, PyTorch provides functions that are stochastic like generating random numbers. However, a very good practice is to setup your code to be reproducible with the exact same random numbers. This is why we set a seed below.

[3]:
```
torch.manual_seed(42) # Setting the seed
```

[3]:
```
<torch._C.Generator at 0x7fa327d6da90>
```

Tensors

Tensors are the PyTorch equivalent to Numpy arrays, with the addition to also have support for GPU acceleration (more on that later). The name "tensor" is a generalization of concepts you already know. For instance, a vector is a 1-D tensor, and a matrix a 2-D tensor. When working with neural networks, we will use tensors of various shapes and number of dimensions.

Most common functions you know from numpy can be used on tensors as well. Actually, since numpy arrays are so similar to tensors, we can convert most tensors to numpy arrays (and back) but we don't need it too often.

Initialization

Let's first start by looking at different ways of creating a tensor. There are many possible options, the simplest one is to call `torch.Tensor` passing the desired shape as input argument:

[4]:
```
x = torch.Tensor(2, 3, 4)
print(x)
```

```
tensor([[[ 6.5254e+10,  3.0890e-41,  4.2039e-45, -6.3663e-15],
         [ 6.5246e+10,  3.0890e-41,  1.6367e-42,  4.5787e-41],
         [ 6.5254e+10,  3.0890e-41,  4.2039e-45,  4.5787e-41]],

        [[ 6.5255e+10,  3.0890e-41,  1.4013e-45,  0.0000e+00],
         [ 6.5255e+10,  3.0890e-41,  6.5246e+10,  3.0890e-41],
         [ 1.7404e-42, -5.0820e+26,  6.5255e+10,  3.0890e-41]]])
```

The function `torch.Tensor` allocates memory for the desired tensor, but reuses any values that have already been in the memory. To directly assign values to the tensor during initialization, there are many alternatives including:

- `torch.zeros`: Creates a tensor filled with zeros
- `torch.ones`: Creates a tensor filled with ones
- `torch.rand`: Creates a tensor with random values uniformly sampled between 0 and 1
- `torch.randn`: Creates a tensor with random values sampled from a normal distribution with mean 0 and variance 1
- `torch.arange`: Creates a tensor containing the values $N, N+1, N+2, ..., M$
- `torch.Tensor` (input list): Creates a tensor from the list elements you provide

[5]:
```
# Create a tensor from a (nested) list
x = torch.Tensor([[1, 2], [3, 4]])
print(x)
```

```
tensor([[1., 2.],
        [3., 4.]])
```

[6]:
```
# Create a tensor with random values between 0 and 1 with the shape [2, 3, 4]
x = torch.rand(2, 3, 4)
print(x)
```

```
tensor([[[0.8823, 0.9150, 0.3829, 0.9593],
         [0.3904, 0.6009, 0.2566, 0.7936],
         [0.9408, 0.1332, 0.9346, 0.5936]],
```

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```
        [[0.8694, 0.5677, 0.7411, 0.4294],
         [0.8854, 0.5739, 0.2666, 0.6274],
         [0.2696, 0.4414, 0.2969, 0.8317]]])
```

You can obtain the shape of a tensor in the same way as in numpy (`x.shape`), or using the `.size` method:

[7]:
```
shape = x.shape
print("Shape:", x.shape)

size = x.size()
print("Size:", size)

dim1, dim2, dim3 = x.size()
print("Size:", dim1, dim2, dim3)
```

```
Shape: torch.Size([2, 3, 4])
Size: torch.Size([2, 3, 4])
Size: 2 3 4
```

Tensor to Numpy, and Numpy to Tensor

Tensors can be converted to numpy arrays, and numpy arrays back to tensors. To transform a numpy array into a tensor, we can use the function `torch.from_numpy`:

[8]:
```
np_arr = np.array([[1, 2], [3, 4]])
tensor = torch.from_numpy(np_arr)

print("Numpy array:", np_arr)
print("PyTorch tensor:", tensor)
```

```
Numpy array: [[1 2]
 [3 4]]
PyTorch tensor: tensor([[1, 2],
        [3, 4]])
```

To transform a PyTorch tensor back to a numpy array, we can use the function `.numpy()` on tensors:

[9]:
```
tensor = torch.arange(4)
np_arr = tensor.numpy()

print("PyTorch tensor:", tensor)
print("Numpy array:", np_arr)
```

```
PyTorch tensor: tensor([0, 1, 2, 3])
Numpy array: [0 1 2 3]
```

The conversion of tensors to numpy require the tensor to be on the CPU, and not the GPU (more on GPU support in a later section). In case you have a tensor on GPU, you need to call `.cpu()` on the tensor beforehand. Hence, you get a line like `np_arr = tensor.cpu().numpy()`.

Operations

Most operations that exist in numpy, also exist in PyTorch. A full list of operations can be found in the PyTorch documentation, but we will review the most important ones here.

The simplest operation is to add two tensors:

[10]:
```
x1 = torch.rand(2, 3)
x2 = torch.rand(2, 3)
y = x1 + x2

print("X1", x1)
print("X2", x2)
print("Y", y)
```

```
X1 tensor([[0.1053, 0.2695, 0.3588],
        [0.1994, 0.5472, 0.0062]])
X2 tensor([[0.9516, 0.0753, 0.8860],
        [0.5832, 0.3376, 0.8090]])
Y tensor([[1.0569, 0.3448, 1.2448],
        [0.7826, 0.8848, 0.8151]])
```

Calling `x1 + x2` creates a new tensor containing the sum of the two inputs. However, we can also use in-place operations that are applied directly on the memory of a tensor. We therefore change the values of `x2` without the chance to re-accessing the values of `x2` before the operation. An example is shown below:

[11]:
```
x1 = torch.rand(2, 3)
x2 = torch.rand(2, 3)
print("X1 (before)", x1)
print("X2 (before)", x2)

x2.add_(x1)
print("X1 (after)", x1)
print("X2 (after)", x2)
```

```
X1 (before) tensor([[0.5779, 0.9040, 0.5547],
        [0.3423, 0.6343, 0.3644]])
X2 (before) tensor([[0.7104, 0.9464, 0.7890],
        [0.2814, 0.7886, 0.5895]])
X1 (after) tensor([[0.5779, 0.9040, 0.5547],
        [0.3423, 0.6343, 0.3644]])
X2 (after) tensor([[1.2884, 1.8504, 1.3437],
        [0.6237, 1.4230, 0.9539]])
```

In-place operations are usually marked with a underscore postfix (e.g. "add_" instead of "add").

Another common operation aims at changing the shape of a tensor. A tensor of size (2,3) can be re-organized to any other shape with the same number of elements (e.g. a tensor of size (6), or (3,2), ...). In PyTorch, this operation is called `view`:

[12]:
```
x = torch.arange(6)
print("X", x)
```

```
X tensor([0, 1, 2, 3, 4, 5])
```

[13]:
```
x = x.view(2, 3)
print("X", x)
```

```
X tensor([[0, 1, 2],
        [3, 4, 5]])
```

[14]:
```
x = x.permute(1, 0) # Swapping dimension 0 and 1
print("X", x)
```

```
X tensor([[0, 3],
        [1, 4],
        [2, 5]])
```

Other commonly used operations include matrix multiplications, which are essential for neural networks. Quite often, we have an input vector $\mathbf{x}$, which is transformed using a learned weight matrix $\mathbf{W}$. There are multiple ways and functions to perform matrix multiplication, some of which we list below:

- `torch.matmul`: Performs the matrix product over two tensors, where the specific behavior depends on the dimensions. If both inputs are matrices (2-dimensional tensors), it performs the standard matrix product. For higher dimensional inputs, the function supports broadcasting (for details see the documentation). Can also be written as `a @ b`, similar to numpy.
- `torch.mm`: Performs the matrix product over two matrices, but doesn't support broadcasting (see documentation)
- `torch.bmm`: Performs the matrix product with a support batch dimension. If the first tensor T is of shape $(b \times n \times m)$, and the second tensor R $(b \times m \times p)$, the output O is of shape $(b \times n \times p)$, and has been calculated by performing b matrix multiplications of the submatrices of T and R: $O_i = T_i @ R_i$
- `torch.einsum`: Performs matrix multiplications and more (i.e. sums of products) using the Einstein summation convention. Explanation of the Einstein sum can be found in assignment 1.

Usually, we use `torch.matmul` or `torch.bmm`. We can try a matrix multiplication with `torch.matmul` below.

[15]:
```
x = torch.arange(6)
x = x.view(2, 3)
print("X", x)
```

```
X tensor([[0, 1, 2],
        [3, 4, 5]])
```

[16]:
```
W = torch.arange(9).view(3, 3) # We can also stack multiple operations in a single line
print("W", W)
```

```
W tensor([[0, 1, 2],
        [3, 4, 5],
        [6, 7, 8]])
```

[17]:
```
h = torch.matmul(x, W) # Verify the result by calculating it by hand too!
print("h", h)
```

```
h tensor([[15, 18, 21],
        [42, 54, 66]])
```

Indexing

We often have the situation where we need to select a part of a tensor. Indexing works just like in numpy, so let's try it:

[18]:
```
x = torch.arange(12).view(3, 4)
print("X", x)
```

```
X tensor([[ 0,  1,  2,  3],
        [ 4,  5,  6,  7],
        [ 8,  9, 10, 11]])
```

[19]:
```
print(x[:, 1])   # Second column
```

```
tensor([1, 5, 9])
```

[20]:
```
print(x[0])      # First row
```

```
tensor([0, 1, 2, 3])
```

[21]:
```
print(x[:2, -1]) # First two rows, last column
```

```
tensor([3, 7])
```

[22]:
```
print(x[1:3, :]) # Middle two rows
```

```
tensor([[ 4,  5,  6,  7],
        [ 8,  9, 10, 11]])
```

Dynamic Computation Graph and Backpropagation

One of the main reasons for using PyTorch in Deep Learning projects is that we can automatically get **gradients/derivatives** of functions that we define. We will mainly use PyTorch for implementing neural networks, and they are just fancy functions. If we use weight matrices in our function that we want to learn, then those are called the **parameters** or simply the **weights**.

If our neural network would output a single scalar value, we would talk about taking the **derivative**, but you will see that quite often we will have **multiple** output variables ("values"); in that case we talk about **gradients**. It's a more general term.

Given an input $\mathbf{x}$, we define our function by **manipulating** that input, usually by matrix-multiplications with weight matrices and additions with so-called bias vectors. As we manipulate our input, we are automatically creating a **computational graph**. This graph shows how to arrive at our output from our input. PyTorch is a **define-by-run** framework; this means that we can just do our manipulations, and PyTorch will keep track of that graph for us. Thus, we create a dynamic computation graph along the way.

So, to recap: the only thing we have to do is to compute the **output**, and then we can ask PyTorch to automatically get the **gradients**.

> **Note: Why do we want gradients?** Consider that we have defined a function, a neural net, that is supposed to compute a certain output y for an input vector $\mathbf{x}$. We then define an **error measure** that tells us how wrong our network is; how bad it is in predicting output y from input $\mathbf{x}$. Based on this error measure, we can use the gradients to **update** the weights $\mathbf{W}$ that were responsible for the output, so that the next time we present input $\mathbf{x}$ to our network, the output will be closer to what we want.

The first thing we have to do is to specify which tensors require gradients. By default, when we create a tensor, it does not require gradients.

[23]:
```
x = torch.ones((3,))
print(x.requires_grad)
```

```
False
```

We can change this for an existing tensor using the function `requires_grad_()` (underscore indicating that this is a in-place operation). Alternatively, when creating a tensor, you can pass the argument `requires_grad=True` to most initializers we have seen above.

[24]:
```
x.requires_grad_(True)
print(x.requires_grad)
```

```
True
```

In order to get familiar with the concept of a computation graph, we will create one for the following function:

$$y = \frac{1}{\ell(x)} \sum_i \left[(x_i + 2)^2 + 3\right],$$

where we use $\ell(x)$ to denote the number of elements in x. In other words, we are taking a mean here over the operation within the sum. You could imagine that x are our parameters, and we want to optimize (either maximize or minimize) the output y. For this, we want to obtain the gradients $\partial y / \partial \mathbf{x}$. For our example, we'll use $\mathbf{x} = [0, 1, 2]$ as our input.

[25]:
```
x = torch.arange(3, dtype=torch.float32, requires_grad=True) # Only float tensors can␣
↪have gradients
print("X", x)
```

```
X tensor([0., 1., 2.], requires_grad=True)
```

Now let's build the computation graph step by step. You can combine multiple operations in a single line, but we will separate them here to get a better understanding of how each operation is added to the computation graph.

[26]:
```
a = x + 2
b = a ** 2
c = b + 3
y = c.mean()
print("Y", y)
```

```
Y tensor(12.6667, grad_fn=<MeanBackward0>)
```

Using the statements above, we have created a computation graph that looks similar to the figure below:

We calculate a based on the inputs x and the constant 2, b is a squared, and so on. The visualization is an abstraction of the dependencies between inputs and outputs of the operations we have applied. Each node of the computation graph has automatically defined a function for calculating the gradients with respect to its inputs, `grad_fn`. You can see this when we printed the output tensor y. This is why the computation graph is usually visualized in the reverse direction (arrows point from the result to the inputs). We can perform backpropagation on the computation graph by calling the function `backward()` on the last output, which effectively calculates the gradients for each tensor that has the property `requires_grad=True`:

[27]:
```
y.backward()
```

`x.grad` will now contain the gradient $\partial y / \partial \S$, and this gradient indicates how a change in $\mathbf{x}$ will affect output y given the current input $\mathbf{x} = [0, 1, 2]$:

[28]:
```
print(x.grad)
```

```
tensor([1.3333, 2.0000, 2.6667])
```

We can also verify these gradients by hand. We will calculate the gradients using the chain rule, in the same way as PyTorch did it:

$$\frac{\partial y}{\partial x_i} = \frac{\partial y}{\partial c_i}\frac{\partial c_i}{\partial b_i}\frac{\partial b_i}{\partial a_i}\frac{\partial a_i}{\partial x_i}$$

Note that we have simplified this equation to index notation, and by using the fact that all operation besides the mean do not combine the elements in the tensor. The partial derivatives are:

$$\frac{\partial a_i}{\partial x_i} = 1, \qquad \frac{\partial b_i}{\partial a_i} = 2 \cdot a_i \qquad \frac{\partial c_i}{\partial b_i} = 1 \qquad \frac{\partial y}{\partial c_i} = \frac{1}{3}$$

Hence, with the input being $\mathbf{x} = [0, 1, 2]$, our gradients are $\partial y / \partial \mathbf{x} = [4/3, 2, 8/3]$. The previous code cell should have printed the same result.

GPU support

A crucial feature of PyTorch is the support of GPUs, short for Graphics Processing Unit. A GPU can perform many thousands of small operations in parallel, making it very well suitable for performing large matrix operations in neural networks. When comparing GPUs to CPUs, we can list the following main differences (credit: Kevin Krewell, 2009)

CPU	GPU
Central Processing Unit	Graphics Processing Unit
Several cores	Many cores
Low latency	High throughput
Good for serial processing	Good for parallel processing
Can do a handful of operations at once	Can do thousands of operations at once

CPUs and GPUs have both different advantages and disadvantages, which is why many computers contain both components and use them for different tasks. In case you are not familiar with GPUs, you can read up more details in this NVIDIA blog post or here.

GPUs can accelerate the training of your network up to a factor of 100 which is essential for large neural networks. PyTorch implements a lot of functionality for supporting GPUs (mostly those of NVIDIA due to the libraries CUDA and cuDNN). First, let's check whether you have a GPU available:

[29]:
```
gpu_avail = torch.cuda.is_available()
print(f"Is the GPU available? {gpu_avail}")
```

```
Is the GPU available? True
```

If you have a GPU on your computer but the command above returns False, make sure you have the correct CUDA-version installed. The `dl2023` environment comes with the CUDA 11.8, which is selected for the Snellius supercomputer. Please change it if necessary (CUDA 11.3 is currently common on Colab). On Google Colab, make sure that you have selected a GPU in your runtime setup (in the menu, check under `Runtime -> Change runtime type`).

By default, all tensors you create are stored on the CPU. We can push a tensor to the GPU by using the function `.to(..)`, or `.cuda()`. However, it is often a good practice to define a `device` object in your code which points to the GPU if you have one, and otherwise to the CPU. Then, you can write your code with respect to this device object, and it allows you to run the same code on both a CPU-only system, and one with a GPU. Let's try it below. We can specify the device as follows:

[30]:
```
device = torch.device("cuda") if torch.cuda.is_available() else torch.device("cpu")
print("Device", device)
```

```
Device cuda
```

Now let's create a tensor and push it to the device:

[31]:
```
x = torch.zeros(2, 3)
x = x.to(device)
print("X", x)
```

```
X tensor([[0., 0., 0.],
        [0., 0., 0.]], device='cuda:0')
```

In case you have a GPU, you should now see the attribute `device='cuda:0'` being printed next to your tensor. The zero next to cuda indicates that this is the zero-th GPU device on your computer. PyTorch also supports multi-GPU systems, but this you will only need once you have very big networks to train (if interested, see the PyTorch documentation). We can also compare the runtime of a large matrix multiplication on the CPU with a operation on the GPU:

[32]:
```
x = torch.randn(5000, 5000)

## CPU version
start_time = time.time()
_ = torch.matmul(x, x)
end_time = time.time()
print(f"CPU time: {(end_time - start_time):6.5f}s")

## GPU version
x = x.to(device)
_ = torch.matmul(x, x)  # First operation to 'burn in' GPU
# CUDA is asynchronous, so we need to use different timing functions
start = torch.cuda.Event(enable_timing=True)
end = torch.cuda.Event(enable_timing=True)
start.record()
_ = torch.matmul(x, x)
end.record()
torch.cuda.synchronize()  # Waits for everything to finish running on the GPU
print(f"GPU time: {0.001 * start.elapsed_time(end):6.5f}s")  # Milliseconds to seconds
```

```
CPU time: 0.20694s
GPU time: 0.00985s
```

Depending on the size of the operation and the CPU/GPU in your system, the speedup of this operation can be >50x. As `matmul` operations are very common in neural networks, we can already see the great benefit of training a NN on a GPU. The time estimate can be relatively noisy here because we haven't run it for multiple times. Feel free to extend this, but it also takes longer to run.

When generating random numbers, the seed between CPU and GPU is not synchronized. Hence, we need to set the seed on the GPU separately to ensure a reproducible code. Note that due to different GPU architectures, running the same code on different GPUs does not guarantee the same random numbers. Still, we don't want that our code gives us a different output every time we run it on the exact same hardware. Hence, we also set the seed on the GPU:

[33]:
```
# GPU operations have a separate seed we also want to set
if torch.cuda.is_available():
    torch.cuda.manual_seed(42)
    torch.cuda.manual_seed_all(42)

# Additionally, some operations on a GPU are implemented stochastic for efficiency
# We want to ensure that all operations are deterministic on GPU (if used) for␣
↪reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False
```

4.16.2 Learning by example: Continuous XOR

If we want to build a neural network in PyTorch, we could specify all our parameters (weight matrices, bias vectors) using `Tensors` (with `requires_grad=True`), ask PyTorch to calculate the gradients and then adjust the parameters. But things can quickly get cumbersome if we have a lot of parameters. In PyTorch, there is a package called `torch.nn` that makes building neural networks more convenient.

We will introduce the libraries and all additional parts you might need to train a neural network in PyTorch, using a simple example classifier on a simple yet well known example: XOR. Given two binary inputs x_1 and x_2, the label to predict is 1 if either x_1 or x_2 is 1 while the other is 0, or the label is 0 in all other cases. The example became famous by the fact that a single neuron, i.e. a linear classifier, cannot learn this simple function. Hence, we will learn how to build a small neural network that can learn this function. To make it a little bit more interesting, we move the XOR into continuous space and introduce some gaussian noise on the binary inputs. Our desired separation of an XOR dataset could look as follows:

The model

The package `torch.nn` defines a series of useful classes like linear networks layers, activation functions, loss functions etc. A full list can be found here. In case you need a certain network layer, check the documentation of the package first before writing the layer yourself as the package likely contains the code for it already. We import it below:

[34]:
```
import torch.nn as nn
```

Additionally to `torch.nn`, there is also `torch.nn.functional`. It contains functions that are used in network layers. This is in contrast to `torch.nn` which defines them as `nn.Modules` (more on it below), and `torch.nn` actually uses a lot of functionalities from `torch.nn.functional`. Hence, the functional package is useful in many situations, and so we import it as well here.

[35]:
```
import torch.nn.functional as F
```

nn.Module

In PyTorch, a neural network is built up out of modules. Modules can contain other modules, and a neural network is considered to be a module itself as well. The basic template of a module is as follows:

[36]:
```
class MyModule(nn.Module):

    def __init__(self):
        super().__init__()
        # Some init for my module

    def forward(self, x):
        # Function for performing the calculation of the module.
        pass
```

The forward function is where the computation of the module is taken place, and is executed when you call the module (`nn = MyModule(); nn(x)`). In the init function, we usually create the parameters of the module, using `nn.Parameter`, or defining other modules that are used in the forward function. The backward calculation is done automatically, but could be overwritten as well if wanted.

Simple classifier

We can now make use of the pre-defined modules in the `torch.nn` package, and define our own small neural network. We will use a minimal network with a input layer, one hidden layer with tanh as activation function, and a output layer. In other words, our networks should look something like this:

The input neurons are shown in blue, which represent the coordinates x_1 and x_2 of a data point. The hidden neurons including a tanh activation are shown in white, and the output neuron in red. In PyTorch, we can define this as follows:

[37]:
```
class SimpleClassifier(nn.Module):

    def __init__(self, num_inputs, num_hidden, num_outputs):
        super().__init__()
        # Initialize the modules we need to build the network
        self.linear1 = nn.Linear(num_inputs, num_hidden)
        self.act_fn = nn.Tanh()
        self.linear2 = nn.Linear(num_hidden, num_outputs)

    def forward(self, x):
        # Perform the calculation of the model to determine the prediction
        x = self.linear1(x)
        x = self.act_fn(x)
        x = self.linear2(x)
        return x
```

For the examples in this notebook, we will use a tiny neural network with two input neurons and four hidden neurons. As we perform binary classification, we will use a single output neuron. Note that we do not apply a sigmoid on the output yet. This is because other functions, especially the loss, are more efficient and precise to calculate on the original outputs instead of the sigmoid output. We will discuss the detailed reason later.

[38]:
```
model = SimpleClassifier(num_inputs=2, num_hidden=4, num_outputs=1)
# Printing a module shows all its submodules
print(model)
```

```
SimpleClassifier(
  (linear1): Linear(in_features=2, out_features=4, bias=True)
  (act_fn): Tanh()
  (linear2): Linear(in_features=4, out_features=1, bias=True)
)
```

Printing the model lists all submodules it contains. The parameters of a module can be obtained by using its `parameters()` functions, or `named_parameters()` to get a name to each parameter object. For our small neural network, we have the following parameters:

[39]:
```
for name, param in model.named_parameters():
    print(f"Parameter {name}, shape {param.shape}")
```

```
Parameter linear1.weight, shape torch.Size([4, 2])
Parameter linear1.bias, shape torch.Size([4])
Parameter linear2.weight, shape torch.Size([1, 4])
Parameter linear2.bias, shape torch.Size([1])
```

Each linear layer has a weight matrix of the shape `[output, input]`, and a bias of the shape `[output]`. The tanh activation function does not have any parameters. Note that parameters are only registered for `nn.Module` objects that are direct object attributes, i.e. `self.a = ...`. If you define a list of modules, the parameters of those are not registered for the outer module and can cause some issues when you try to optimize your module. There are alternatives, like `nn.ModuleList`, `nn.ModuleDict` and `nn.Sequential`, that allow you to have different data structures of modules. We will use them in a few later tutorials and explain them there.

The data

PyTorch also provides a few functionalities to load the training and test data efficiently, summarized in the package `torch.utils.data`.

[40]:
```
import torch.utils.data as data
```

The data package defines two classes which are the standard interface for handling data in PyTorch: `data.Dataset`, and `data.DataLoader`. The dataset class provides an uniform interface to access the training/test data, while the data loader makes sure to efficiently load and stack the data points from the dataset into batches during training.

The dataset class

The dataset class summarizes the basic functionality of a dataset in a natural way. To define a dataset in PyTorch, we simply specify two functions: `__getitem__`, and `__len__`. The get-item function has to return the i-th data point in the dataset, while the len function returns the size of the dataset. For the XOR dataset, we can define the dataset class as follows:

[41]:
```
class XORDataset(data.Dataset):

    def __init__(self, size, std=0.1):
        """
        Inputs:
```

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```
            size - Number of data points we want to generate
            std - Standard deviation of the noise (see generate_continuous_xor function)
        """
        super().__init__()
        self.size = size
        self.std = std
        self.generate_continuous_xor()

    def generate_continuous_xor(self):
        # Each data point in the XOR dataset has two variables, x and y, that can be␣
↪either 0 or 1
        # The label is their XOR combination, i.e. 1 if only x or only y is 1 while the␣
↪other is 0.
        # If x=y, the label is 0.
        data = torch.randint(low=0, high=2, size=(self.size, 2), dtype=torch.float32)
        label = (data.sum(dim=1) == 1).to(torch.long)
        # To make it slightly more challenging, we add a bit of gaussian noise to the␣
↪data points.
        data += self.std * torch.randn(data.shape)

        self.data = data
        self.label = label

    def __len__(self):
        # Number of data point we have. Alternatively self.data.shape[0], or self.label.
↪shape[0]
        return self.size

    def __getitem__(self, idx):
        # Return the idx-th data point of the dataset
        # If we have multiple things to return (data point and label), we can return␣
↪them as tuple
        data_point = self.data[idx]
        data_label = self.label[idx]
        return data_point, data_label
```

Let's try to create such a dataset and inspect it:

[42]:
```
dataset = XORDataset(size=200)
print("Size of dataset:", len(dataset))
print("Data point 0:", dataset[0])
```

```
Size of dataset: 200
Data point 0: (tensor([0.9632, 0.1117]), tensor(1))
```

To better relate to the dataset, we visualize the samples below.

[43]:
```
def visualize_samples(data, label):
    if isinstance(data, torch.Tensor):
        data = data.cpu().numpy()
    if isinstance(label, torch.Tensor):
        label = label.cpu().numpy()
    data_0 = data[label == 0]
```

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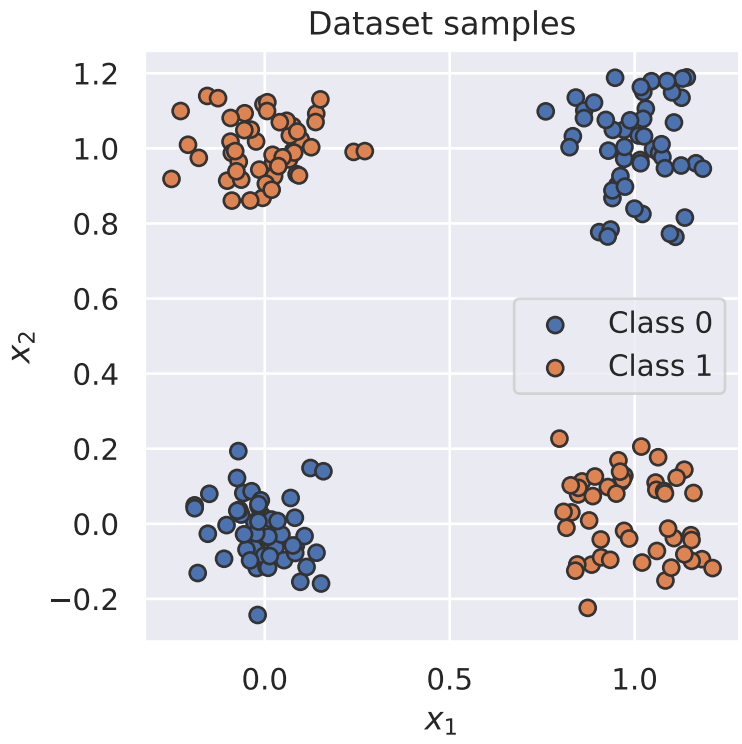
```
    data_1 = data[label == 1]

    plt.figure(figsize=(4,4))
    plt.scatter(data_0[:,0], data_0[:,1], edgecolor="#333", label="Class 0")
    plt.scatter(data_1[:,0], data_1[:,1], edgecolor="#333", label="Class 1")
    plt.title("Dataset samples")
    plt.ylabel(r"$x_2$")
    plt.xlabel(r"$x_1$")
    plt.legend()
```

[44]:
```
visualize_samples(dataset.data, dataset.label)
plt.show()
```



The data loader class

The class `torch.utils.data.DataLoader` represents a Python iterable over a dataset with support for automatic batching, multi-process data loading and many more features. The data loader communicates with the dataset using the function `__getitem__`, and stacks its outputs as tensors over the first dimension to form a batch. In contrast to the dataset class, we usually don't have to define our own data loader class, but can just create an object of it with the dataset as input. Additionally, we can configure our data loader with the following input arguments (only a selection, see full list here):

- `batch_size`: Number of samples to stack per batch
- `shuffle`: If True, the data is returned in a random order. This is important during training for introducing stochasticity.
- `num_workers`: Number of subprocesses to use for data loading. The default, 0, means that the data will be loaded

in the main process which can slow down training for datasets where loading a data point takes a considerable amount of time (e.g. large images). More workers are recommended for those, but can cause issues on Windows computers. For tiny datasets as ours, 0 workers are usually faster.

- `pin_memory`: If True, the data loader will copy Tensors into CUDA pinned memory before returning them. This can save some time for large data points on GPUs. Usually a good practice to use for a training set, but not necessarily for validation and test to save memory on the GPU.
- `drop_last`: If True, the last batch is dropped in case it is smaller than the specified batch size. This occurs when the dataset size is not a multiple of the batch size. Only potentially helpful during training to keep a consistent batch size.

Let's create a simple data loader below:

[45]:
```
data_loader = data.DataLoader(dataset, batch_size=8, shuffle=True)
```

[46]:
```
# next(iter(...)) catches the first batch of the data loader
# If shuffle is True, this will return a different batch every time we run this cell
# For iterating over the whole dataset, we can simple use "for batch in data_loader: ..."
data_inputs, data_labels = next(iter(data_loader))

# The shape of the outputs are [batch_size, d_1,...,d_N] where d_1,...,d_N are the
# dimensions of the data point returned from the dataset class
print("Data inputs", data_inputs.shape, "\n", data_inputs)
print("Data labels", data_labels.shape, "\n", data_labels)
```

```
Data inputs torch.Size([8, 2])
 tensor([[-0.0890,  0.8608],
        [ 1.0905, -0.0128],
        [ 0.7967,  0.2268],
        [-0.0688,  0.0371],
        [ 0.8732, -0.2240],
        [-0.0559, -0.0282],
        [ 0.9277,  0.0978],
        [ 1.0150,  0.9689]])
Data labels torch.Size([8])
 tensor([1, 1, 1, 0, 1, 0, 1, 0])
```

Optimization

After defining the model and the dataset, it is time to prepare the optimization of the model. During training, we will perform the following steps:

1. Get a batch from the data loader
2. Obtain the predictions from the model for the batch
3. Calculate the loss based on the difference between predictions and labels
4. Backpropagation: calculate the gradients for every parameter with respect to the loss
5. Update the parameters of the model in the direction of the gradients

We have seen how we can do step 1, 2 and 4 in PyTorch. Now, we will look at step 3 and 5.

Loss modules

We can calculate the loss for a batch by simply performing a few tensor operations as those are automatically added to the computation graph. For instance, for binary classification, we can use Binary Cross Entropy (BCE) which is defined as follows:

$$\mathcal{L}_{BCE} = -\sum_i \left[y_i \log x_i + (1 - y_i) \log(1 - x_i) \right]$$

where y are our labels, and x our predictions, both in the range of $[0, 1]$. However, PyTorch already provides a list of predefined loss functions which we can use (see here for a full list). For instance, for BCE, PyTorch has two modules: `nn.BCELoss()`, `nn.BCEWithLogitsLoss()`. While `nn.BCELoss` expects the inputs x to be in the range $[0, 1]$, i.e. the output of a sigmoid, `nn.BCEWithLogitsLoss` combines a sigmoid layer and the BCE loss in a single class. This version is numerically more stable than using a plain Sigmoid followed by a BCE loss because of the logarithms applied in the loss function. Hence, it is adviced to use loss functions applied on "logits" where possible (remember to not apply a sigmoid on the output of the model in this case!). For our model defined above, we therefore use the module `nn.BCEWithLogitsLoss`.

[47]:
```
loss_module = nn.BCEWithLogitsLoss()
```

Stochastic Gradient Descent

For updating the parameters, PyTorch provides the package `torch.optim` that has most popular optimizers implemented. We will discuss the specific optimizers and their differences later in the course, but will for now use the simplest of them: `torch.optim.SGD`. Stochastic Gradient Descent updates parameters by multiplying the gradients with a small constant, called learning rate, and subtracting those from the parameters (hence minimizing the loss). Therefore, we slowly move towards the direction of minimizing the loss. A good default value of the learning rate for a small network as ours is 0.1.

[48]:
```
# Input to the optimizer are the parameters of the model: model.parameters()
optimizer = torch.optim.SGD(model.parameters(), lr=0.1)
```

The optimizer provides two useful functions: `optimizer.step()`, and `optimizer.zero_grad()`. The step function updates the parameters based on the gradients as explained above. The function `optimizer.zero_grad()` sets the gradients of all parameters to zero. While this function seems less relevant at first, it is a crucial pre-step before performing backpropagation. If we call the `backward` function on the loss while the parameter gradients are non-zero from the previous batch, the new gradients would actually be added to the previous ones instead of overwriting them. This is done because a parameter might occur multiple times in a computation graph, and we need to sum the gradients in this case instead of replacing them. Hence, remember to call `optimizer.zero_grad()` before calculating the gradients of a batch.

Training

Finally, we are ready to train our model. As a first step, we create a slightly larger dataset and specify a data loader with a larger batch size.

[49]:
```
train_dataset = XORDataset(size=2500)
train_data_loader = data.DataLoader(train_dataset, batch_size=128, shuffle=True)
```

Now, we can write a small training function. Remember our five steps: load a batch, obtain the predictions, calculate the loss, backpropagate, and update. Additionally, we have to push all data and model parameters to the device of our choice (GPU if available). For the tiny neural network we have, communicating the data to the GPU actually takes much more time than we could save from running the operation on CPU. For large networks, the communication time

is significantly smaller than the actual runtime making a GPU crucial in these cases. Still, to practice, we will push the data to GPU here.

[50]:
```
# Push model to device. Has to be only done once
model.to(device)
```

[50]:
```
SimpleClassifier(
  (linear1): Linear(in_features=2, out_features=4, bias=True)
  (act_fn): Tanh()
  (linear2): Linear(in_features=4, out_features=1, bias=True)
)
```

In addition, we set our model to training mode. This is done by calling `model.train()`. There exist certain modules that need to perform a different forward step during training than during testing (e.g. BatchNorm and Dropout), and we can switch between them using `model.train()` and `model.eval()`.

[51]:
```
def train_model(model, optimizer, data_loader, loss_module, num_epochs=100):
    # Set model to train mode
    model.train()

    # Training loop
    for epoch in tqdm(range(num_epochs)):
        for data_inputs, data_labels in data_loader:

            ## Step 1: Move input data to device (only strictly necessary if we use GPU)
            data_inputs = data_inputs.to(device)
            data_labels = data_labels.to(device)

            ## Step 2: Run the model on the input data
            preds = model(data_inputs)
            preds = preds.squeeze(dim=1) # Output is [Batch size, 1], but we want [Batch␣
↪size]

            ## Step 3: Calculate the loss
            loss = loss_module(preds, data_labels.float())

            ## Step 4: Perform backpropagation
            # Before calculating the gradients, we need to ensure that they are all zero.
            # The gradients would not be overwritten, but actually added to the existing␣
↪ones.
            optimizer.zero_grad()
            # Perform backpropagation
            loss.backward()

            ## Step 5: Update the parameters
            optimizer.step()
```

[52]:
```
train_model(model, optimizer, train_data_loader, loss_module)
```

```
  0%|          | 0/100 [00:00<?, ?it/s]
```

Saving a model

After finish training a model, we save the model to disk so that we can load the same weights at a later time. For this, we extract the so-called `state_dict` from the model which contains all learnable parameters. For our simple model, the state dict contains the following entries:

[53]:
```
state_dict = model.state_dict()
print(state_dict)
```

```
OrderedDict([('linear1.weight', tensor([[-2.6034, -3.3292],
        [ 1.9774, -2.4076],
        [-2.5968, -1.5908],
        [-0.5717, -0.8101]], device='cuda:0')), ('linear1.bias', tensor([ 1.4459, -1.
↪3992,  2.9882, -0.1375], device='cuda:0')), ('linear2.weight', tensor([[-4.4623,  3.
↪0885,  4.4030, -0.1377]], device='cuda:0')), ('linear2.bias', tensor([-1.6853], device=
↪'cuda:0'))])
```

To save the state dictionary, we can use `torch.save`:

[54]:
```
# torch.save(object, filename). For the filename, any extension can be used
torch.save(state_dict, "our_model.tar")
```

To load a model from a state dict, we use the function `torch.load` to load the state dict from the disk, and the module function `load_state_dict` to overwrite our parameters with the new values:

[55]:
```
# Load state dict from the disk (make sure it is the same name as above)
state_dict = torch.load("our_model.tar")

# Create a new model and load the state
new_model = SimpleClassifier(num_inputs=2, num_hidden=4, num_outputs=1)
new_model.load_state_dict(state_dict)

# Verify that the parameters are the same
print("Original model\n", model.state_dict())
print("\nLoaded model\n", new_model.state_dict())
```

```
Original model
 OrderedDict([('linear1.weight', tensor([[-2.6034, -3.3292],
        [ 1.9774, -2.4076],
        [-2.5968, -1.5908],
        [-0.5717, -0.8101]], device='cuda:0')), ('linear1.bias', tensor([ 1.4459, -1.
↪3992,  2.9882, -0.1375], device='cuda:0')), ('linear2.weight', tensor([[-4.4623,  3.
↪0885,  4.4030, -0.1377]], device='cuda:0')), ('linear2.bias', tensor([-1.6853], device=
↪'cuda:0'))])

Loaded model
 OrderedDict([('linear1.weight', tensor([[-2.6034, -3.3292],
        [ 1.9774, -2.4076],
        [-2.5968, -1.5908],
        [-0.5717, -0.8101]])), ('linear1.bias', tensor([ 1.4459, -1.3992,  2.9882, -0.
↪1375])), ('linear2.weight', tensor([[-4.4623,  3.0885,  4.4030, -0.1377]])), ('linear2.
↪bias', tensor([-1.6853]))])
```

A detailed tutorial on saving and loading models in PyTorch can be found here.

Evaluation

Once we have trained a model, it is time to evaluate it on a held-out test set. As our dataset consist of randomly generated data points, we need to first create a test set with a corresponding data loader.

[56]:
```
test_dataset = XORDataset(size=500)
# drop_last -> Don't drop the last batch although it is smaller than 128
test_data_loader = data.DataLoader(test_dataset, batch_size=128, shuffle=False, drop_
↪last=False)
```

As metric, we will use accuracy which is calculated as follows:

$$acc = \frac{\#\text{correct predictions}}{\#\text{all predictions}} = \frac{TP+TN}{TP+TN+FP+FN}$$

where TP are the true positives, TN true negatives, FP false positives, and FN the fale negatives.

When evaluating the model, we don't need to keep track of the computation graph as we don't intend to calculate the gradients. This reduces the required memory and speed up the model. In PyTorch, we can deactivate the computation graph using `with torch.no_grad(): ...`. Remember to additionally set the model to eval mode.

[57]:
```
def eval_model(model, data_loader):
    model.eval() # Set model to eval mode
    true_preds, num_preds = 0., 0.

    with torch.no_grad(): # Deactivate gradients for the following code
        for data_inputs, data_labels in data_loader:

            # Determine prediction of model on dev set
            data_inputs, data_labels = data_inputs.to(device), data_labels.to(device)
            preds = model(data_inputs)
            preds = preds.squeeze(dim=1)
            preds = torch.sigmoid(preds) # Sigmoid to map predictions between 0 and 1
            pred_labels = (preds >= 0.5).long() # Binarize predictions to 0 and 1

            # Keep records of predictions for the accuracy metric (true_preds=TP+TN, num_
↪preds=TP+TN+FP+FN)
            true_preds += (pred_labels == data_labels).sum()
            num_preds += data_labels.shape[0]

    acc = true_preds / num_preds
    print(f"Accuracy of the model: {100.0*acc:4.2f}%")
```

[58]:
```
eval_model(model, test_data_loader)
```

```
Accuracy of the model: 100.00%
```

If we trained our model correctly, we should see a score close to 100% accuracy. However, this is only possible because of our simple task, and unfortunately, we usually don't get such high scores on test sets of more complex tasks.

Visualizing classification boundaries

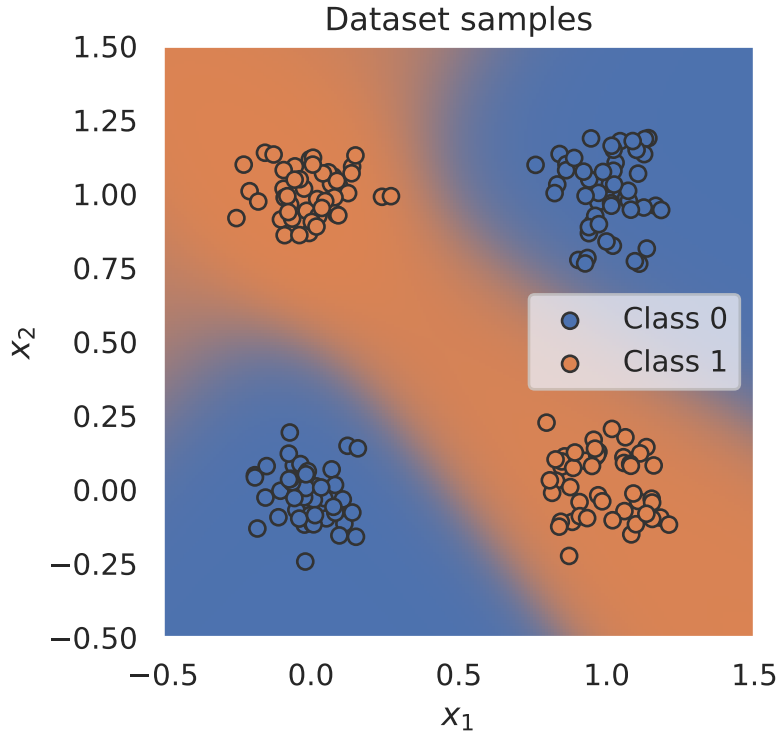
To visualize what our model has learned, we can perform a prediction for every data point in a range of $[-0.5, 1.5]$, and visualize the predicted class as in the sample figure at the beginning of this section. This shows where the model has created decision boundaries, and which points would be classified as 0, and which as 1. We therefore get a background image out of blue (class 0) and orange (class 1). The spots where the model is uncertain we will see a blurry overlap. The specific code is less relevant compared to the output figure which should hopefully show us a clear separation of classes:

[59]:
```
@torch.no_grad() # Decorator, same effect as "with torch.no_grad(): ..." over the whole␣
↪function.
def visualize_classification(model, data, label):
    if isinstance(data, torch.Tensor):
        data = data.cpu().numpy()
    if isinstance(label, torch.Tensor):
        label = label.cpu().numpy()
    data_0 = data[label == 0]
    data_1 = data[label == 1]

    fig = plt.figure(figsize=(4,4), dpi=500)
    plt.scatter(data_0[:,0], data_0[:,1], edgecolor="#333", label="Class 0")
    plt.scatter(data_1[:,0], data_1[:,1], edgecolor="#333", label="Class 1")
    plt.title("Dataset samples")
    plt.ylabel(r"$x_2$")
    plt.xlabel(r"$x_1$")
    plt.legend()

    # Let's make use of a lot of operations we have learned above
    model.to(device)
    c0 = torch.Tensor(to_rgba("C0")).to(device)
    c1 = torch.Tensor(to_rgba("C1")).to(device)
    x1 = torch.arange(-0.5, 1.5, step=0.01, device=device)
    x2 = torch.arange(-0.5, 1.5, step=0.01, device=device)
    xx1, xx2 = torch.meshgrid(x1, x2, indexing='ij')  # Meshgrid function as in numpy
    model_inputs = torch.stack([xx1, xx2], dim=-1)
    preds = model(model_inputs)
    preds = torch.sigmoid(preds)
    output_image = (1 - preds) * c0[None,None] + preds * c1[None,None]  # Specifying
↪"None" in a dimension creates a new one
    output_image = output_image.cpu().numpy()  # Convert to numpy array. This only works␣
↪for tensors on CPU, hence first push to CPU
    plt.imshow(output_image, origin='lower', extent=(-0.5, 1.5, -0.5, 1.5))
    plt.grid(False)
    return fig

_ = visualize_classification(model, dataset.data, dataset.label)
plt.show()
```



The decision boundaries might not look exactly as in the figure in the preamble of this section which can be caused by running it on CPU or a different GPU architecture. Nevertheless, the result on the accuracy metric should be the approximately the same.

4.16.3 Additional features we didn't get to discuss yet

Finally, you are all set to start with your own PyTorch project! In summary, we have looked at how we can build neural networks in PyTorch, and train and test them on data. However, there is still much more to PyTorch we haven't discussed yet. In the coming series of Jupyter notebooks, we will discover more and more functionalities of PyTorch, so that you also get familiar to PyTorch concepts beyond the basics. If you are already interested in learning more of PyTorch, we recommend the official tutorial website that contains many tutorials on various topics. Especially logging with Tensorboard (official tutorial here) is a good practice that we will explore further from Tutorial 5 on in combination with PyTorch Lightning. Nonetheless, let's check it shortly out how we could use TensorBoard in our small example.

TensorBoard logging

TensorBoard is a logging and visualization tool that is a popular choice for training deep learning models. Although initially published for TensorFlow, TensorBoard is also integrated in PyTorch allowing us to easily use it. First, let's import it below.

[60]:
```
# Import tensorboard logger from PyTorch
from torch.utils.tensorboard import SummaryWriter

# Load tensorboard extension for Jupyter Notebook, only need to start TB in the notebook
%load_ext tensorboard
```

The last line is required if you want to run TensorBoard directly in the Jupyter Notebook. Otherwise, you can start TensorBoard from the terminal.

PyTorch's TensorBoard API is simple to use. We start the logging process by creating a new object, `writer = SummaryWriter(...)`, where we specify the directory in which the logging file should be saved. With this object, we can log different aspects of our model by calling functions of the style `writer.add_...`. For example, we can visualize the computation graph with the function `writer.add_graph`, or add a scalar value like the loss with `writer.add_scalar`. Let's adapt our initial training function with adding a TensorBoard logger below.

[61]:
```
def train_model_with_logger(model, optimizer, data_loader, loss_module, val_dataset, num_
↪epochs=100, logging_dir='runs/our_experiment'):
    # Create TensorBoard logger
    writer = SummaryWriter(logging_dir)
    model_plotted = False

    # Set model to train mode
    model.train()

    # Training loop
    for epoch in tqdm(range(num_epochs)):
        epoch_loss = 0.0
        for data_inputs, data_labels in data_loader:

            ## Step 1: Move input data to device (only strictly necessary if we use GPU)
            data_inputs = data_inputs.to(device)
            data_labels = data_labels.to(device)

            # For the very first batch, we visualize the computation graph in TensorBoard
            if not model_plotted:
                writer.add_graph(model, data_inputs)
                model_plotted = True

            ## Step 2: Run the model on the input data
            preds = model(data_inputs)
            preds = preds.squeeze(dim=1) # Output is [Batch size, 1], but we want [Batch␣
↪size]

            ## Step 3: Calculate the loss
            loss = loss_module(preds, data_labels.float())

            ## Step 4: Perform backpropagation
            # Before calculating the gradients, we need to ensure that they are all zero.
            # The gradients would not be overwritten, but actually added to the existing␣
↪ones.
            optimizer.zero_grad()
            # Perform backpropagation
            loss.backward()

            ## Step 5: Update the parameters
            optimizer.step()

            ## Step 6: Take the running average of the loss
            epoch_loss += loss.item()
```

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```
        # Add average loss to TensorBoard
        epoch_loss /= len(data_loader)
        writer.add_scalar('training_loss',
                          epoch_loss,
                          global_step = epoch + 1)

        # Visualize prediction and add figure to TensorBoard
        # Since matplotlib figures can be slow in rendering, we only do it every 10th␣
↪epoch
        if (epoch + 1) % 10 == 0:
            fig = visualize_classification(model, val_dataset.data, val_dataset.label)
            writer.add_figure('predictions',
                              fig,
                              global_step = epoch + 1)

    writer.close()
```

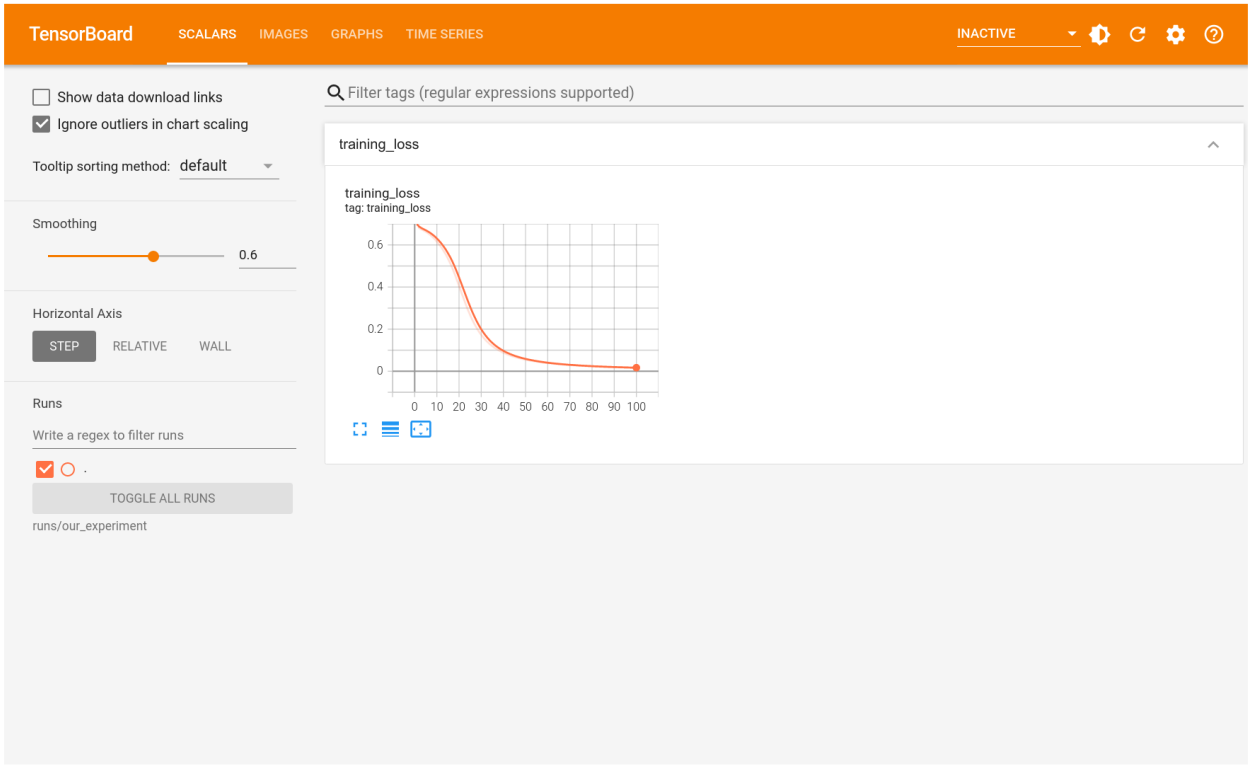
Let's use this method to train a model as before, with a new model and optimizer.

[62]:
```
model = SimpleClassifier(num_inputs=2, num_hidden=4, num_outputs=1).to(device)
optimizer = torch.optim.SGD(model.parameters(), lr=0.1)
train_model_with_logger(model, optimizer, train_data_loader, loss_module, val_
↪dataset=dataset)
```

```
  0%|          | 0/100 [00:00<?, ?it/s]
```

The TensorBoard file in the folder `runs/our_experiment` now contains a loss curve, the computation graph of our network, and a visualization of the learned predictions over number of epochs. To start the TensorBoard visualizer, simply run the following statement:

[63]:
```
%tensorboard --logdir runs/our_experiment
```



TensorBoard visualizations can help to identify possible issues with your model, and identify situations such as overfitting. You can also track the training progress while a model is training, since the logger automatically writes everything added to it to the logging file. Feel free to explore the TensorBoard functionalities, and we will make use of TensorBoards a couple of times from Tutorial 5 on.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.17 Tutorial 3: Activation Functions

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will take a closer look at (popular) activation functions and investigate their effect on optimization properties in neural networks. Activation functions are a crucial part of deep learning models as they add the non-linearity to neural networks. There is a great variety of activation functions in the literature, and some are more beneficial than others. The goal of this tutorial is to show the importance of choosing a good activation function (and how to do so), and what problems might occur if we don't.

Before we start, we import our standard libraries and set up basic functions:

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import seaborn as sns
sns.set()

## Progress bar
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
```

We will define a function to set a seed on all libraries we might interact with in this tutorial (here numpy and torch). This allows us to make our training reproducible. However, note that in contrast to the CPU, the same seed on different GPU architectures can give different results. All models here have been trained on an NVIDIA GTX1080Ti.

Additionally, the following cell defines two paths: `DATASET_PATH` and `CHECKPOINT_PATH`. The dataset path is the directory where we will download datasets used in the notebooks. It is recommended to store all datasets from PyTorch in one joined directory to prevent duplicate downloads. The checkpoint path is the directory where we will store trained model weights and additional files. The needed files will be automatically downloaded. In case you are on Google Colab, it is recommended to change the directories to start from the current directory (i.e. remove `../` for both dataset and checkpoint path).

[2]:
```
# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial3"

# Function for setting the seed
def set_seed(seed):
    np.random.seed(seed)
```

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```
    torch.manual_seed(seed)
    if torch.cuda.is_available(): # GPU operation have separate seed
        torch.cuda.manual_seed(seed)
        torch.cuda.manual_seed_all(seed)
set_seed(42)

# Additionally, some operations on a GPU are implemented stochastic for efficiency
# We want to ensure that all operations are deterministic on GPU (if used) for␣
↪reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

# Fetching the device that will be used throughout this notebook
device = torch.device("cpu") if not torch.cuda.is_available() else torch.device("cuda:0")
print("Using device", device)
```

```
Using device cuda:0
```

The following cell downloads all pretrained models we will use in this notebook. The files are stored on a separate repository to reduce the size of the notebook repository, especially for building the documentation on ReadTheDocs. In case the download below fails, you can download the models from a Google Drive folder. Please let me (Phillip) know if an error occurs so it can be fixed for all students.

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial3/"
# Files to download
pretrained_files = ["FashionMNIST_elu.config", "FashionMNIST_elu.tar",
                    "FashionMNIST_leakyrelu.config", "FashionMNIST_leakyrelu.tar",
                    "FashionMNIST_relu.config", "FashionMNIST_relu.tar",
                    "FashionMNIST_sigmoid.config", "FashionMNIST_sigmoid.tar",
                    "FashionMNIST_swish.config", "FashionMNIST_swish.tar",
                    "FashionMNIST_tanh.config", "FashionMNIST_tanh.tar"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.17.1 Common activation functions

As a first step, we will implement some common activation functions by ourselves. Of course, most of them can also be found in the `torch.nn` package (see the documentation for an overview). However, we'll write our own functions here for a better understanding and insights.

For an easier time of comparing various activation functions, we start with defining a base class from which all our future modules will inherit:

[4]:
```
class ActivationFunction(nn.Module):

    def __init__(self):
        super().__init__()
        self.name = self.__class__.__name__
        self.config = {"name": self.name}
```

Every activation function will be an `nn.Module` so that we can integrate them nicely in a network. We will use the `config` dictionary to store adjustable parameters for some activation functions.

Next, we implement two of the "oldest" activation functions that are still commonly used for various tasks: sigmoid and tanh. Both the sigmoid and tanh activation can be also found as PyTorch functions (`torch.sigmoid`, `torch.tanh`) or as modules (`nn.Sigmoid`, `nn.Tanh`). Here, we implement them by hand:

[5]:
```
##############################

class Sigmoid(ActivationFunction):

    def forward(self, x):
        return 1 / (1 + torch.exp(-x))

##############################

class Tanh(ActivationFunction):

    def forward(self, x):
        x_exp, neg_x_exp = torch.exp(x), torch.exp(-x)
        return (x_exp - neg_x_exp) / (x_exp + neg_x_exp)

##############################
```

Another popular activation function that has allowed the training of deeper networks, is the Rectified Linear Unit (ReLU). Despite its simplicity of being a piecewise linear function, ReLU has one major benefit compared to sigmoid and tanh: a strong, stable gradient for a large range of values. Based on this idea, a lot of variations of ReLU have been proposed, of which we will implement the following three: LeakyReLU, ELU, and Swish. LeakyReLU replaces the zero settings in the negative part with a smaller slope to allow gradients to flow also in this part of the input. Similarly, ELU replaces the negative part with an exponential decay. The third, most recently proposed activation function is Swish, which is actually the result of a large experiment with the purpose of finding the "optimal" activation function. Compared to the other activation functions, Swish is both smooth and non-monotonic (i.e. contains a change of sign in the gradient). This has been shown to prevent dead neurons as in standard ReLU activation, especially for deep networks. If interested, a more detailed discussion of the benefits of Swish can be found in this paper [1].

Let's implement the four activation functions below:

[6]:
```
##############################

```

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```
class ReLU(ActivationFunction):

    def forward(self, x):
        return x * (x > 0).float()

###############################

class LeakyReLU(ActivationFunction):

    def __init__(self, alpha=0.1):
        super().__init__()
        self.config["alpha"] = alpha

    def forward(self, x):
        return torch.where(x > 0, x, self.config["alpha"] * x)

###############################

class ELU(ActivationFunction):

    def forward(self, x):
        return torch.where(x > 0, x, torch.exp(x)-1)

###############################

class Swish(ActivationFunction):

    def forward(self, x):
        return x * torch.sigmoid(x)

###############################
```

For later usage, we summarize all our activation functions in a dictionary mapping the name to the class object. In case you implement a new activation function by yourself, add it here to include it in future comparisons as well:

[7]:
```
act_fn_by_name = {
    "sigmoid": Sigmoid,
    "tanh": Tanh,
    "relu": ReLU,
    "leakyrelu": LeakyReLU,
    "elu": ELU,
    "swish": Swish
}
```

Visualizing activation functions

To get an idea of what each activation function actually does, we will visualize them in the following. Next to the actual activation value, the gradient of the function is an important aspect as it is crucial for optimizing the neural network. PyTorch allows us to compute the gradients simply by calling the `backward` function:

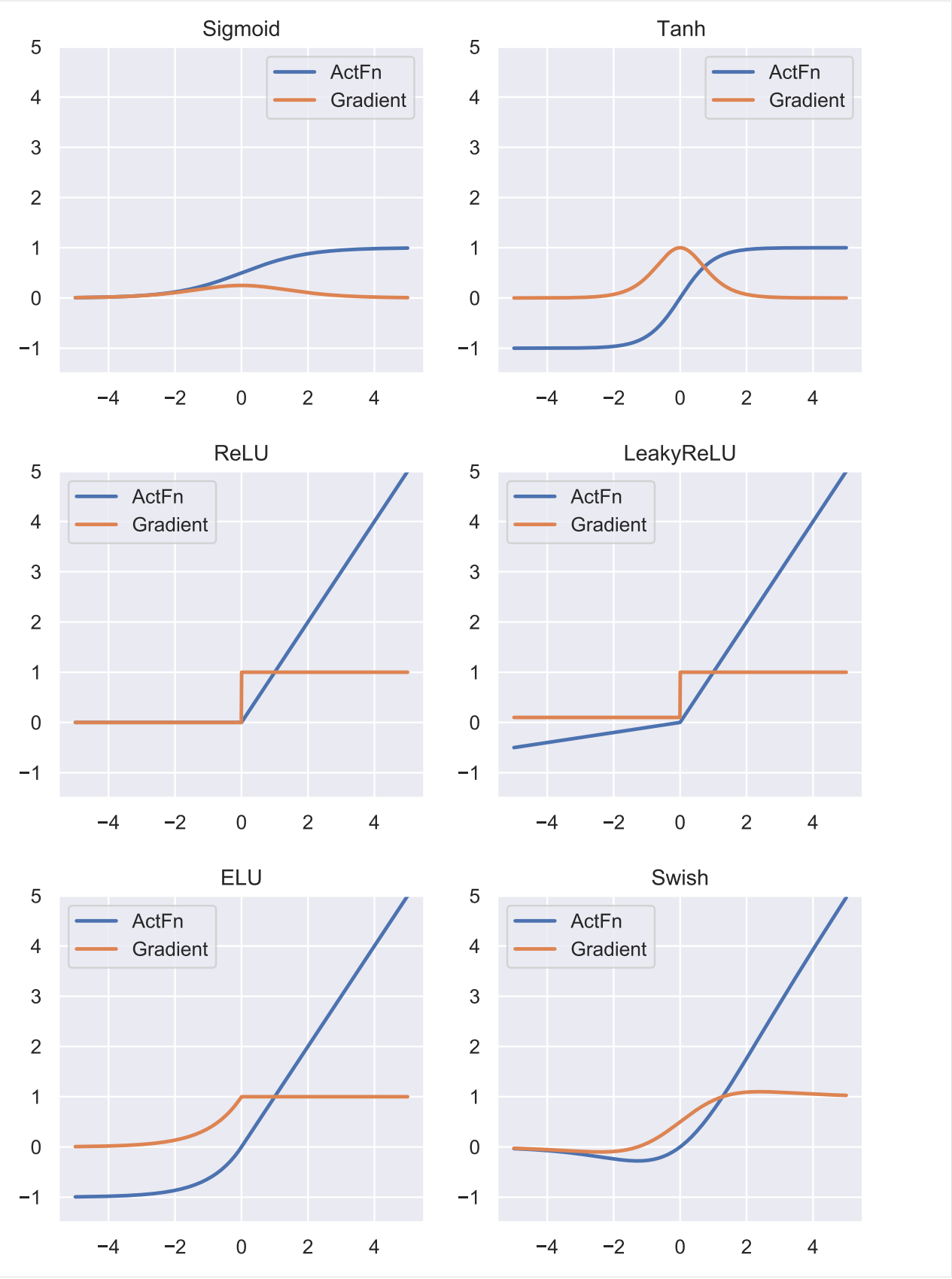
[8]:
```
def get_grads(act_fn, x):
    """
    Computes the gradients of an activation function at specified positions.

    Inputs:
        act_fn - An object of the class "ActivationFunction" with an implemented forward␣
↪pass.
        x - 1D input tensor.
    Output:
        A tensor with the same size of x containing the gradients of act_fn at x.
    """
    x = x.clone().requires_grad_() # Mark the input as tensor for which we want to store␣
↪gradients
    out = act_fn(x)
    out.sum().backward() # Summing results in an equal gradient flow to each element in x
    return x.grad # Accessing the gradients of x by "x.grad"
```

Now we can visualize all our activation functions including their gradients:

[9]:
```
def vis_act_fn(act_fn, ax, x):
    # Run activation function
    y = act_fn(x)
    y_grads = get_grads(act_fn, x)
    # Push x, y and gradients back to cpu for plotting
    x, y, y_grads = x.cpu().numpy(), y.cpu().numpy(), y_grads.cpu().numpy()
    ## Plotting
    ax.plot(x, y, linewidth=2, label="ActFn")
    ax.plot(x, y_grads, linewidth=2, label="Gradient")
    ax.set_title(act_fn.name)
    ax.legend()
    ax.set_ylim(-1.5, x.max())

# Add activation functions if wanted
act_fns = [act_fn() for act_fn in act_fn_by_name.values()]
x = torch.linspace(-5, 5, 1000) # Range on which we want to visualize the activation␣
↪functions
## Plotting
rows = math.ceil(len(act_fns)/2.0)
fig, ax = plt.subplots(rows, 2, figsize=(8, rows*4))
for i, act_fn in enumerate(act_fns):
    vis_act_fn(act_fn, ax[divmod(i,2)], x)
fig.subplots_adjust(hspace=0.3)
plt.show()
```


Sigmoid
Tanh
ReLU
LeakyReLU
ELU
Swish
ActFn
Gradient
5
4
3
2
1
0
−1
−4
−2
0
2
4

4.17.2 Analysing the effect of activation functions

After implementing and visualizing the activation functions, we are aiming to gain insights into their effect. We do this by using a simple neural network trained on FashionMNIST and examine various aspects of the model, including the performance and gradient flow.

Setup

Firstly, let's set up a neural network. The chosen network views the images as 1D tensors and pushes them through a sequence of linear layers and a specified activation function. Feel free to experiment with other network architectures.

[10]:
```
class BaseNetwork(nn.Module):

    def __init__(self, act_fn, input_size=784, num_classes=10, hidden_sizes=[512, 256,␣
↪256, 128]):
        """
        Inputs:
            act_fn - Object of the activation function that should be used as non-
↪linearity in the network.
            input_size - Size of the input images in pixels
            num_classes - Number of classes we want to predict
            hidden_sizes - A list of integers specifying the hidden layer sizes in the NN
        """
        super().__init__()

        # Create the network based on the specified hidden sizes
        layers = []
        layer_sizes = [input_size] + hidden_sizes
        for layer_index in range(1, len(layer_sizes)):
            layers += [nn.Linear(layer_sizes[layer_index-1], layer_sizes[layer_index]),
                       act_fn]
        layers += [nn.Linear(layer_sizes[-1], num_classes)]
        self.layers = nn.Sequential(*layers) # nn.Sequential summarizes a list of␣
↪modules into a single module, applying them in sequence

        # We store all hyperparameters in a dictionary for saving and loading of the␣
↪model
        self.config = {"act_fn": act_fn.config, "input_size": input_size, "num_classes":␣
↪num_classes, "hidden_sizes": hidden_sizes}

    def forward(self, x):
        x = x.view(x.size(0), -1) # Reshape images to a flat vector
        out = self.layers(x)
        return out
```

We also add functions for loading and saving the model. The hyperparameters are stored in a configuration file (simple json file):

[11]:
```
def _get_config_file(model_path, model_name):
    # Name of the file for storing hyperparameter details
    return os.path.join(model_path, model_name + ".config")

def _get_model_file(model_path, model_name):
```

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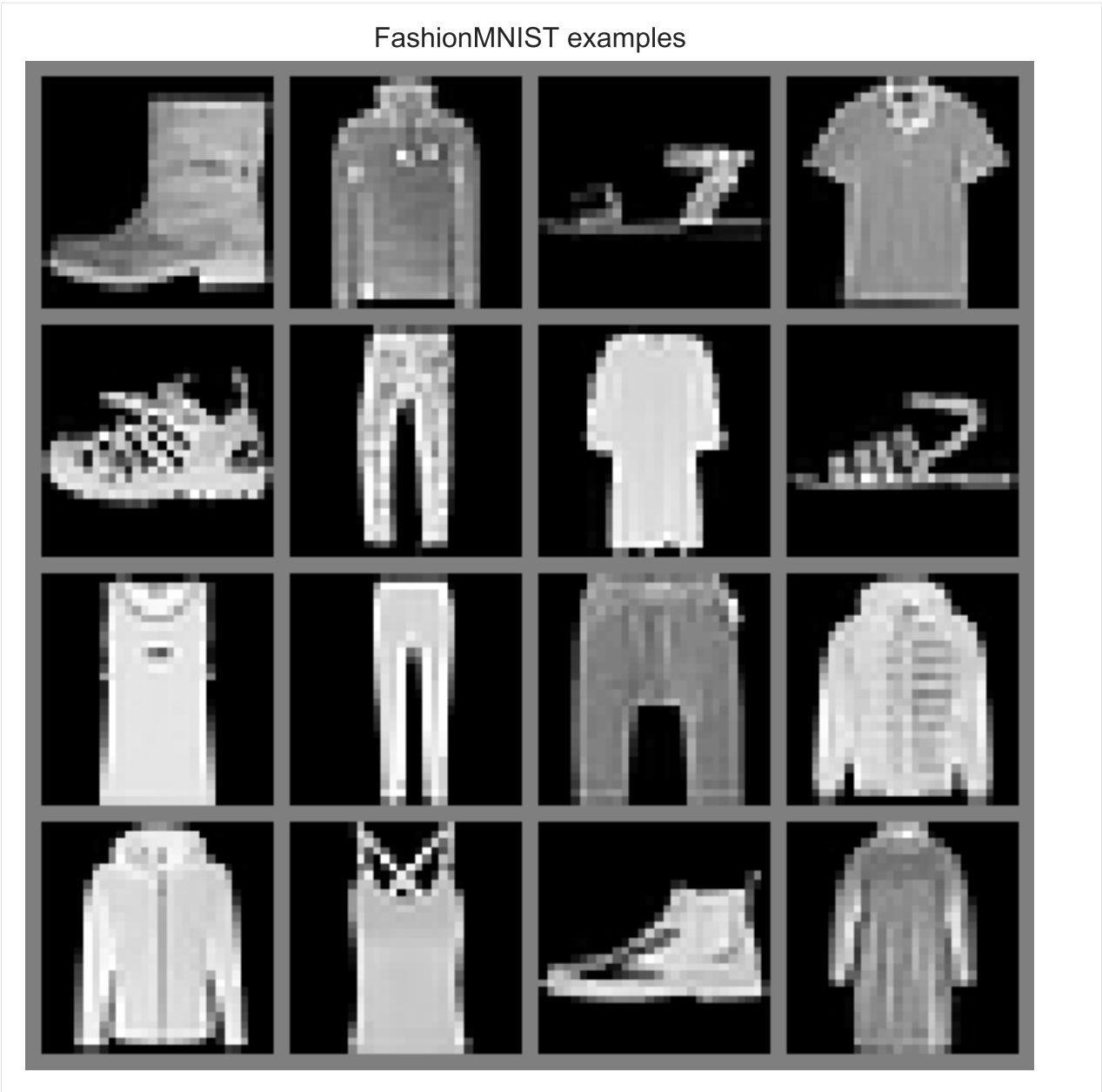
```
    # Name of the file for storing network parameters
    return os.path.join(model_path, model_name + ".tar")

def load_model(model_path, model_name, net=None):
    """
    Loads a saved model from disk.

    Inputs:
        model_path - Path of the checkpoint directory
        model_name - Name of the model (str)
        net - (Optional) If given, the state dict is loaded into this model. Otherwise,␣
↪a new model is created.
    """
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_
↪file(model_path, model_name)
    assert os.path.isfile(config_file), f"Could not find the config file \"{config_file}\
↪". Are you sure this is the correct path and you have your model config stored here?"
    assert os.path.isfile(model_file), f"Could not find the model file \"{model_file}\".␣
↪Are you sure this is the correct path and you have your model stored here?"
    with open(config_file, "r") as f:
        config_dict = json.load(f)
    if net is None:
        act_fn_name = config_dict["act_fn"].pop("name").lower()
        act_fn = act_fn_by_name[act_fn_name](**config_dict.pop("act_fn"))
        net = BaseNetwork(act_fn=act_fn, **config_dict)
    net.load_state_dict(torch.load(model_file, map_location=device))
    return net

def save_model(model, model_path, model_name):
    """
    Given a model, we save the state_dict and hyperparameters.

    Inputs:
        model - Network object to save parameters from
        model_path - Path of the checkpoint directory
        model_name - Name of the model (str)
    """
    config_dict = model.config
    os.makedirs(model_path, exist_ok=True)
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_
↪file(model_path, model_name)
    with open(config_file, "w") as f:
        json.dump(config_dict, f)
    torch.save(model.state_dict(), model_file)
```

We also set up the dataset we want to train it on, namely FashionMNIST. FashionMNIST is a more complex version of MNIST and contains black-and-white images of clothes instead of digits. The 10 classes include trousers, coats, shoes, bags and more. To load this dataset, we will make use of yet another PyTorch package, namely `torchvision` (documentation). The `torchvision` package consists of popular datasets, model architectures, and common image transformations for computer vision. We will use the package for many of the notebooks in this course to simplify our dataset handling.

Let's load the dataset below, and visualize a few images to get an impression of the data.

[12]:
```
import torchvision
from torchvision.datasets import FashionMNIST
from torchvision import transforms

# Transformations applied on each image => first make them a tensor, then normalize them␣
↪in the range -1 to 1
transform = transforms.Compose([transforms.ToTensor(),
                                transforms.Normalize((0.5,), (0.5,))])

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = FashionMNIST(root=DATASET_PATH, train=True, transform=transform,␣
↪download=True)
train_set, val_set = torch.utils.data.random_split(train_dataset, [50000, 10000])

# Loading the test set
test_set = FashionMNIST(root=DATASET_PATH, train=False, transform=transform,␣
↪download=True)

# We define a set of data loaders that we can use for various purposes later.
# Note that for actually training a model, we will use different data loaders
# with a lower batch size.
train_loader = data.DataLoader(train_set, batch_size=1024, shuffle=True, drop_last=False)
val_loader = data.DataLoader(val_set, batch_size=1024, shuffle=False, drop_last=False)
test_loader = data.DataLoader(test_set, batch_size=1024, shuffle=False, drop_last=False)
```

[13]:
```
exmp_imgs = [train_set[i][0] for i in range(16)]
# Organize the images into a grid for nicer visualization
img_grid = torchvision.utils.make_grid(torch.stack(exmp_imgs, dim=0), nrow=4,␣
↪normalize=True, pad_value=0.5)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("FashionMNIST examples")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```



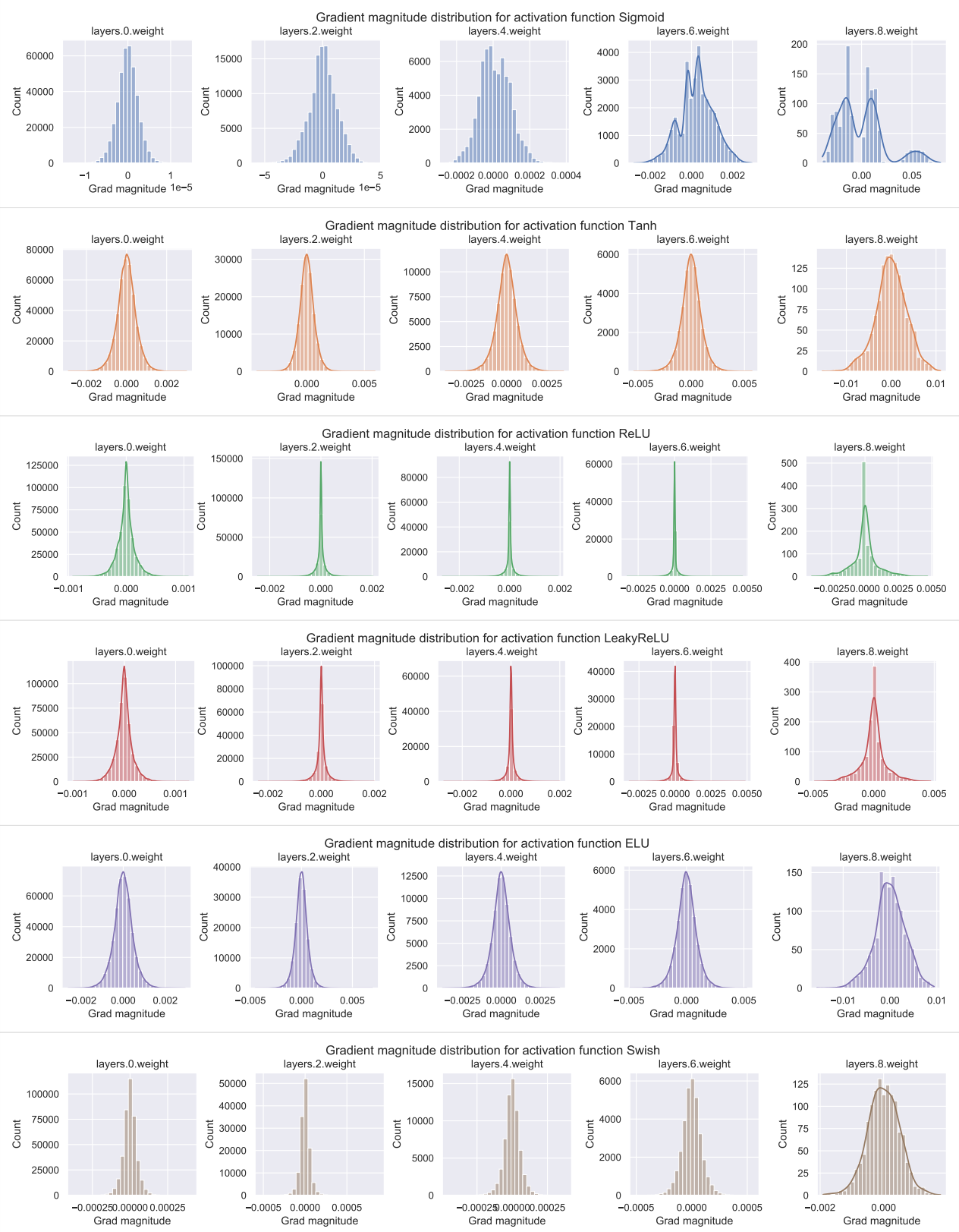
Visualizing the gradient flow after initialization

As mentioned previously, one important aspect of activation functions is how they propagate gradients through the network. Imagine we have a very deep neural network with more than 50 layers. The gradients for the input layer, i.e. the very first layer, have passed >50 times the activation function, but we still want them to be of a reasonable size. If the gradient through the activation function is (in expectation) considerably smaller than 1, our gradients will vanish until they reach the input layer. If the gradient through the activation function is larger than 1, the gradients exponentially increase and might explode.

To get a feeling of how every activation function influences the gradients, we can look at a freshly initialized network and measure the gradients for each parameter for a batch of 256 images:

[14]:
```
def visualize_gradients(net, color="C0"):
    """
    Inputs:
        net - Object of class BaseNetwork
        color - Color in which we want to visualize the histogram (for easier separation␣
↪of activation functions)
    """
    net.eval()
    small_loader = data.DataLoader(train_set, batch_size=256, shuffle=False)
    imgs, labels = next(iter(small_loader))
    imgs, labels = imgs.to(device), labels.to(device)

    # Pass one batch through the network, and calculate the gradients for the weights
    net.zero_grad()
    preds = net(imgs)
    loss = F.cross_entropy(preds, labels)
    loss.backward()
    # We limit our visualization to the weight parameters and exclude the bias to reduce␣
↪the number of plots
    grads = {name: params.grad.data.view(-1).cpu().clone().numpy() for name, params in␣
↪net.named_parameters() if "weight" in name}
    net.zero_grad()

    ## Plotting
    columns = len(grads)
    fig, ax = plt.subplots(1, columns, figsize=(columns*3.5, 2.5))
    fig_index = 0
    for key in grads:
        key_ax = ax[fig_index%columns]
        sns.histplot(data=grads[key], bins=30, ax=key_ax, color=color, kde=True)
        key_ax.set_title(str(key))
        key_ax.set_xlabel("Grad magnitude")
        fig_index += 1
    fig.suptitle(f"Gradient magnitude distribution for activation function {net.config[
↪'act_fn']['name']}", fontsize=14, y=1.05)
    fig.subplots_adjust(wspace=0.45)
    plt.show()
    plt.close()
```

[15]:
```
# Seaborn prints warnings if histogram has small values. We can ignore them for now
import warnings
warnings.filterwarnings('ignore')
## Create a plot for every activation function
for i, act_fn_name in enumerate(act_fn_by_name):
    set_seed(42) # Setting the seed ensures that we have the same weight initialization␣
↪for each activation function
    act_fn = act_fn_by_name[act_fn_name]()
    net_actfn = BaseNetwork(act_fn=act_fn).to(device)
    visualize_gradients(net_actfn, color=f"C{i}")
```



The sigmoid activation function shows a clearly undesirable behavior. While the gradients for the output layer are very large with up to 0.1, the input layer has the lowest gradient norm across all activation functions with only 1e-5. This

is due to its small maximum gradient of 1/4, and finding a suitable learning rate across all layers is not possible in this setup. All the other activation functions show to have similar gradient norms across all layers. Interestingly, the ReLU activation has a spike around 0 which is caused by its zero-part on the left, and dead neurons (we will take a closer look at this later on).

Note that additionally to the activation, the initialization of the weight parameters can be crucial. By default, PyTorch uses the Kaiming initialization for linear layers optimized for ReLU activations. In Tutorial 4, we will take a closer look at initialization, but assume for now that the Kaiming initialization works for all activation functions reasonably well.

Training a model

Next, we want to train our model with different activation functions on FashionMNIST and compare the gained performance. All in all, our final goal is to achieve the best possible performance on a dataset of our choice. Therefore, we write a training loop in the next cell including a validation after every epoch and a final test on the best model:

[16]:
```
def train_model(net, model_name, max_epochs=50, patience=7, batch_size=256,␣
↪overwrite=False):
    """
    Train a model on the training set of FashionMNIST

    Inputs:
        net - Object of BaseNetwork
        model_name - (str) Name of the model, used for creating the checkpoint names
        max_epochs - Number of epochs we want to (maximally) train for
        patience - If the performance on the validation set has not improved for
↪#patience epochs, we stop training early
        batch_size - Size of batches used in training
        overwrite - Determines how to handle the case when there already exists a␣
↪checkpoint. If True, it will be overwritten. Otherwise, we skip training.
    """
    file_exists = os.path.isfile(_get_model_file(CHECKPOINT_PATH, model_name))
    if file_exists and not overwrite:
        print("Model file already exists. Skipping training...")
    else:
        if file_exists:
            print("Model file exists, but will be overwritten...")

        # Defining optimizer, loss and data loader
        optimizer = optim.SGD(net.parameters(), lr=1e-2, momentum=0.9) # Default␣
↪parameters, feel free to change
        loss_module = nn.CrossEntropyLoss()
        train_loader_local = data.DataLoader(train_set, batch_size=batch_size,␣
↪shuffle=True, drop_last=True, pin_memory=True)

        val_scores = []
        best_val_epoch = -1
        for epoch in range(max_epochs):
            ############
            # Training #
            ############
            net.train()
            true_preds, count = 0., 0
```

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```
            for imgs, labels in tqdm(train_loader_local, desc=f"Epoch {epoch+1}",␣
↪leave=False):
                imgs, labels = imgs.to(device), labels.to(device) # To GPU
                optimizer.zero_grad() # Zero-grad can be placed anywhere before "loss.
↪backward()"
                preds = net(imgs)
                loss = loss_module(preds, labels)
                loss.backward()
                optimizer.step()
                # Record statistics during training
                true_preds += (preds.argmax(dim=-1) == labels).sum()
                count += labels.shape[0]
            train_acc = true_preds / count

            ###############
            # Validation #
            ###############
            val_acc = test_model(net, val_loader)
            val_scores.append(val_acc)
            print(f"[Epoch {epoch+1:2d}] Training accuracy: {train_acc*100.0:05.2f}%,␣
↪Validation accuracy: {val_acc*100.0:05.2f}%")

            if len(val_scores) == 1 or val_acc > val_scores[best_val_epoch]:
                print("\t   (New best performance, saving model...)")
                save_model(net, CHECKPOINT_PATH, model_name)
                best_val_epoch = epoch
            elif best_val_epoch <= epoch - patience:
                print(f"Early stopping due to no improvement over the last {patience}␣
↪epochs")
                break

        # Plot a curve of the validation accuracy
        plt.plot([i for i in range(1,len(val_scores)+1)], val_scores)
        plt.xlabel("Epochs")
        plt.ylabel("Validation accuracy")
        plt.title(f"Validation performance of {model_name}")
        plt.show()
        plt.close()

    load_model(CHECKPOINT_PATH, model_name, net=net)
    test_acc = test_model(net, test_loader)
    print((f" Test accuracy: {test_acc*100.0:4.2f}% ").center(50, "=")+"\n")
    return test_acc


def test_model(net, data_loader):
    """
    Test a model on a specified dataset.

    Inputs:
        net - Trained model of type BaseNetwork
        data_loader - DataLoader object of the dataset to test on (validation or test)
```

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```
    """
    net.eval()
    true_preds, count = 0., 0
    for imgs, labels in data_loader:
        imgs, labels = imgs.to(device), labels.to(device)
        with torch.no_grad():
            preds = net(imgs).argmax(dim=-1)
            true_preds += (preds == labels).sum().item()
            count += labels.shape[0]
    test_acc = true_preds / count
    return test_acc
```

We train one model for each activation function. We recommend using the pretrained models to save time if you are running this notebook on CPU.

[17]:
```
for act_fn_name in act_fn_by_name:
    print(f"Training BaseNetwork with {act_fn_name} activation...")
    set_seed(42)
    act_fn = act_fn_by_name[act_fn_name]()
    net_actfn = BaseNetwork(act_fn=act_fn).to(device)
    train_model(net_actfn, f"FashionMNIST_{act_fn_name}", overwrite=False)
```

```
Training BaseNetwork with sigmoid activation...
Model file already exists. Skipping training...
============= Test accuracy: 10.00% ==============

Training BaseNetwork with tanh activation...
Model file already exists. Skipping training...
============= Test accuracy: 87.59% ==============

Training BaseNetwork with relu activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.62% ==============

Training BaseNetwork with leakyrelu activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.92% ==============

Training BaseNetwork with elu activation...
Model file already exists. Skipping training...
============= Test accuracy: 87.27% ==============

Training BaseNetwork with swish activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.73% ==============
```

Not surprisingly, the model using the sigmoid activation function shows to fail and does not improve upon random performance (10 classes => 1/10 for random chance).

All the other activation functions gain similar performance. To have a more accurate conclusion, we would have to train the models for multiple seeds and look at the averages. However, the "optimal" activation function also depends on many other factors (hidden sizes, number of layers, type of layers, task, dataset, optimizer, learning rate, etc.) so that a thorough grid search would not be useful in our case. In the literature, activation functions that have shown to

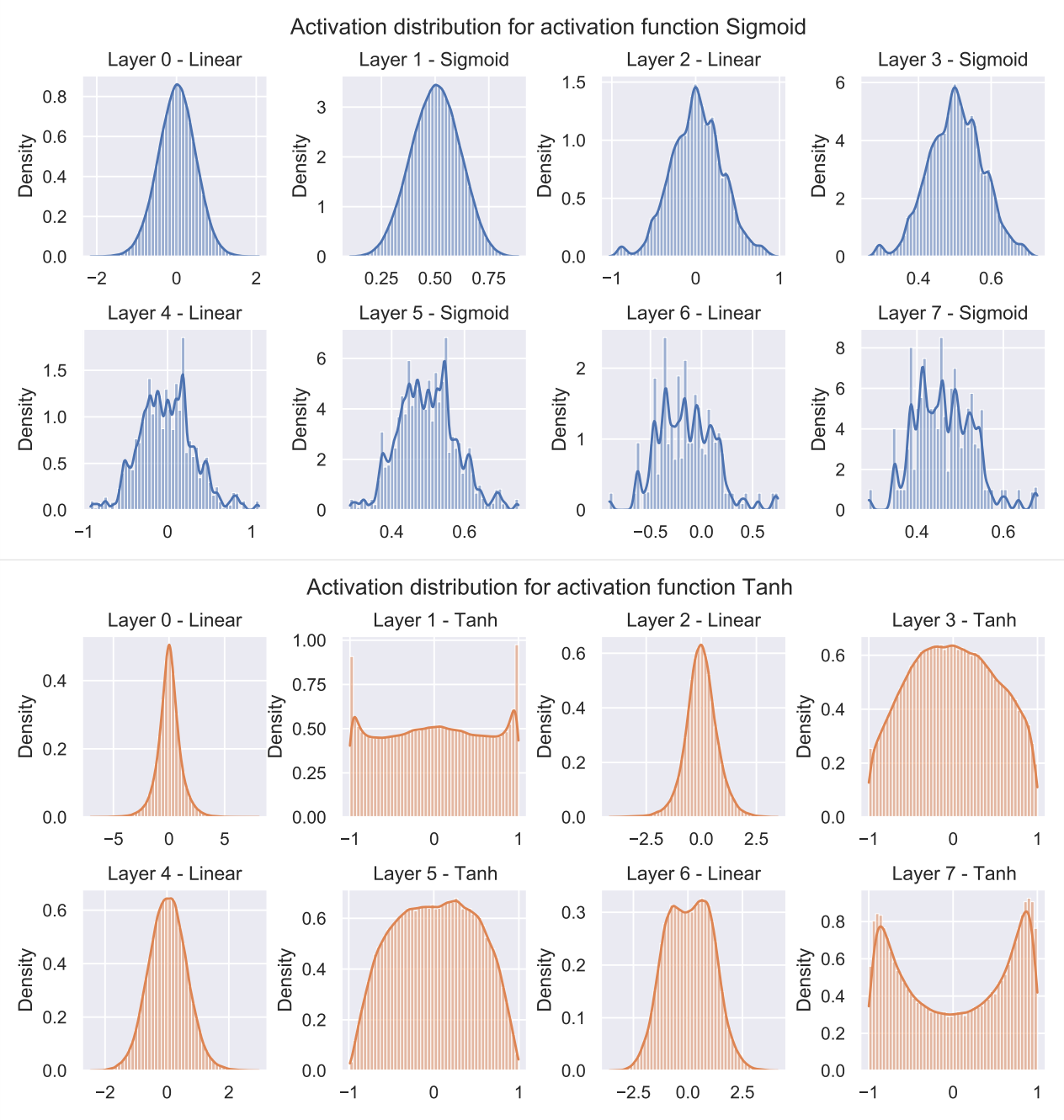
work well with deep networks are all types of ReLU functions we experiment with here, with small gains for specific activation functions in specific networks.

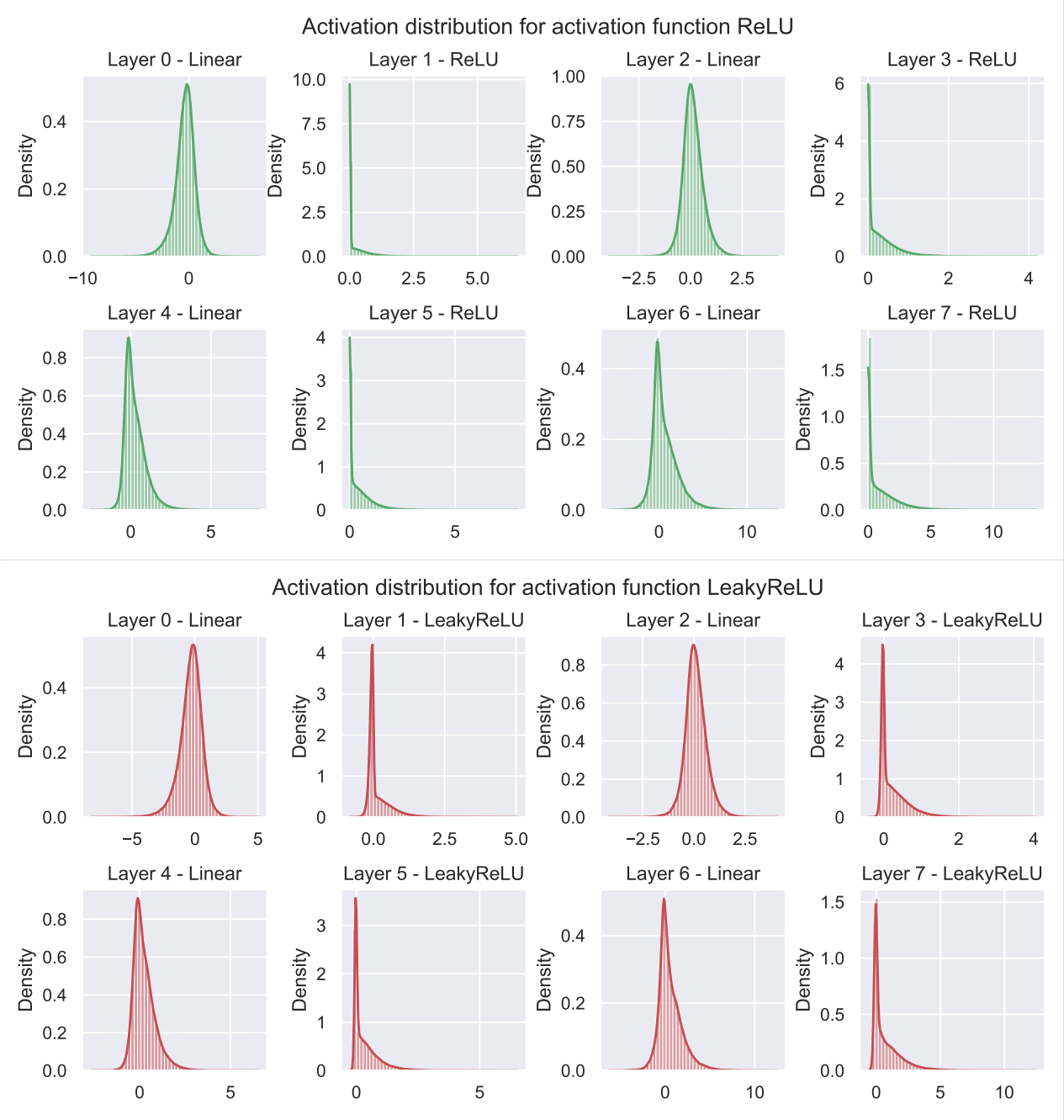
Visualizing the activation distribution

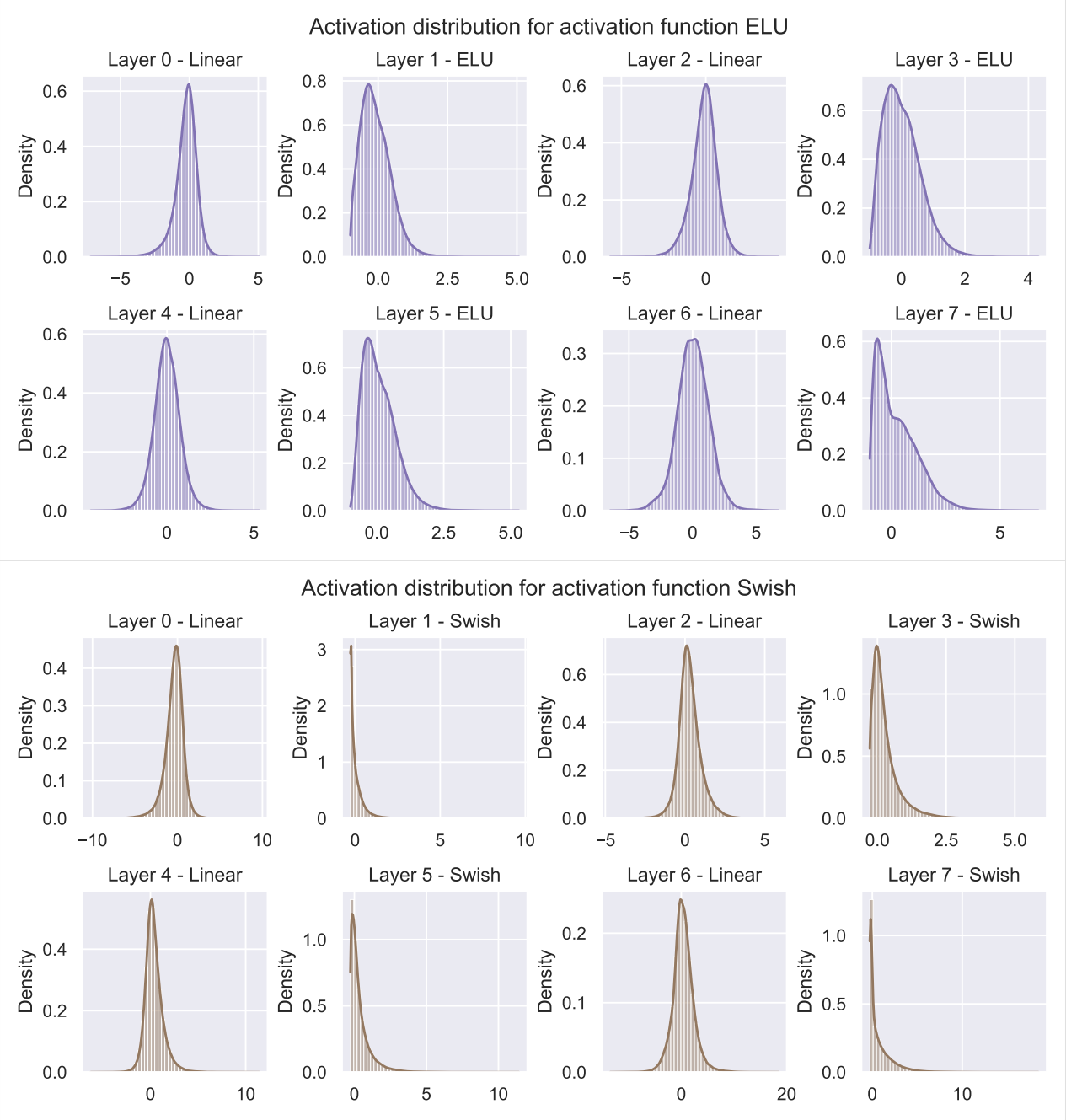
After we have trained the models, we can look at the actual activation values that find inside the model. For instance, how many neurons are set to zero in ReLU? Where do we find most values in Tanh? To answer these questions, we can write a simple function which takes a trained model, applies it to a batch of images, and plots the histogram of the activations inside the network:

[18]:
```
def visualize_activations(net, color="C0"):
    activations = {}

    net.eval()
    small_loader = data.DataLoader(train_set, batch_size=1024)
    imgs, labels = next(iter(small_loader))
    with torch.no_grad():
        layer_index = 0
        imgs = imgs.to(device)
        imgs = imgs.view(imgs.size(0), -1)
        # We need to manually loop through the layers to save all activations
        for layer_index, layer in enumerate(net.layers[:-1]):
            imgs = layer(imgs)
            activations[layer_index] = imgs.view(-1).cpu().numpy()

    ## Plotting
    columns = 4
    rows = math.ceil(len(activations)/columns)
    fig, ax = plt.subplots(rows, columns, figsize=(columns*2.7, rows*2.5))
    fig_index = 0
    for key in activations:
        key_ax = ax[fig_index//columns][fig_index%columns]
        sns.histplot(data=activations[key], bins=50, ax=key_ax, color=color, kde=True,␣
↪stat="density")
        key_ax.set_title(f"Layer {key} - {net.layers[key].__class__.__name__}")
        fig_index += 1
    fig.suptitle(f"Activation distribution for activation function {net.config['act_fn']['
↪'name']}", fontsize=14)
    fig.subplots_adjust(hspace=0.4, wspace=0.4)
    plt.show()
    plt.close()
```

[19]:
```
for i, act_fn_name in enumerate(act_fn_by_name):
    net_actfn = load_model(model_path=CHECKPOINT_PATH, model_name=f"FashionMNIST_{act_fn_
↪name}").to(device)
    visualize_activations(net_actfn, color=f"C{i}")
```


Activation distribution for activation function Sigmoid
Layer 0 - Linear
Layer 1 - Sigmoid
Layer 2 - Linear
Layer 3 - Sigmoid
Layer 4 - Linear
Layer 5 - Sigmoid
Layer 6 - Linear
Layer 7 - Sigmoid
Activation distribution for activation function Tanh
Layer 0 - Linear
Layer 1 - Tanh
Layer 2 - Linear
Layer 3 - Tanh
Layer 4 - Linear
Layer 5 - Tanh
Layer 6 - Linear
Layer 7 - Tanh
Density


Activation distribution for activation function ReLU
Layer 0 - Linear
Layer 1 - ReLU
Layer 2 - Linear
Layer 3 - ReLU
Layer 4 - Linear
Layer 5 - ReLU
Layer 6 - Linear
Layer 7 - ReLU
Activation distribution for activation function LeakyReLU
Layer 0 - Linear
Layer 1 - LeakyReLU
Layer 2 - Linear
Layer 3 - LeakyReLU
Layer 4 - Linear
Layer 5 - LeakyReLU
Layer 6 - Linear
Layer 7 - LeakyReLU
Density



As the model with sigmoid activation was not able to train properly, the activations are also less informative and all gathered around 0.5 (the activation at input 0).

The tanh shows a more diverse behavior. While for the input layer we experience a larger amount of neurons to be close to -1 and 1, where the gradients are close to zero, the activations in the two consecutive layers are closer to zero. This is probably because the input layers look for specific features in the input image, and the consecutive layers combine those together. The activations for the last layer are again more biased to the extreme points because the classification layer can be seen as a weighted average of those values (the gradients push the activations to those extremes).

The ReLU has a strong peak at 0, as we initially expected. The effect of having no gradients for negative values is that the network does not have a Gaussian-like distribution after the linear layers, but a longer tail towards the positive values. The LeakyReLU shows a very similar behavior while ELU follows again a more Gaussian-like distribution.

The Swish activation seems to lie in between, although it is worth noting that Swish uses significantly higher values than other activation functions (up to 20).

As all activation functions show slightly different behavior although obtaining similar performance for our simple network, it becomes apparent that the selection of the "optimal" activation function really depends on many factors, and is not the same for all possible networks.

Finding dead neurons in ReLU networks

One known drawback of the ReLU activation is the occurrence of "dead neurons", i.e. neurons with no gradient for any training input. The issue of dead neurons is that as no gradient is provided for the layer, we cannot train the parameters of this neuron in the previous layer to obtain output values besides zero. For dead neurons to happen, the output value of a specific neuron of the linear layer before the ReLU has to be negative for all input images. Considering the large number of neurons we have in a neural network, it is not unlikely for this to happen.

To get a better understanding of how much of a problem this is, and when we need to be careful, we will measure how many dead neurons different networks have. For this, we implement a function which runs the network on the whole training set and records whether a neuron is exactly 0 for all data points or not:

[20]:
```
def measure_number_dead_neurons(net):

    # For each neuron, we create a boolean variable initially set to 1. If it has an␣
↪activation unequals 0 at any time,
    # we set this variable to 0. After running through the whole training set, only dead␣
↪neurons will have a 1.
    neurons_dead = [
        torch.ones(layer.weight.shape[0], device=device, dtype=torch.bool) for layer in␣
↪net.layers[:-1] if isinstance(layer, nn.Linear)
    ] # Same shapes as hidden size in BaseNetwork

    net.eval()
    with torch.no_grad():
        for imgs, labels in tqdm(train_loader, leave=False): # Run through whole␣
↪training set
            layer_index = 0
            imgs = imgs.to(device)
            imgs = imgs.view(imgs.size(0), -1)
            for layer in net.layers[:-1]:
                imgs = layer(imgs)
                if isinstance(layer, ActivationFunction):
                    # Are all activations == 0 in the batch, and we did not record the␣
↪opposite in the last batches?
                    neurons_dead[layer_index] = torch.logical_and(neurons_dead[layer_
↪index], (imgs == 0).all(dim=0))
                    layer_index += 1
    number_neurons_dead = [t.sum().item() for t in neurons_dead]
    print("Number of dead neurons:", number_neurons_dead)
    print("In percentage:", ", ".join([f"{(100.0 * num_dead / tens.shape[0]):4.2f}%" for␣
↪tens, num_dead in zip(neurons_dead, number_neurons_dead)]))
```

First, we can measure the number of dead neurons for an untrained network:

[21]:
```
set_seed(42)
net_relu = BaseNetwork(act_fn=ReLU()).to(device)
```

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```
measure_number_dead_neurons(net_relu)
```

```
HBox(children=(FloatProgress(value=0.0, max=49.0), HTML(value='')))
```

```
Number of dead neurons: [0, 0, 3, 10]
In percentage: 0.00%, 0.00%, 1.17%, 7.81%
```

We see that only a minor amount of neurons are dead, but that they increase with the depth of the layer. However, this is not a problem for the small number of dead neurons we have as the input to later layers is changed due to updates to the weights of previous layers. Therefore, dead neurons in later layers can potentially become "alive"/active again.

How does this look like for a trained network (with the same initialization)?

[22]:
```
net_relu = load_model(model_path=CHECKPOINT_PATH, model_name="FashionMNIST_relu").
↪to(device)
measure_number_dead_neurons(net_relu)
```

```
HBox(children=(FloatProgress(value=0.0, max=49.0), HTML(value='')))
```

```
Number of dead neurons: [0, 0, 0, 3]
In percentage: 0.00%, 0.00%, 0.00%, 2.34%
```

The number of dead neurons indeed decreased in the later layers. However, it should be noted that dead neurons are especially problematic in the input layer. As the input does not change over epochs (the training set is kept as it is), training the network cannot turn those neurons back active. Still, the input data has usually a sufficiently high standard deviation to reduce the risk of dead neurons.

Finally, we check how the number of dead neurons behaves with increasing layer depth. For instance, let's take the following 10-layer neural network:

[23]:
```
set_seed(42)
net_relu = BaseNetwork(act_fn=ReLU(), hidden_sizes=[256, 256, 256, 256, 256, 128, 128,␣
↪128, 128, 128]).to(device)
measure_number_dead_neurons(net_relu)
```

```
HBox(children=(FloatProgress(value=0.0, max=49.0), HTML(value='')))
```

```
Number of dead neurons: [0, 0, 7, 27, 89, 60, 58, 61, 72, 56]
In percentage: 0.00%, 0.00%, 2.73%, 10.55%, 34.77%, 46.88%, 45.31%, 47.66%, 56.25%, 43.75
↪%
```

The number of dead neurons is significantly higher than before which harms the gradient flow especially in the first iterations. For instance, more than 56% of the neurons in the pre-last layer are dead which creates a considerable bottleneck. Hence, it is advisible to use other nonlinearities like Swish for very deep networks.

4.17.3 Conclusion

In this notebook, we have reviewed a set of six activation functions (sigmoid, tanh, ReLU, LeakyReLU, ELU, and Swish) in neural networks, and discussed how they influence the gradient distribution across layers. Sigmoid tends to fail deep neural networks as the highest gradient it provides is 0.25 leading to vanishing gradients in early layers. All ReLU-based activation functions have shown to perform well, and besides the original ReLU, do not have the issue of dead neurons. When implementing your own neural network, it is recommended to start with a ReLU-based network and select the specific activation function based on the properties of the network.

4.17.4 References

[1] Ramachandran, Prajit, Barret Zoph, and Quoc V. Le. "Searching for activation functions." arXiv preprint arXiv:1710.05941 (2017). Paper link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.18 Tutorial 4: Optimization and Initialization

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will review techniques for optimization and initialization of neural networks. When increasing the depth of neural networks, there are various challenges we face. Most importantly, we need to have a stable gradient flow through the network, as otherwise, we might encounter vanishing or exploding gradients. This is why we will take a closer look at the following concepts: initialization and optimization.

In the first half of the notebook, we will review different initialization techniques, and go step by step from the simplest initialization to methods that are nowadays used in very deep networks. In the second half, we focus on optimization comparing the optimizers SGD, SGD with Momentum, and Adam.

Let's start with importing our standard libraries:

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
import copy

## Imports for plotting
import matplotlib.pyplot as plt
from matplotlib import cm
%matplotlib inline
from IPython.display import set_matplotlib_formats
```

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```
set_matplotlib_formats('svg', 'pdf') # For export
import seaborn as sns
sns.set()

## Progress bar
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
```

We will use the same `set_seed` function as in Tutorial 3, as well as the path variables `DATASET_PATH` and `CHECKPOINT_PATH`. Adjust the paths if necessary.

[2]:
```
# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial4"

# Function for setting the seed
def set_seed(seed):
    np.random.seed(seed)
    torch.manual_seed(seed)
    if torch.cuda.is_available():
        torch.cuda.manual_seed(seed)
        torch.cuda.manual_seed_all(seed)
set_seed(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

# Fetching the device that will be used throughout this notebook
device = torch.device("cpu") if not torch.cuda.is_available() else torch.device("cuda:0")
print("Using device", device)
```

```
Using device cuda:0
```

In the last part of the notebook, we will train models using three different optimizers. The pretrained models for those are downloaded below.

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial4/"
# Files to download
pretrained_files = ["FashionMNIST_SGD.config",    "FashionMNIST_SGD_results.json",
↪"FashionMNIST_SGD.tar",
                    "FashionMNIST_SGDMom.config", "FashionMNIST_SGDMom_results.json",
↪"FashionMNIST_SGDMom.tar",
```

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```
                    "FashionMNIST_Adam.config",   "FashionMNIST_Adam_results.json",
↪"FashionMNIST_Adam.tar"   ]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.18.1 Preparation

Throughout this notebook, we will use a deep fully connected network, similar to our previous tutorial. We will also again apply the network to FashionMNIST, so you can relate to the results of Tutorial 3. We start by loading the FashionMNIST dataset:

[4]:
```
from torchvision.datasets import FashionMNIST
from torchvision import transforms

# Transformations applied on each image => first make them a tensor, then normalize them␣
↪with mean 0 and std 1
transform = transforms.Compose([transforms.ToTensor(),
                                transforms.Normalize((0.2861,), (0.3530,))
                               ])

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = FashionMNIST(root=DATASET_PATH, train=True, transform=transform,␣
↪download=True)
train_set, val_set = torch.utils.data.random_split(train_dataset, [50000, 10000])

# Loading the test set
test_set = FashionMNIST(root=DATASET_PATH, train=False, transform=transform,␣
↪download=True)

# We define a set of data loaders that we can use for various purposes later.
# Note that for actually training a model, we will use different data loaders
# with a lower batch size.
train_loader = data.DataLoader(train_set, batch_size=1024, shuffle=True, drop_last=False)
val_loader = data.DataLoader(val_set, batch_size=1024, shuffle=False, drop_last=False)
test_loader = data.DataLoader(test_set, batch_size=1024, shuffle=False, drop_last=False)
```

In comparison to the previous tutorial, we have changed the parameters of the normalization transformation `transforms.Normalize`. The normalization is now designed to give us an expected mean of 0 and a standard deviation of 1 across pixels. This will be particularly relevant for the discussion about initialization we will look at below,

and hence we change it here. It should be noted that in most classification tasks, both normalization techniques (between -1 and 1 or mean 0 and stddev 1) have shown to work well. We can calculate the normalization parameters by determining the mean and standard deviation on the original images:

[5]:
```
print("Mean", (train_dataset.data.float() / 255.0).mean().item())
print("Std", (train_dataset.data.float() / 255.0).std().item())
```

```
Mean 0.2860923707485199
Std 0.3530242443084717
```

We can verify the transformation by looking at the statistics of a single batch:

[6]:
```
imgs, _ = next(iter(train_loader))
print(f"Mean: {imgs.mean().item():5.3f}")
print(f"Standard deviation: {imgs.std().item():5.3f}")
print(f"Maximum: {imgs.max().item():5.3f}")
print(f"Minimum: {imgs.min().item():5.3f}")
```

```
Mean: 0.002
Standard deviation: 1.001
Maximum: 2.022
Minimum: -0.810
```

Note that the maximum and minimum are not 1 and -1 anymore, but shifted towards the positive values. This is because FashionMNIST contains a lot of black pixels, similar to MNIST.

Next, we create a linear neural network. We use the same setup as in the previous tutorial.

[7]:
```
class BaseNetwork(nn.Module):

    def __init__(self, act_fn, input_size=784, num_classes=10, hidden_sizes=[512, 256,␣
↪256, 128]):
        """
        Inputs:
            act_fn - Object of the activation function that should be used as non-
↪linearity in the network.
            input_size - Size of the input images in pixels
            num_classes - Number of classes we want to predict
            hidden_sizes - A list of integers specifying the hidden layer sizes in the NN
        """
        super().__init__()

        # Create the network based on the specified hidden sizes
        layers = []
        layer_sizes = [input_size] + hidden_sizes
        for layer_index in range(1, len(layer_sizes)):
            layers += [nn.Linear(layer_sizes[layer_index-1], layer_sizes[layer_index]),
                       act_fn]
        layers += [nn.Linear(layer_sizes[-1], num_classes)]
        self.layers = nn.ModuleList(layers) # A module list registers a list of modules␣
↪as submodules (e.g. for parameters)

        self.config = {"act_fn": act_fn.__class__.__name__, "input_size": input_size,
↪"num_classes": num_classes, "hidden_sizes": hidden_sizes}
```

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```
    def forward(self, x):
        x = x.view(x.size(0), -1)
        for l in self.layers:
            x = l(x)
        return x
```

For the activation functions, we make use of PyTorch's `torch.nn` library instead of implementing ourselves. However, we also define an `Identity` activation function. Although this activation function would significantly limit the network's modeling capabilities, we will use it in the first steps of our discussion about initialization (for simplicity).

[8]:
```
class Identity(nn.Module):
    def forward(self, x):
        return x

act_fn_by_name = {
    "tanh": nn.Tanh,
    "relu": nn.ReLU,
    "identity": Identity
}
```

Finally, we define a few plotting functions that we will use for our discussions. These functions help us to (1) visualize the weight/parameter distribution inside a network, (2) visualize the gradients that the parameters at different layers receive, and (3) the activations, i.e. the output of the linear layers. The detailed code is not important, but feel free to take a closer look if interested.

[9]:
```
##################################################################

def plot_dists(val_dict, color="C0", xlabel=None, stat="count", use_kde=True):
    columns = len(val_dict)
    fig, ax = plt.subplots(1, columns, figsize=(columns*3, 2.5))
    fig_index = 0
    for key in sorted(val_dict.keys()):
        key_ax = ax[fig_index%columns]
        sns.histplot(val_dict[key], ax=key_ax, color=color, bins=50, stat=stat,
                     kde=use_kde and ((val_dict[key].max()-val_dict[key].min())>1e-8)) #␣
↪Only plot kde if there is variance
        key_ax.set_title(f"{key} " + (r"(%i $\to$ %i)" % (val_dict[key].shape[1], val_
↪dict[key].shape[0]) if len(val_dict[key].shape)>1 else ""))
        if xlabel is not None:
            key_ax.set_xlabel(xlabel)
        fig_index += 1
    fig.subplots_adjust(wspace=0.4)
    return fig

##################################################################

def visualize_weight_distribution(model, color="C0"):
    weights = {}
    for name, param in model.named_parameters():
        if name.endswith(".bias"):
            continue
        key_name = f"Layer {name.split('.')[1]}"
```

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```
        weights[key_name] = param.detach().view(-1).cpu().numpy()

    ## Plotting
    fig = plot_dists(weights, color=color, xlabel="Weight vals")
    fig.suptitle("Weight distribution", fontsize=14, y=1.05)
    plt.show()
    plt.close()

################################################################

def visualize_gradients(model, color="C0", print_variance=False):
    """
    Inputs:
        net - Object of class BaseNetwork
        color - Color in which we want to visualize the histogram (for easier separation␣
↪of activation functions)
    """
    model.eval()
    small_loader = data.DataLoader(train_set, batch_size=1024, shuffle=False)
    imgs, labels = next(iter(small_loader))
    imgs, labels = imgs.to(device), labels.to(device)

    # Pass one batch through the network, and calculate the gradients for the weights
    model.zero_grad()
    preds = model(imgs)
    loss = F.cross_entropy(preds, labels) # Same as nn.CrossEntropyLoss, but as a␣
↪function instead of module
    loss.backward()
    # We limit our visualization to the weight parameters and exclude the bias to reduce␣
↪the number of plots
    grads = {name: params.grad.view(-1).cpu().clone().numpy() for name, params in model.
↪named_parameters() if "weight" in name}
    model.zero_grad()

    ## Plotting
    fig = plot_dists(grads, color=color, xlabel="Grad magnitude")
    fig.suptitle("Gradient distribution", fontsize=14, y=1.05)
    plt.show()
    plt.close()

    if print_variance:
        for key in sorted(grads.keys()):
            print(f"{key} - Variance: {np.var(grads[key])}")

################################################################

def visualize_activations(model, color="C0", print_variance=False):
    model.eval()
    small_loader = data.DataLoader(train_set, batch_size=1024, shuffle=False)
    imgs, labels = next(iter(small_loader))
    imgs, labels = imgs.to(device), labels.to(device)
```

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```
    # Pass one batch through the network, and calculate the gradients for the weights
    feats = imgs.view(imgs.shape[0], -1)
    activations = {}
    with torch.no_grad():
        for layer_index, layer in enumerate(model.layers):
            feats = layer(feats)
            if isinstance(layer, nn.Linear):
                activations[f"Layer {layer_index}"] = feats.view(-1).detach().cpu().
↪numpy()

    ## Plotting
    fig = plot_dists(activations, color=color, stat="density", xlabel="Activation vals")
    fig.suptitle("Activation distribution", fontsize=14, y=1.05)
    plt.show()
    plt.close()

    if print_variance:
        for key in sorted(activations.keys()):
            print(f"{key} - Variance: {np.var(activations[key])}")


##############################################################
```

4.18.2 Initialization

Before starting our discussion about initialization, it should be noted that there exist many very good blog posts about the topic of neural network initialization (for example deeplearning.ai, or a more math-focused blog post). In case something remains unclear after this tutorial, we recommend skimming through these blog posts as well.

When initializing a neural network, there are a few properties we would like to have. First, the variance of the input should be propagated through the model to the last layer, so that we have a similar standard deviation for the output neurons. If the variance would vanish the deeper we go in our model, it becomes much harder to optimize the model as the input to the next layer is basically a single constant value. Similarly, if the variance increases, it is likely to explode (i.e. head to infinity) the deeper we design our model. The second property we look out for in initialization techniques is a gradient distribution with equal variance across layers. If the first layer receives much smaller gradients than the last layer, we will have difficulties in choosing an appropriate learning rate.

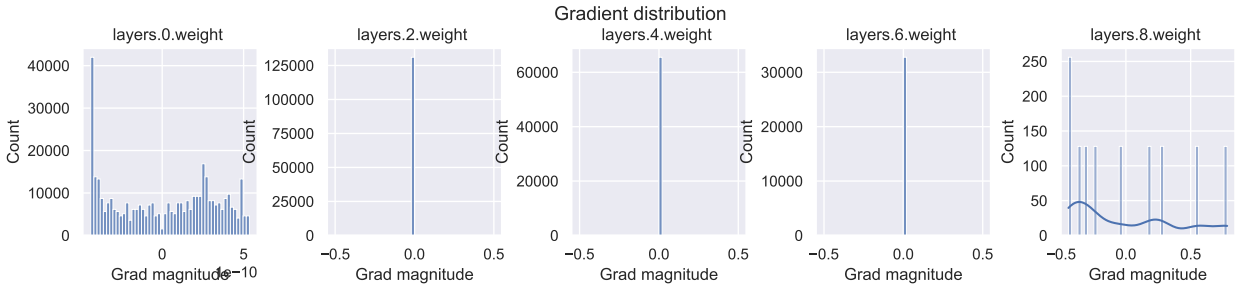
As a starting point for finding a good method, we will analyze different initialization based on our linear neural network with no activation function (i.e. an identity). We do this because initializations depend on the specific activation function used in the network, and we can adjust the initialization schemes later on for our specific choice.

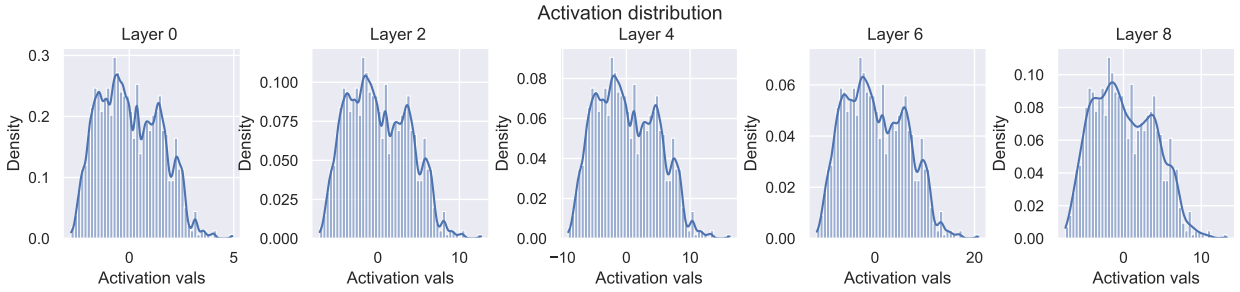
[10]:
```
model = BaseNetwork(act_fn=Identity()).to(device)
```

Constant initialization

The first initialization we can consider is to initialize all weights with the same constant value. Intuitively, setting all weights to zero is not a good idea as the propagated gradient will be zero. However, what happens if we set all weights to a value slightly larger or smaller than 0? To find out, we can implement a function for setting all parameters below and visualize the gradients.

[11]:
```
def const_init(model, c=0.0):
    for name, param in model.named_parameters():
        param.data.fill_(c)

const_init(model, c=0.005)
visualize_gradients(model)
visualize_activations(model, print_variance=True)
```





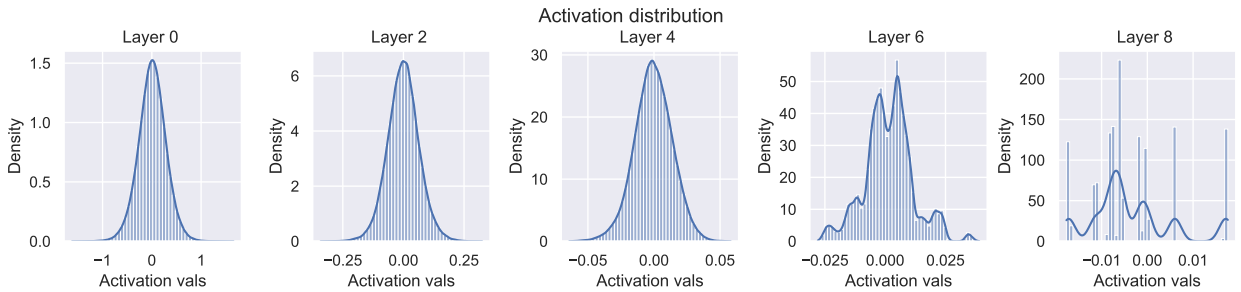

```
Layer 0 - Variance: 2.058276
Layer 2 - Variance: 13.489119
Layer 4 - Variance: 22.100567
Layer 6 - Variance: 36.209572
Layer 8 - Variance: 14.831439
```

As we can see, only the first and the last layer have diverse gradient distributions while the other three layers have the same gradient for all weights (note that this value is unequal 0, but often very close to it). Having the same gradient for parameters that have been initialized with the same values means that we will always have the same value for those parameters. This would make our layer useless and reduce our effective number of parameters to 1. Thus, we cannot use a constant initialization to train our networks.

Constant variance

From the experiment above, we have seen that a constant value is not working. So instead, how about we initialize the parameters by randomly sampling from a distribution like a Gaussian? The most intuitive way would be to choose one variance that is used for all layers in the network. Let's implement it below, and visualize the activation distribution across layers.

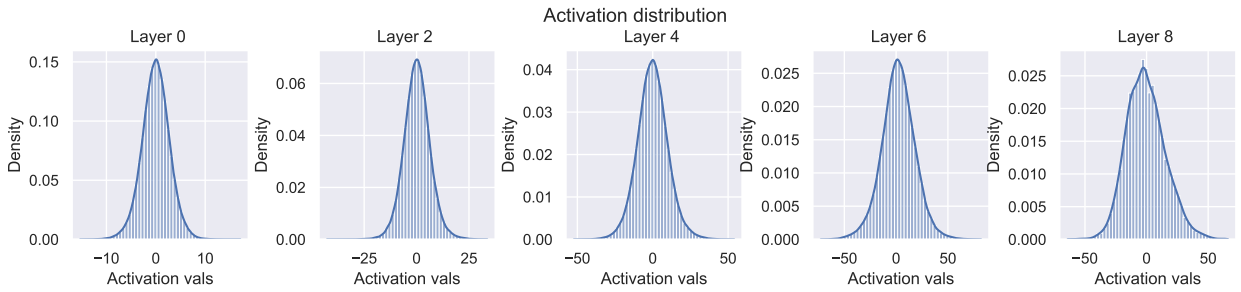
[12]:
```
def var_init(model, std=0.01):
    for name, param in model.named_parameters():
        param.data.normal_(std=std)

var_init(model, std=0.01)
visualize_activations(model, print_variance=True)
```




```
Layer 0 - Variance: 0.077930
Layer 2 - Variance: 0.004179
Layer 4 - Variance: 0.000207
Layer 6 - Variance: 0.000102
Layer 8 - Variance: 0.000083
```

The variance of the activation becomes smaller and smaller across layers, and almost vanishes in the last layer. Alternatively, we could use a higher standard deviation:

[13]:
```
var_init(model, std=0.1)
visualize_activations(model, print_variance=True)
```




```
Layer 0 - Variance: 7.901733
Layer 2 - Variance: 38.941471
Layer 4 - Variance: 103.246284
Layer 6 - Variance: 262.478546
Layer 8 - Variance: 248.354202
```

With a higher standard deviation, the activations are likely to explode. You can play around with the specific standard deviation values, but it will be hard to find one that gives us a good activation distribution across layers and is very specific to our model. If we would change the hidden sizes or number of layers, you would have to search all over again, which is neither efficient nor recommended.

How to find appropriate initialization values

From our experiments above, we have seen that we need to sample the weights from a distribution, but are not sure which one exactly. As a next step, we will try to find the optimal initialization from the perspective of the activation distribution. For this, we state two requirements:

1. The mean of the activations should be zero
2. The variance of the activations should stay the same across every layer

Suppose we want to design an initialization for the following layer: $y = Wx + b$ with $y \in \mathbb{R}^{d_y}$, $x \in \mathbb{R}^{d_x}$. Our goal is that the variance of each element of y is the same as the input, i.e. $\text{Var}(y_i) = \text{Var}(x_i) = \sigma_x^2$, and that the mean is zero. We assume x to also have a mean of zero, because, in deep neural networks, y would be the input of another layer. This requires the bias and weight to have an expectation of 0. Actually, as b is a single element per output neuron and is constant across different inputs, we set it to 0 overall.

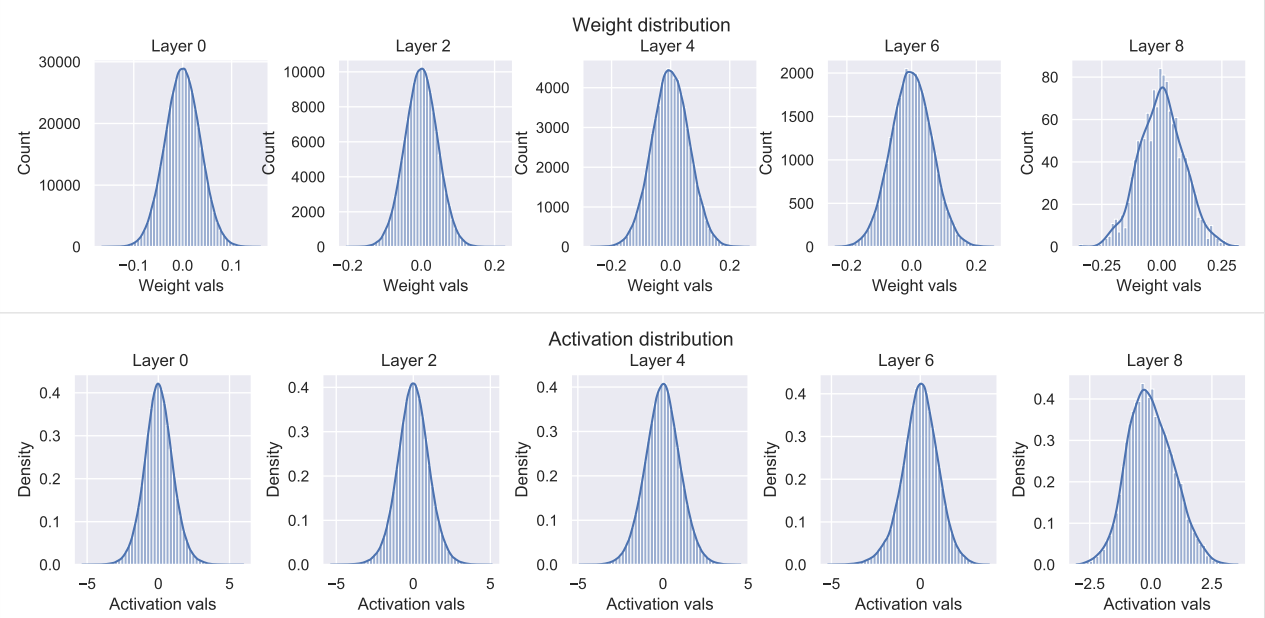
Next, we need to calculate the variance with which we need to initialize the weight parameters. Along the calculation, we will need the following variance rule: given two independent variables, the variance of their product is $\text{Var}(X \cdot Y) = \mathbb{E}(Y)^2\text{Var}(X) + \mathbb{E}(X)^2\text{Var}(Y) + \text{Var}(X)\text{Var}(Y) = \mathbb{E}(Y^2)\mathbb{E}(X^2) - \mathbb{E}(Y)^2\mathbb{E}(X)^2$ (X and Y are not refering to x and y, but any random variable).

The needed variance of the weights, $\text{Var}(w_{ij})$, is calculated as follows:

$$
\begin{aligned}
y_i &= \sum_j w_{ij} x_j && \text{Calculation of a single output neuron without bias} \\
\text{Var}(y_i) = \sigma_x^2 &= \text{Var}\left(\sum_j w_{ij} x_j\right) \\
&= \sum_j \text{Var}(w_{ij} x_j) && \text{Inputs and weights are independent of each other} \\
&= \sum_j \text{Var}(w_{ij}) \cdot \text{Var}(x_j) && \text{Variance rule (see above) with expectations being zero} \\
&= d_x \cdot \text{Var}(w_{ij}) \cdot \text{Var}(x_j) && \text{Variance equal for all } d_x \text{ elements} \\
&= \sigma_x^2 \cdot d_x \cdot \text{Var}(w_{ij}) \\
\Rightarrow \text{Var}(w_{ij}) = \sigma_W^2 &= \frac{1}{d_x}
\end{aligned}
$$

Thus, we should initialize the weight distribution with a variance of the inverse of the input dimension d_x. Let's implement it below and check whether this holds:

[14]:
```
def equal_var_init(model):
    for name, param in model.named_parameters():
        if name.endswith(".bias"):
            param.data.fill_(0)
        else:
            param.data.normal_(std=1.0/math.sqrt(param.shape[1]))

equal_var_init(model)
visualize_weight_distribution(model)
visualize_activations(model, print_variance=True)
```




```
Layer 0 - Variance: 1.020319
Layer 2 - Variance: 1.049295
Layer 4 - Variance: 1.031418
Layer 6 - Variance: 1.025792
Layer 8 - Variance: 0.872356
```

As we expected, the variance stays indeed constant across layers. Note that our initialization does not restrict us to a normal distribution, but allows any other distribution with a mean of 0 and variance of $1/d_x$. You often see that a uniform distribution is used for initialization. A small benefit of using a uniform instead of a normal distribution is that we can exclude the chance of initializing very large or small weights.

Besides the variance of the activations, another variance we would like to stabilize is the one of the gradients. This ensures a stable optimization for deep networks. It turns out that we can do the same calculation as above starting from $\Delta x = W\Delta y$, and come to the conclusion that we should initialize our layers with $1/d_y$ where d_y is the number of output neurons. You can do the calculation as a practice, or check a thorough explanation in this blog post. As a compromise between both constraints, Glorot and Bengio (2010) proposed to use the harmonic mean of both values. This leads us to the well-known Xavier initialization:

$$W \sim \mathcal{N}\left(0, \frac{2}{d_x + d_y}\right)$$

If we use a uniform distribution, we would initialize the weights with:

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{d_x + d_y}}, \frac{\sqrt{6}}{\sqrt{d_x + d_y}}\right]$$

Let's shortly implement it and validate its effectiveness:

[15]:
```
def xavier_init(model):
    for name, param in model.named_parameters():
        if name.endswith(".bias"):
            param.data.fill_(0)
        else:
            bound = math.sqrt(6)/math.sqrt(param.shape[0]+param.shape[1])
```

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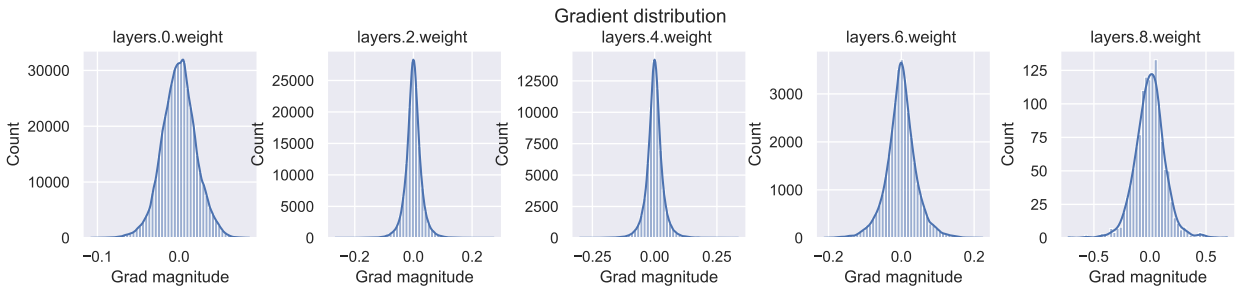
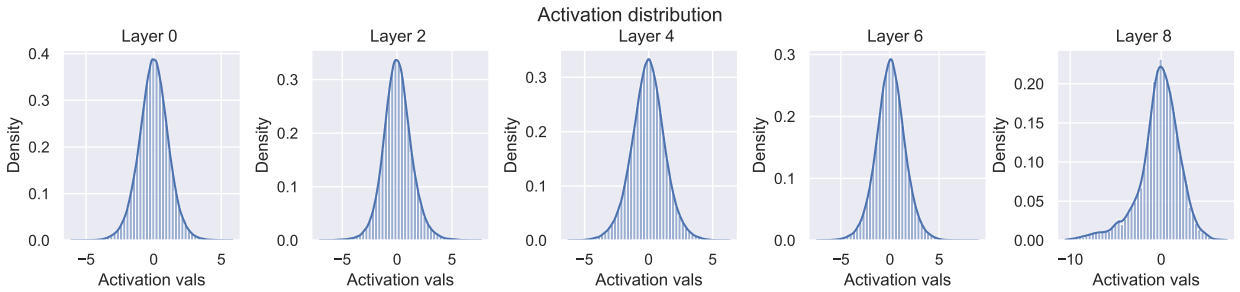
```
            param.data.uniform_(-bound, bound)

xavier_init(model)
visualize_gradients(model, print_variance=True)
visualize_activations(model, print_variance=True)
```



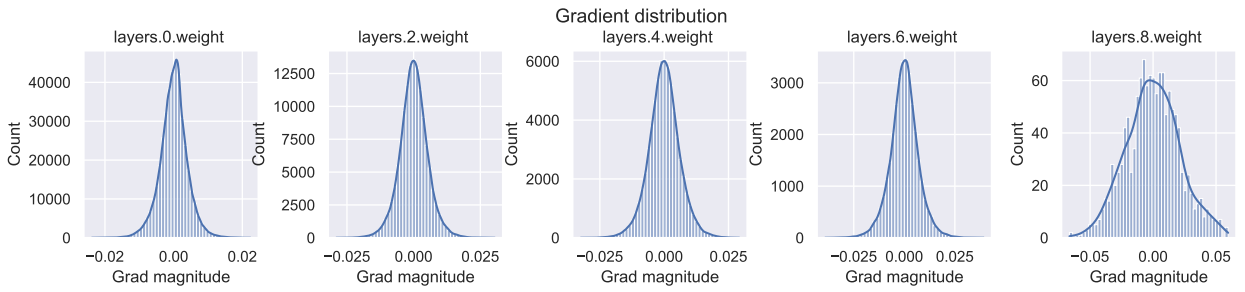

```
layers.0.weight - Variance: 0.000436
layers.2.weight - Variance: 0.000747
layers.4.weight - Variance: 0.001149
layers.6.weight - Variance: 0.001744
layers.8.weight - Variance: 0.017655
```



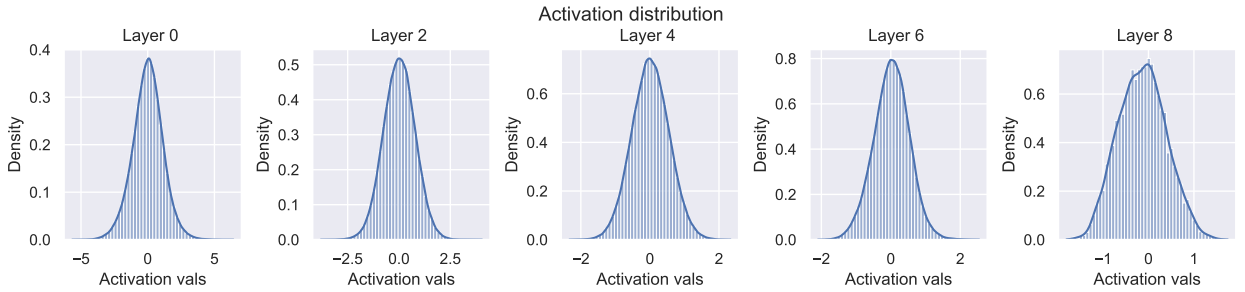

```
Layer 0 - Variance: 1.216592
Layer 2 - Variance: 1.719161
Layer 4 - Variance: 1.714506
Layer 6 - Variance: 2.224779
Layer 8 - Variance: 5.297660
```

We see that the Xavier initialization balances the variance of gradients and activations. Note that the significantly higher variance for the output layer is due to the large difference of input and output dimension (128 vs 10). However, we currently assumed the activation function to be linear. So what happens if we add a non-linearity? In a tanh-based network, a common assumption is that for small values during the initial steps in training, the tanh works as a linear function such that we don't have to adjust our calculation. We can check if that is the case for us as well:

[16]:
```
model = BaseNetwork(act_fn=nn.Tanh()).to(device)
xavier_init(model)
visualize_gradients(model, print_variance=True)
visualize_activations(model, print_variance=True)
```




```
layers.0.weight - Variance: 0.000016
layers.2.weight - Variance: 0.000027
layers.4.weight - Variance: 0.000036
layers.6.weight - Variance: 0.000049
layers.8.weight - Variance: 0.000455
```




```
Layer 0 - Variance: 1.295969
Layer 2 - Variance: 0.583388
Layer 4 - Variance: 0.291432
Layer 6 - Variance: 0.265237
Layer 8 - Variance: 0.274929
```

Although the variance decreases over depth, it is apparent that the activation distribution becomes more focused on the low values. Therefore, our variance will stabilize around 0.25 if we would go even deeper. Hence, we can conclude that the Xavier initialization works well for Tanh networks. But what about ReLU networks? Here, we cannot take the previous assumption of the non-linearity becoming linear for small values. The ReLU activation function sets (in expectation) half of the inputs to 0 so that also the expectation of the input is not zero. However, as long as the expectation of W is zero and $b = 0$, the expectation of the output is zero. The part where the calculation of the ReLU initialization differs from the identity is when determining $\text{Var}(w_{ij}x_j)$:

$$\text{Var}(w_{ij}x_j) = \underbrace{\mathbb{E}[w_{ij}^2]}_{=\text{Var}(w_{ij})}\ \mathbb{E}[x_j^2] - \underbrace{\mathbb{E}[w_{ij}]^2}_{=0}\mathbb{E}[x_j]^2 = \text{Var}(w_{ij})\mathbb{E}[x_j^2]$$

If we assume now that x is the output of a ReLU activation (from a previous layer, $x = max(0, \tilde{y})$), we can calculate the expectation as follows:

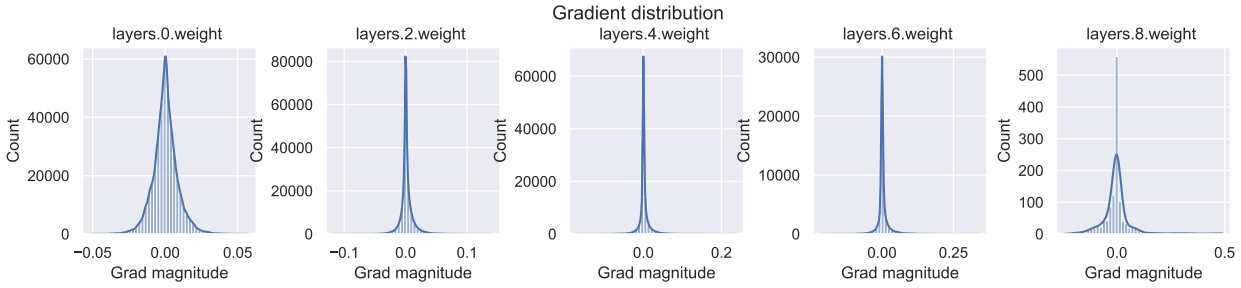
$$\begin{aligned}
\mathbb{E}[x^2] &= \mathbb{E}[\max(0, \tilde{y})^2] \\
&= \frac{1}{2}\mathbb{E}[\tilde{y}^2] && \tilde{y} \text{ is zero-centered and symmetric} \\
&= \frac{1}{2}\text{Var}(\tilde{y})
\end{aligned}$$

Thus, we see that we have an additional factor of 1/2 in the equation, so that our desired weight variance becomes $2/d_x$. This gives us the Kaiming initialization (see He, K. et al. (2015)). Note that the Kaiming initialization does not use the harmonic mean between input and output size. In their paper (Section 2.2, Backward Propagation, last paragraph),

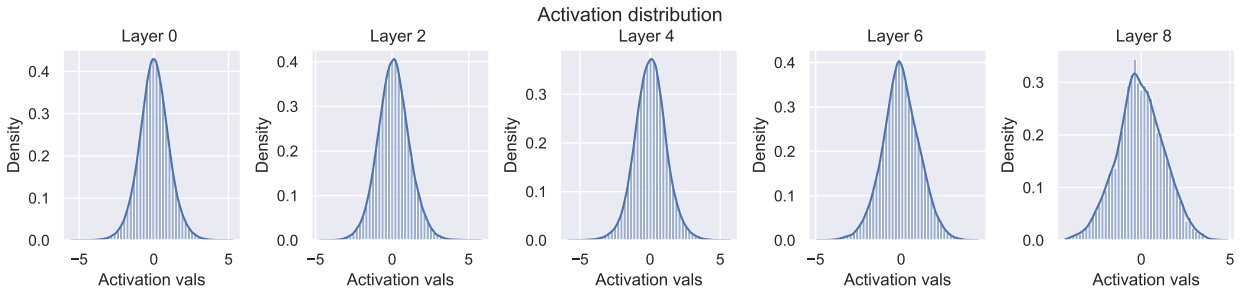
they argue that using d_x or d_y both lead to stable gradients throughout the network, and only depend on the overall input and output size of the network. Hence, we can use here only the input d_x:

[17]:
```
def kaiming_init(model):
    for name, param in model.named_parameters():
        if name.endswith(".bias"):
            param.data.fill_(0)
        elif name.startswith("layers.0"): # The first layer does not have ReLU applied␣
↪on its input
            param.data.normal_(0, 1/math.sqrt(param.shape[1]))
        else:
            param.data.normal_(0, math.sqrt(2)/math.sqrt(param.shape[1]))

model = BaseNetwork(act_fn=nn.ReLU()).to(device)
kaiming_init(model)
visualize_gradients(model, print_variance=True)
visualize_activations(model, print_variance=True)
```




```
layers.0.weight - Variance: 0.000075
layers.2.weight - Variance: 0.000108
layers.4.weight - Variance: 0.000185
layers.6.weight - Variance: 0.000444
layers.8.weight - Variance: 0.005548
```




```
Layer 0 - Variance: 1.012342
Layer 2 - Variance: 1.092432
Layer 4 - Variance: 1.268176
Layer 6 - Variance: 1.193706
Layer 8 - Variance: 1.760064
```

The variance stays stable across layers. We can conclude that the Kaiming initialization indeed works well for ReLU-based networks. Note that for Leaky-ReLU etc., we have to slightly adjust the factor of 2 in the variance as half of the values are not set to zero anymore. PyTorch provides a function to calculate this factor for many activation function, see `torch.nn.init.calculate_gain` (link).

4.18.3 Optimization

Besides initialization, selecting a suitable optimization algorithm can be an important choice for deep neural networks. Before taking a closer look at them, we should define code for training the models. Most of the following code is copied from the previous tutorial, and only slightly altered to fit our needs.

[18]:
```
def _get_config_file(model_path, model_name):
    return os.path.join(model_path, model_name + ".config")

def _get_model_file(model_path, model_name):
    return os.path.join(model_path, model_name + ".tar")

def _get_result_file(model_path, model_name):
    return os.path.join(model_path, model_name + "_results.json")

def load_model(model_path, model_name, net=None):
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_
↪file(model_path, model_name)
    assert os.path.isfile(config_file), f"Could not find the config file \"{config_file}\
↪". Are you sure this is the correct path and you have your model config stored here?"
    assert os.path.isfile(model_file), f"Could not find the model file \"{model_file}\".␣
↪Are you sure this is the correct path and you have your model stored here?"
    with open(config_file, "r") as f:
        config_dict = json.load(f)
    if net is None:
        act_fn_name = config_dict["act_fn"].pop("name").lower()
        assert act_fn_name in act_fn_by_name, f"Unknown activation function \"{act_fn_
↪name}\". Please add it to the \"act_fn_by_name\" dict."
        act_fn = act_fn_by_name[act_fn_name]()
        net = BaseNetwork(act_fn=act_fn, **config_dict)
    net.load_state_dict(torch.load(model_file))
    return net

def save_model(model, model_path, model_name):
    config_dict = model.config
    os.makedirs(model_path, exist_ok=True)
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_
↪file(model_path, model_name)
    with open(config_file, "w") as f:
        json.dump(config_dict, f)
    torch.save(model.state_dict(), model_file)

def train_model(net, model_name, optim_func, max_epochs=50, batch_size=256,␣
↪overwrite=False):
    """
    Train a model on the training set of FashionMNIST

    Inputs:
        net - Object of BaseNetwork
        model_name - (str) Name of the model, used for creating the checkpoint names
        max_epochs - Number of epochs we want to (maximally) train for
        patience - If the performance on the validation set has not improved for
↪#patience epochs, we stop training early
```

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```
        batch_size - Size of batches used in training
        overwrite - Determines how to handle the case when there already exists a␣
↪checkpoint. If True, it will be overwritten. Otherwise, we skip training.
    """
    file_exists = os.path.isfile(_get_model_file(CHECKPOINT_PATH, model_name))
    if file_exists and not overwrite:
        print(f"Model file of \"{model_name}\" already exists. Skipping training...")
        with open(_get_result_file(CHECKPOINT_PATH, model_name), "r") as f:
            results = json.load(f)
    else:
        if file_exists:
            print("Model file exists, but will be overwritten...")

        # Defining optimizer, loss and data loader
        optimizer =  optim_func(net.parameters())
        loss_module = nn.CrossEntropyLoss()
        train_loader_local = data.DataLoader(train_set, batch_size=batch_size,␣
↪shuffle=True, drop_last=True, pin_memory=True)

        results = None
        val_scores = []
        train_losses, train_scores = [], []
        best_val_epoch = -1
        for epoch in range(max_epochs):
            ############
            # Training #
            ############
            net.train()
            true_preds, count = 0., 0
            t = tqdm(train_loader_local, leave=False)
            for imgs, labels in t:
                imgs, labels = imgs.to(device), labels.to(device)
                optimizer.zero_grad()
                preds = net(imgs)
                loss = loss_module(preds, labels)
                loss.backward()
                optimizer.step()
                # Record statistics during training
                true_preds += (preds.argmax(dim=-1) == labels).sum().item()
                count += labels.shape[0]
                t.set_description(f"Epoch {epoch+1}: loss={loss.item():4.2f}")
                train_losses.append(loss.item())
            train_acc = true_preds / count
            train_scores.append(train_acc)

            ##############
            # Validation #
            ##############
            val_acc = test_model(net, val_loader)
            val_scores.append(val_acc)
            print(f"[Epoch {epoch+1:2d}] Training accuracy: {train_acc*100.0:05.2f}%,␣
↪Validation accuracy: {val_acc*100.0:05.2f}%")
```

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```
            if len(val_scores) == 1 or val_acc > val_scores[best_val_epoch]:
                print("\t   (New best performance, saving model...)")
                save_model(net, CHECKPOINT_PATH, model_name)
                best_val_epoch = epoch

    if results is None:
        load_model(CHECKPOINT_PATH, model_name, net=net)
        test_acc = test_model(net, test_loader)
        results = {"test_acc": test_acc, "val_scores": val_scores, "train_losses": train_
↪losses, "train_scores": train_scores}
        with open(_get_result_file(CHECKPOINT_PATH, model_name), "w") as f:
            json.dump(results, f)

    # Plot a curve of the validation accuracy
    sns.set()
    plt.plot([i for i in range(1,len(results["train_scores"])+1)], results["train_scores
↪"], label="Train")
    plt.plot([i for i in range(1,len(results["val_scores"])+1)], results["val_scores"],␣
↪label="Val")
    plt.xlabel("Epochs")
    plt.ylabel("Validation accuracy")
    plt.ylim(min(results["val_scores"]), max(results["train_scores"])*1.01)
    plt.title(f"Validation performance of {model_name}")
    plt.legend()
    plt.show()
    plt.close()

    print((f" Test accuracy: {results['test_acc']*100.0:4.2f}% ").center(50, "=")+"\n")
    return results


def test_model(net, data_loader):
    """
    Test a model on a specified dataset.

    Inputs:
        net - Trained model of type BaseNetwork
        data_loader - DataLoader object of the dataset to test on (validation or test)
    """
    net.eval()
    true_preds, count = 0., 0
    for imgs, labels in data_loader:
        imgs, labels = imgs.to(device), labels.to(device)
        with torch.no_grad():
            preds = net(imgs).argmax(dim=-1)
            true_preds += (preds == labels).sum().item()
            count += labels.shape[0]
    test_acc = true_preds / count
    return test_acc
```

First, we need to understand what an optimizer actually does. The optimizer is responsible to update the network's parameters given the gradients. Hence, we effectively implement a function $w^t = f(w^{t-1}, g^t, ...)$ with w being the

parameters, and $g^t = \nabla_{w^{(t-1)}} \mathcal{L}^{(t)}$ the gradients at time step t. A common, additional parameter to this function is the learning rate, here denoted by η. Usually, the learning rate can be seen as the "step size" of the update. A higher learning rate means that we change the weights more in the direction of the gradients, a smaller means we take shorter steps.

As most optimizers only differ in the implementation of f, we can define a template for an optimizer in PyTorch below. We take as input the parameters of a model and a learning rate. The function `zero_grad` sets the gradients of all parameters to zero, which we have to do before calling `loss.backward()`. Finally, the `step()` function tells the optimizer to update all weights based on their gradients. The template is setup below:

[19]:
```
class OptimizerTemplate:

    def __init__(self, params, lr):
        self.params = list(params)
        self.lr = lr

    def zero_grad(self):
        ## Set gradients of all parameters to zero
        for p in self.params:
            if p.grad is not None:
                p.grad.detach_() # For second-order optimizers important
                p.grad.zero_()

    @torch.no_grad()
    def step(self):
        ## Apply update step to all parameters
        for p in self.params:
            if p.grad is None: # We skip parameters without any gradients
                continue
            self.update_param(p)

    def update_param(self, p):
        # To be implemented in optimizer-specific classes
        raise NotImplementedError
```

The first optimizer we are going to implement is the standard Stochastic Gradient Descent (SGD). SGD updates the parameters using the following equation:

$$w^{(t)} = w^{(t-1)} - \eta \cdot g^{(t)}$$

As simple as the equation is also our implementation of SGD:

[20]:
```
class SGD(OptimizerTemplate):

    def __init__(self, params, lr):
        super().__init__(params, lr)

    def update_param(self, p):
        p_update = -self.lr * p.grad
        p.add_(p_update) # In-place update => saves memory and does not create␣
↪computation graph
```

In the lecture, we also have discussed the concept of momentum which replaces the gradient in the update by an

exponential average of all past gradients including the current one:

$$m^{(t)} = \beta_1 m^{(t-1)} + (1 - \beta_1) \cdot g^{(t)}$$
$$w^{(t)} = w^{(t-1)} - \eta \cdot m^{(t)}$$

Let's also implement it below:

[21]:
```
class SGDMomentum(OptimizerTemplate):

    def __init__(self, params, lr, momentum=0.0):
        super().__init__(params, lr)
        self.momentum = momentum # Corresponds to beta_1 in the equation above
        self.param_momentum = {p: torch.zeros_like(p.data) for p in self.params} # Dict␣
↪to store m_t

    def update_param(self, p):
        self.param_momentum[p] = (1 - self.momentum) * p.grad + self.momentum * self.
↪param_momentum[p]
        p_update = -self.lr * self.param_momentum[p]
        p.add_(p_update)
```

Finally, we arrive at Adam. Adam combines the idea of momentum with an adaptive learning rate, which is based on an exponential average of the squared gradients, i.e. the gradients norm. Furthermore, we add a bias correction for the momentum and adaptive learning rate for the first iterations:

$$m^{(t)} = \beta_1 m^{(t-1)} + (1 - \beta_1) \cdot g^{(t)}$$
$$v^{(t)} = \beta_2 v^{(t-1)} + (1 - \beta_2) \cdot \left(g^{(t)}\right)^2$$
$$\hat{m}^{(t)} = \frac{m^{(t)}}{1 - \beta_1^t}, \hat{v}^{(t)} = \frac{v^{(t)}}{1 - \beta_2^t}$$
$$w^{(t)} = w^{(t-1)} - \frac{\eta}{\sqrt{\hat{v}^{(t)}} + \epsilon} \circ \hat{m}^{(t)}$$

Epsilon is a small constant used to improve numerical stability for very small gradient norms. Remember that the adaptive learning rate does not replace the learning rate hyperparameter η, but rather acts as an extra factor and ensures that the gradients of various parameters have a similar norm.

[22]:
```
class Adam(OptimizerTemplate):

    def __init__(self, params, lr, beta1=0.9, beta2=0.999, eps=1e-8):
        super().__init__(params, lr)
        self.beta1 = beta1
        self.beta2 = beta2
        self.eps = eps
        self.param_step = {p: 0 for p in self.params} # Remembers "t" for each parameter␣
↪for bias correction
        self.param_momentum = {p: torch.zeros_like(p.data) for p in self.params}
        self.param_2nd_momentum = {p: torch.zeros_like(p.data) for p in self.params}

    def update_param(self, p):
        self.param_step[p] += 1

        self.param_momentum[p] = (1 - self.beta1) * p.grad + self.beta1 * self.param_
↪momentum[p]
```

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```
        self.param_2nd_momentum[p] = (1 - self.beta2) * (p.grad)**2 + self.beta2 * self.
↪param_2nd_momentum[p]

        bias_correction_1 = 1 - self.beta1 ** self.param_step[p]
        bias_correction_2 = 1 - self.beta2 ** self.param_step[p]

        p_2nd_mom = self.param_2nd_momentum[p] / bias_correction_2
        p_mom = self.param_momentum[p] / bias_correction_1
        p_lr = self.lr / (torch.sqrt(p_2nd_mom) + self.eps)
        p_update = -p_lr * p_mom

        p.add_(p_update)
```

Comparing optimizers on model training

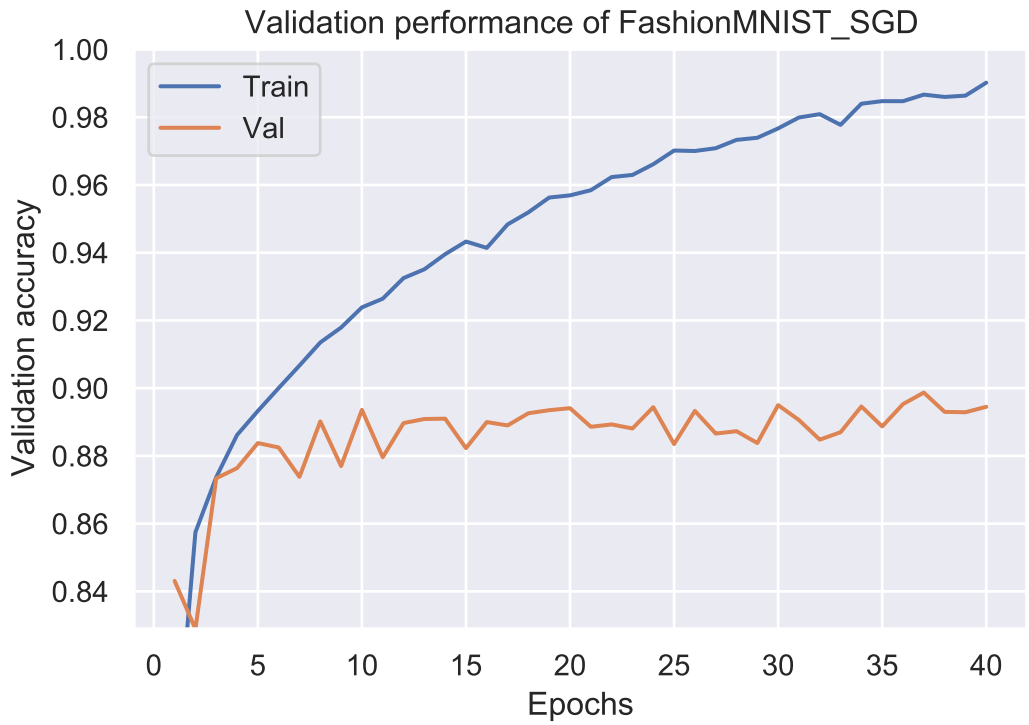
After we have implemented three optimizers (SGD, SGD with momentum, and Adam), we can start to analyze and compare them. First, we test them on how well they can optimize a neural network on the FashionMNIST dataset. We use again our linear network, this time with a ReLU activation and the kaiming initialization, which we have found before to work well for ReLU-based networks. Note that the model is over-parameterized for this task, and we can achieve similar performance with a much smaller network (for example `100,100,100`). However, our main interest is in how well the optimizer can train *deep* neural networks, hence the over-parameterization.

[23]:
```
base_model = BaseNetwork(act_fn=nn.ReLU(), hidden_sizes=[512,256,256,128])
kaiming_init(base_model)
```

For a fair comparison, we train the exact same model with the same seed with the three optimizers below. Feel free to change the hyperparameters if you want (however, you have to train your own model then).

[24]:
```
SGD_model = copy.deepcopy(base_model).to(device)
SGD_results = train_model(SGD_model, "FashionMNIST_SGD",
                          lambda params: SGD(params, lr=1e-1),
                          max_epochs=40, batch_size=256)
```

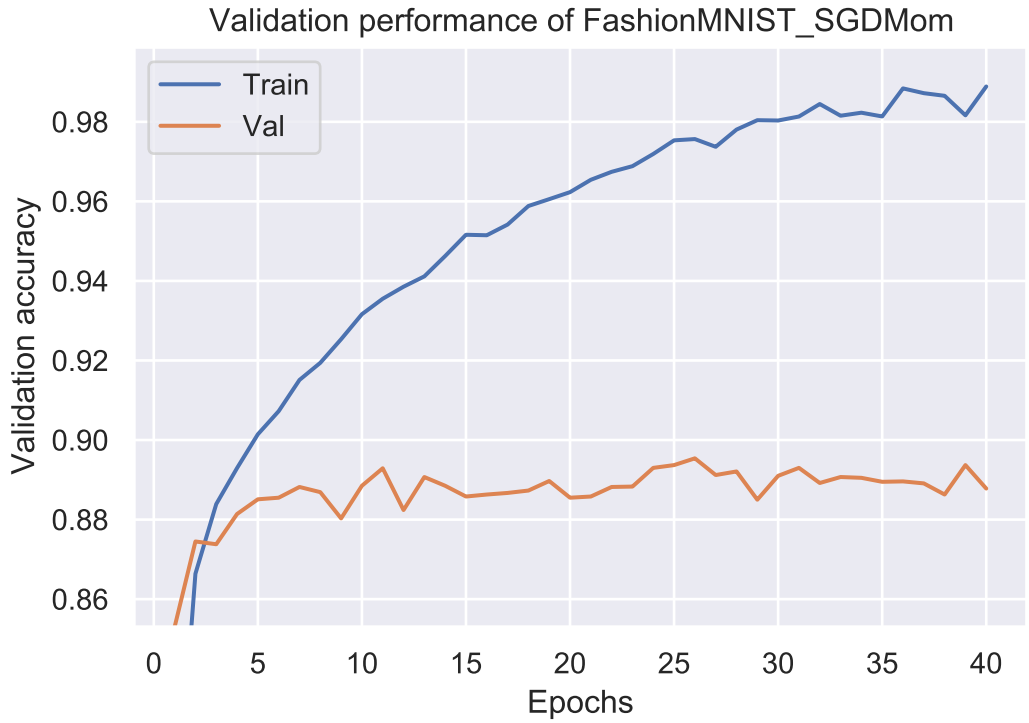
```
Model file of "FashionMNIST_SGD" already exists. Skipping training...
```




```
============= Test accuracy: 89.09% ==============
```

[25]:
```
SGDMom_model = copy.deepcopy(base_model).to(device)
SGDMom_results = train_model(SGDMom_model, "FashionMNIST_SGDMom",
                             lambda params: SGDMomentum(params, lr=1e-1, momentum=0.9),
                             max_epochs=40, batch_size=256)
```

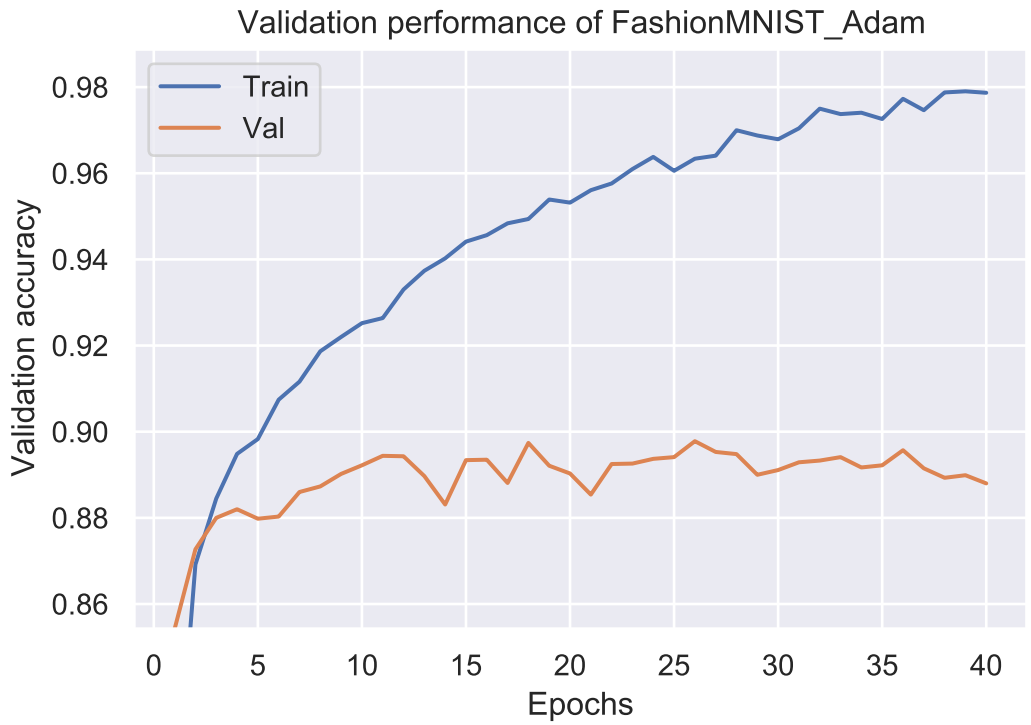
```
Model file of "FashionMNIST_SGDMom" already exists. Skipping training...
```




```
============= Test accuracy: 88.83% ==============
```

[26]:
```
Adam_model = copy.deepcopy(base_model).to(device)
Adam_results = train_model(Adam_model, "FashionMNIST_Adam",
                           lambda params: Adam(params, lr=1e-3),
                           max_epochs=40, batch_size=256)
```

```
Model file of "FashionMNIST_Adam" already exists. Skipping training...
```




```
============= Test accuracy: 89.46% ==============
```

The result is that all optimizers perform similarly well with the given model. The differences are too small to find any significant conclusion. However, keep in mind that this can also be attributed to the initialization we chose. When changing the initialization to worse (e.g. constant initialization), Adam usually shows to be more robust because of its adaptive learning rate. To show the specific benefits of the optimizers, we will continue to look at some possible loss surfaces in which momentum and adaptive learning rate are crucial.

Pathological curvatures

A pathological curvature is a type of surface that is similar to ravines and is particularly tricky for plain SGD optimization. In words, pathological curvatures typically have a steep gradient in one direction with an optimum at the center, while in a second direction we have a slower gradient towards a (global) optimum. Let's first create an example surface of this and visualize it:

[27]:
```
def pathological_curve_loss(w1, w2):
    # Example of a pathological curvature. There are many more possible, feel free to␣
↪experiment here!
    x1_loss = torch.tanh(w1)**2 + 0.01 * torch.abs(w1)
    x2_loss = torch.sigmoid(w2)
    return x1_loss + x2_loss
```

[28]:
```
def plot_curve(curve_fn, x_range=(-5,5), y_range=(-5,5), plot_3d=False, cmap=cm.viridis,␣
↪title="Pathological curvature"):
    fig = plt.figure()
    ax = plt.axes(projection='3d') if plot_3d else plt.axes()
```

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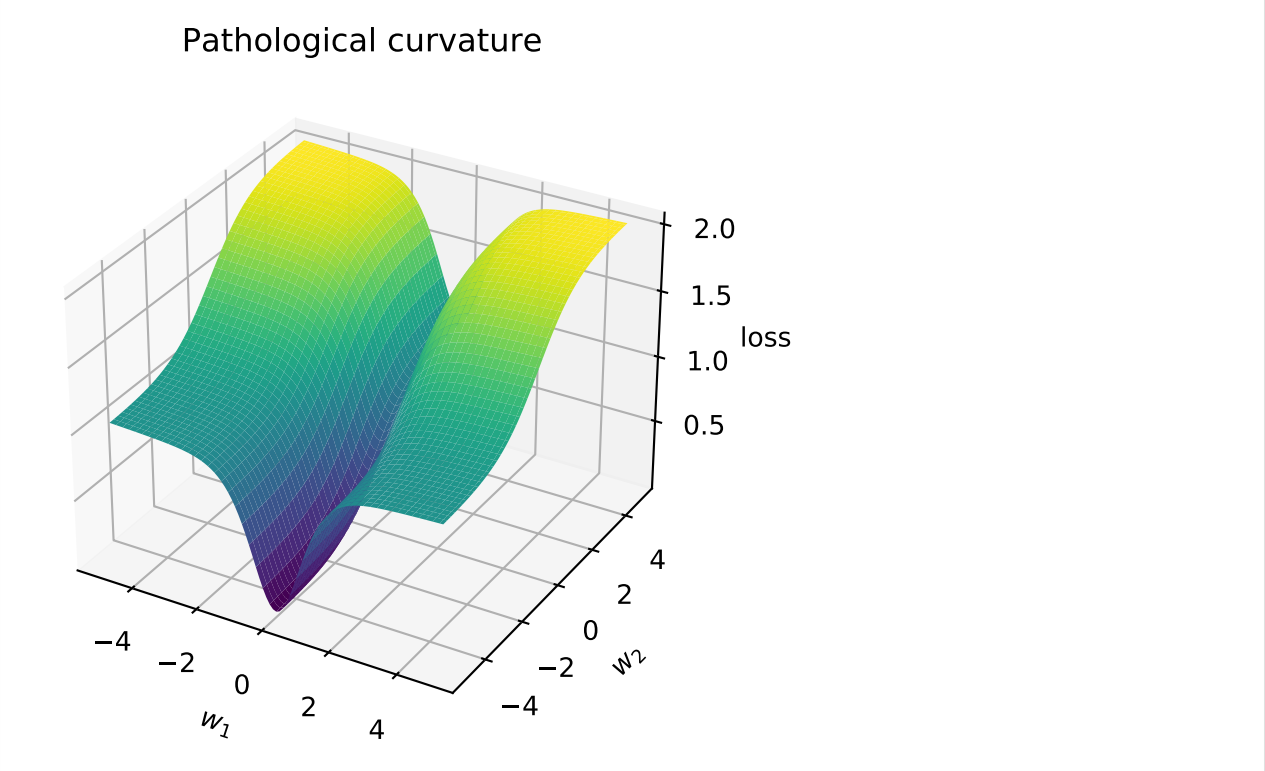
```
    x = torch.arange(x_range[0], x_range[1], (x_range[1]-x_range[0])/100.)
    y = torch.arange(y_range[0], y_range[1], (y_range[1]-y_range[0])/100.)
    x, y = torch.meshgrid(x, y, indexing='xy')
    z = curve_fn(x, y)
    x, y, z = x.numpy(), y.numpy(), z.numpy()

    if plot_3d:
        ax.plot_surface(x, y, z, cmap=cmap, linewidth=1, color="#000", antialiased=False)
        ax.set_zlabel("loss")
    else:
        ax.imshow(z[::-1], cmap=cmap, extent=(x_range[0], x_range[1], y_range[0], y_
↪range[1]))
    plt.title(title)
    ax.set_xlabel(r"$w_1$")
    ax.set_ylabel(r"$w_2$")
    plt.tight_layout()
    return ax

sns.reset_orig()
_ = plot_curve(pathological_curve_loss, plot_3d=True)
plt.show()
```



In terms of optimization, you can image that w_1 and w_2 are weight parameters, and the curvature represents the loss surface over the space of w_1 and w_2. Note that in typical networks, we have many, many more parameters than two, and such curvatures can occur in multi-dimensional spaces as well.

Ideally, our optimization algorithm would find the center of the ravine and focuses on optimizing the parameters towards the direction of w_2. However, if we encounter a point along the ridges, the gradient is much greater in w_1 than w_2, and we might end up jumping from one side to the other. Due to the large gradients, we would have to reduce our learning

rate slowing down learning significantly.

To test our algorithms, we can implement a simple function to train two parameters on such a surface:

[29]:
```
def train_curve(optimizer_func, curve_func=pathological_curve_loss, num_updates=100,␣
↪init=[5,5]):
    """
    Inputs:
        optimizer_func - Constructor of the optimizer to use. Should only take a␣
↪parameter list
        curve_func - Loss function (e.g. pathological curvature)
        num_updates - Number of updates/steps to take when optimizing
        init - Initial values of parameters. Must be a list/tuple with two elements␣
↪representing w_1 and w_2
    Outputs:
        Numpy array of shape [num_updates, 3] with [t,:2] being the parameter values at␣
↪step t, and [t,2] the loss at t.
    """
    weights = nn.Parameter(torch.FloatTensor(init), requires_grad=True)
    optimizer = optimizer_func([weights])

    list_points = []
    for _ in range(num_updates):
        loss = curve_func(weights[0], weights[1])
        list_points.append(torch.cat([weights.data.detach(), loss.unsqueeze(dim=0).
↪detach()], dim=0))
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
    points = torch.stack(list_points, dim=0).numpy()
    return points
```

Next, let's apply the different optimizers on our curvature. Note that we set a much higher learning rate for the optimization algorithms as you would in a standard neural network. This is because we only have 2 parameters instead of tens of thousands or even millions.

[30]:
```
SGD_points = train_curve(lambda params: SGD(params, lr=10))
SGDMom_points = train_curve(lambda params: SGDMomentum(params, lr=10, momentum=0.9))
Adam_points = train_curve(lambda params: Adam(params, lr=1))
```

To understand best how the different algorithms worked, we visualize the update step as a line plot through the loss surface. We will stick with a 2D representation for readability.

[31]:
```
all_points = np.concatenate([SGD_points, SGDMom_points, Adam_points], axis=0)
ax = plot_curve(pathological_curve_loss,
                x_range=(-np.absolute(all_points[:,0]).max(), np.absolute(all_points[:,
↪0]).max()),
                y_range=(all_points[:,1].min(), all_points[:,1].max()),
                plot_3d=False)
ax.plot(SGD_points[:,0], SGD_points[:,1], color="red", marker="o", zorder=1, label="SGD")
ax.plot(SGDMom_points[:,0], SGDMom_points[:,1], color="blue", marker="o", zorder=2,␣
↪label="SGDMom")
ax.plot(Adam_points[:,0], Adam_points[:,1], color="grey", marker="o", zorder=3, label=
↪"Adam")
```

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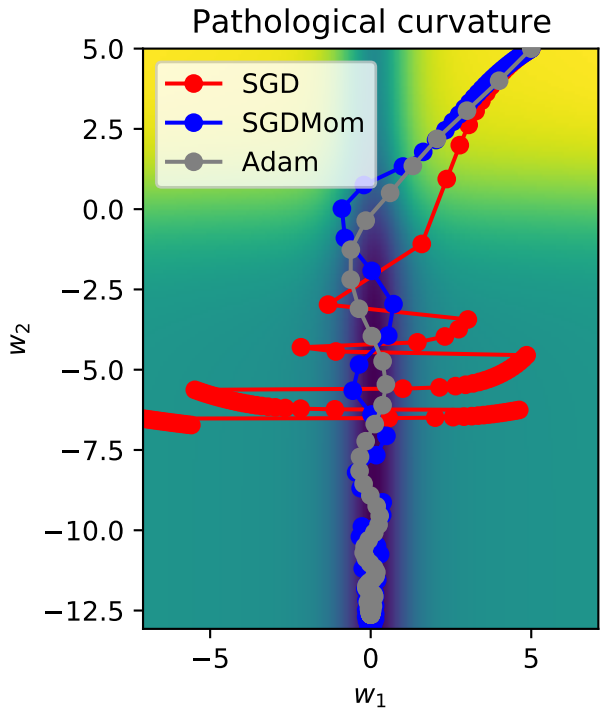
```
plt.legend()
plt.show()
```

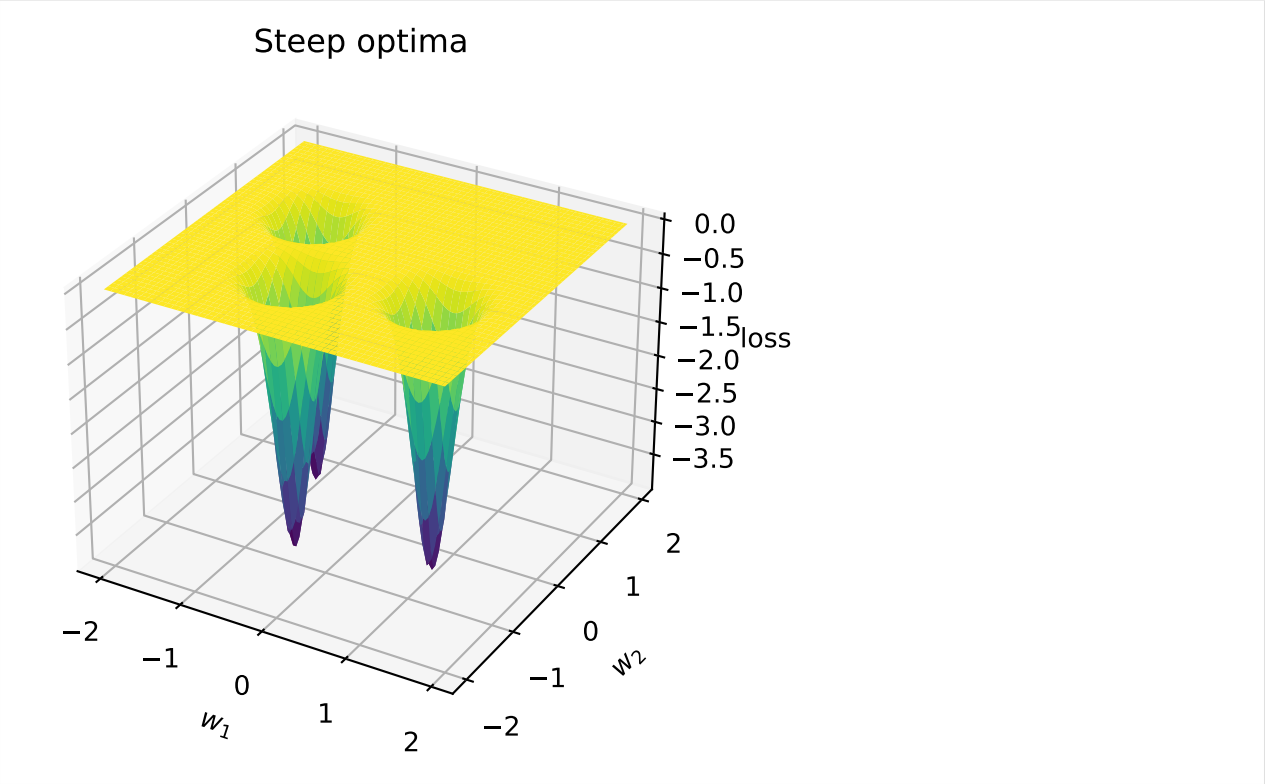


We can clearly see that SGD is not able to find the center of the optimization curve and has a problem converging due to the steep gradients in w_1. In contrast, Adam and SGD with momentum nicely converge as the changing direction of w_1 is canceling itself out. On such surfaces, it is crucial to use momentum.

Steep optima

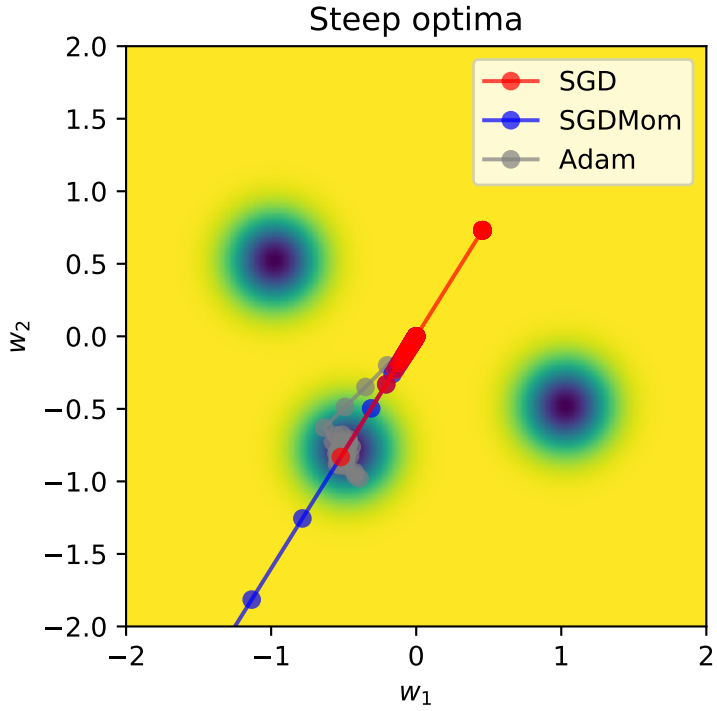
A second type of challenging loss surfaces are steep optima. In those, we have a larger part of the surface having very small gradients while around the optimum, we have very large gradients. For instance, take the following loss surfaces:

[32]:
```
def bivar_gaussian(w1, w2, x_mean=0.0, y_mean=0.0, x_sig=1.0, y_sig=1.0):
    norm = 1 / (2 * np.pi * x_sig * y_sig)
    x_exp = (-1 * (w1 - x_mean)**2) / (2 * x_sig**2)
    y_exp = (-1 * (w2 - y_mean)**2) / (2 * y_sig**2)
    return norm * torch.exp(x_exp + y_exp)

def comb_func(w1, w2):
    z = -bivar_gaussian(w1, w2, x_mean=1.0, y_mean=-0.5, x_sig=0.2, y_sig=0.2)
    z -= bivar_gaussian(w1, w2, x_mean=-1.0, y_mean=0.5, x_sig=0.2, y_sig=0.2)
    z -= bivar_gaussian(w1, w2, x_mean=-0.5, y_mean=-0.8, x_sig=0.2, y_sig=0.2)
    return z

_ = plot_curve(comb_func, x_range=(-2,2), y_range=(-2,2), plot_3d=True, title="Steep␣
↪optima")
```



Most of the loss surface has very little to no gradients. However, close to the optima, we have very steep gradients. To reach the minimum when starting in a region with lower gradients, we expect an adaptive learning rate to be crucial. To verify this hypothesis, we can run our three optimizers on the surface:

[33]:
```
SGD_points = train_curve(lambda params: SGD(params, lr=.5), comb_func, init=[0,0])
SGDMom_points = train_curve(lambda params: SGDMomentum(params, lr=1, momentum=0.9), comb_
↪func, init=[0,0])
Adam_points = train_curve(lambda params: Adam(params, lr=0.2), comb_func, init=[0,0])

all_points = np.concatenate([SGD_points, SGDMom_points, Adam_points], axis=0)
ax = plot_curve(comb_func,
                x_range=(-2, 2),
                y_range=(-2, 2),
                plot_3d=False,
                title="Steep optima")
ax.plot(SGD_points[:,0], SGD_points[:,1], color="red", marker="o", zorder=3, label="SGD",
↪ alpha=0.7)
ax.plot(SGDMom_points[:,0], SGDMom_points[:,1], color="blue", marker="o", zorder=2,␣
↪label="SGDMom", alpha=0.7)
ax.plot(Adam_points[:,0], Adam_points[:,1], color="grey", marker="o", zorder=1, label=
↪"Adam", alpha=0.7)
ax.set_xlim(-2, 2)
ax.set_ylim(-2, 2)
plt.legend()
plt.show()
```



SGD first takes very small steps until it touches the border of the optimum. First reaching a point around $(-0.75, -0.5)$, the gradient direction has changed and pushes the parameters to $(0.8, 0.5)$ from which SGD cannot recover anymore (only with many, many steps). A similar problem has SGD with momentum, only that it continues the direction of the touch of the optimum. The gradients from this time step are so much larger than any other point that the momentum m_t is overpowered by it. Finally, Adam is able to converge in the optimum showing the importance of adaptive learning rates.

What optimizer to take

After seeing the results on optimization, what is our conclusion? Should we always use Adam and never look at SGD anymore? The short answer: no. There are many papers saying that in certain situations, SGD (with momentum) generalizes better where Adam often tends to overfit [5,6]. This is related to the idea of finding wider optima. For instance, see the illustration of different optima below (credit: Keskar et al., 2017):

The black line represents the training loss surface, while the dotted red line is the test loss. Finding sharp, narrow minima can be helpful for finding the minimal training loss. However, this doesn't mean that it also minimizes the test loss as especially flat minima have shown to generalize better. You can imagine that the test dataset has a slightly shifted loss surface due to the different examples than in the training set. A small change can have a significant influence for sharp minima, while flat minima are generally more robust to this change.

In the next tutorial, we will see that some network types can still be better optimized with SGD and learning rate scheduling than Adam. Nevertheless, Adam is the most commonly used optimizer in Deep Learning as it usually performs better than other optimizers, especially for deep networks.

4.18.4 Conclusion

In this tutorial, we have looked at initialization and optimization techniques for neural networks. We have seen that a good initialization has to balance the preservation of the gradient variance as well as the activation variance. This can be achieved with the Xavier initialization for tanh-based networks, and the Kaiming initialization for ReLU-based networks. In optimization, concepts like momentum and adaptive learning rate can help with challenging loss surfaces but don't guarantee an increase in performance for neural networks.

4.18.5 References

[1] Glorot, Xavier, and Yoshua Bengio. "Understanding the difficulty of training deep feedforward neural networks." Proceedings of the thirteenth international conference on artificial intelligence and statistics. 2010. link

[2] He, Kaiming, et al. "Delving deep into rectifiers: Surpassing human-level performance on imagenet classification." Proceedings of the IEEE international conference on computer vision. 2015. link

[3] Kingma, Diederik P. & Ba, Jimmy. "Adam: A Method for Stochastic Optimization." Proceedings of the third international conference for learning representations (ICLR). 2015. link

[4] Keskar, Nitish Shirish, et al. "On large-batch training for deep learning: Generalization gap and sharp minima." Proceedings of the fifth international conference for learning representations (ICLR). 2017. link

[5] Wilson, Ashia C., et al. "The Marginal Value of Adaptive Gradient Methods in Machine Learning." Advances in neural information processing systems. 2017. link

[6] Ruder, Sebastian. "An overview of gradient descent optimization algorithms." arXiv preprint. 2017. link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.19 Tutorial 5: Inception, ResNet and DenseNet

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will implement and discuss variants of modern CNN architectures. There have been many different architectures been proposed over the past few years. Some of the most impactful ones, and still relevant today, are

the following: GoogleNet/Inception architecture (winner of ILSVRC 2014), ResNet (winner of ILSVRC 2015), and DenseNet (best paper award CVPR 2017). All of them were state-of-the-art models when being proposed, and the core ideas of these networks are the foundations for most current state-of-the-art architectures. Thus, it is important to understand these architectures in detail and learn how to implement them.

Let's start with importing our standard libraries here.

[1]:
```
## Standard libraries
import os
import numpy as np
import random
from PIL import Image
from types import SimpleNamespace

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## PyTorch
import torch
import torch.nn as nn
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import CIFAR10
from torchvision import transforms
```

We will use the same `set_seed` function as in the previous tutorials, as well as the path variables `DATASET_PATH` and `CHECKPOINT_PATH`. Adjust the paths if necessary.

[2]:
```
# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial5"

# Function for setting the seed
def set_seed(seed):
    random.seed(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    if torch.cuda.is_available():
        torch.cuda.manual_seed(seed)
        torch.cuda.manual_seed_all(seed)
set_seed(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
```

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```
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
```

We also have pretrained models and Tensorboards (more on this later) for this tutorial, and download them below.

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial5/"
# Files to download
pretrained_files = ["GoogleNet.ckpt", "ResNet.ckpt", "ResNetPreAct.ckpt", "DenseNet.ckpt
↪",
                    "tensorboards/GoogleNet/events.out.tfevents.googlenet",
                    "tensorboards/ResNet/events.out.tfevents.resnet",
                    "tensorboards/ResNetPreAct/events.out.tfevents.resnetpreact",
                    "tensorboards/DenseNet/events.out.tfevents.densenet"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

Throughout this tutorial, we will train and evaluate the models on the CIFAR10 dataset. This allows you to compare the results obtained here with the model you have implemented in the first assignment. As we have learned from the previous tutorial about initialization, it is important to have the data preprocessed with a zero mean. Therefore, as a first step, we will calculate the mean and standard deviation of the CIFAR dataset:

[4]:
```
train_dataset = CIFAR10(root=DATASET_PATH, train=True, download=True)
DATA_MEANS = (train_dataset.data / 255.0).mean(axis=(0,1,2))
DATA_STD = (train_dataset.data / 255.0).std(axis=(0,1,2))
print("Data mean", DATA_MEANS)
print("Data std", DATA_STD)
```

```
Files already downloaded and verified
Data mean [0.49139968 0.48215841 0.44653091]
Data std [0.24703223 0.24348513 0.26158784]
```

We will use this information to define a `transforms.Normalize` module which will normalize our data accordingly. Additionally, we will use data augmentation during training. This reduces the risk of overfitting and helps CNNs to generalize better. Specifically, we will apply two random augmentations.

First, we will flip each image horizontally by a chance of 50% (`transforms.RandomHorizontalFlip`). The object class usually does not change when flipping an image, and we don't expect any image information to be dependent on the horizontal orientation. This would be however different if we would try to detect digits or letters in an image, as those have a certain orientation.

The second augmentation we use is called `transforms.RandomResizedCrop`. This transformation crops the image in a small range, eventually changing the aspect ratio, and scaling it back afterward to the previous size. Therefore, the actual pixel values change while the content or overall semantics of the image stays the same.

We will randomly split the training dataset into a training and a validation set. The validation set will be used for determining early stopping. After finishing the training, we test the models on the CIFAR test set.

[5]:
```
test_transform = transforms.Compose([transforms.ToTensor(),
                                     transforms.Normalize(DATA_MEANS, DATA_STD)
                                     ])
# For training, we add some augmentation. Networks are too powerful and would overfit.
train_transform = transforms.Compose([transforms.RandomHorizontalFlip(),
                                      transforms.RandomResizedCrop((32,32), scale=(0.8,1.
↪0), ratio=(0.9,1.1)),
                                      transforms.ToTensor(),
                                      transforms.Normalize(DATA_MEANS, DATA_STD)
                                     ])
# Loading the training dataset. We need to split it into a training and validation part
# We need to do a little trick because the validation set should not use the␣
↪augmentation.
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=train_transform,␣
↪download=True)
val_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=test_transform,␣
↪download=True)
set_seed(42)
train_set, _ = torch.utils.data.random_split(train_dataset, [45000, 5000])
set_seed(42)
_, val_set = torch.utils.data.random_split(val_dataset, [45000, 5000])

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=test_transform,␣
↪download=True)

# We define a set of data loaders that we can use for various purposes later.
train_loader = data.DataLoader(train_set, batch_size=128, shuffle=True, drop_last=True,␣
↪pin_memory=True, num_workers=4)
val_loader = data.DataLoader(val_set, batch_size=128, shuffle=False, drop_last=False,␣
↪num_workers=4)
test_loader = data.DataLoader(test_set, batch_size=128, shuffle=False, drop_last=False,␣
↪num_workers=4)
```

```
Files already downloaded and verified
Files already downloaded and verified
Files already downloaded and verified
```

To verify that our normalization works, we can print out the mean and standard deviation of the single batch. The mean should be close to 0 and the standard deviation close to 1 for each channel:

[6]:
```
imgs, _ = next(iter(train_loader))
print("Batch mean", imgs.mean(dim=[0,2,3]))
```

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```
print("Batch std", imgs.std(dim=[0,2,3]))
```

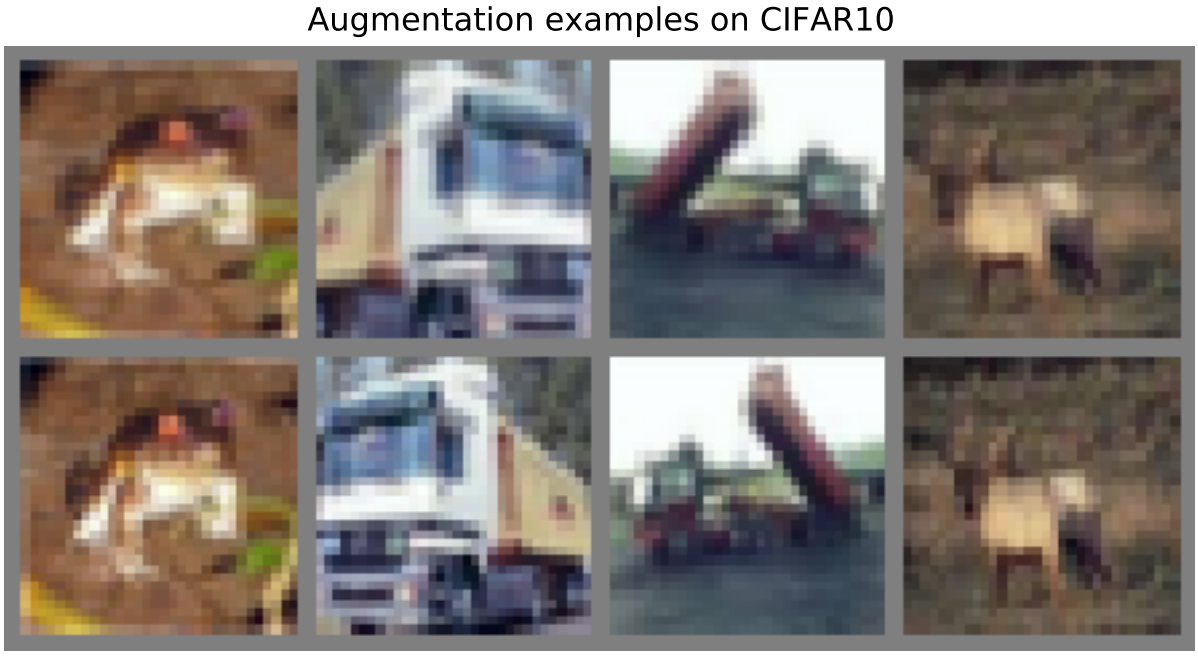
```
Batch mean tensor([-0.0143, -0.0204, -0.0017])
Batch std tensor([0.9772, 0.9650, 0.9809])
```

Finally, let's visualize a few images from the training set, and how they look like after random data augmentation:

[7]:
```
NUM_IMAGES = 4
images = [train_dataset[idx][0] for idx in range(NUM_IMAGES)]
orig_images = [Image.fromarray(train_dataset.data[idx]) for idx in range(NUM_IMAGES)]
orig_images = [test_transform(img) for img in orig_images]

img_grid = torchvision.utils.make_grid(torch.stack(images + orig_images, dim=0), nrow=4,␣
↪normalize=True, pad_value=0.5)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Augmentation examples on CIFAR10")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```



4.19.1 PyTorch Lightning

In this notebook and in many following ones, we will make use of the library PyTorch Lightning. PyTorch Lightning is a framework that simplifies your code needed to train, evaluate, and test a model in PyTorch. It also handles logging into TensorBoard, a visualization toolkit for ML experiments, and saving model checkpoints automatically with minimal code overhead from our side. This is extremely helpful for us as we want to focus on implementing different model architectures and spend little time on other code overhead. Note that at the time of writing/teaching, the framework has been released in version 1.8. Future versions might have a slightly changed interface and thus might not work perfectly with the code (we will try to keep it up-to-date as much as possible).

Now, we will take the first step in PyTorch Lightning, and continue to explore the framework in our other tutorials. First, we import the library:

[8]:
```
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.5
    import pytorch_lightning as pl
```

PyTorch Lightning comes with a lot of useful functions, such as one for setting the seed:

[9]:
```
# Setting the seed
pl.seed_everything(42)
```

[9]:
```
42
```

Thus, in the future, we don't have to define our own `set_seed` function anymore.

In PyTorch Lightning, we define `pl.LightningModule`'s (inheriting from `torch.nn.Module`) that organize our code into 5 main sections:

1. Initialization (`__init__`), where we create all necessary parameters/models
2. Optimizers (`configure_optimizers`) where we create the optimizers, learning rate scheduler, etc.
3. Training loop (`training_step`) where we only have to define the loss calculation for a single batch (the loop of optimizer.zero_grad(), loss.backward() and optimizer.step(), as well as any logging/saving operation, is done in the background)
4. Validation loop (`validation_step`) where similarly to the training, we only have to define what should happen per step
5. Test loop (`test_step`) which is the same as validation, only on a test set.

Therefore, we don't abstract the PyTorch code, but rather organize it and define some default operations that are commonly used. If you need to change something else in your training/validation/test loop, there are many possible functions you can overwrite (see the docs for details).

Now we can look at an example of how a Lightning Module for training a CNN looks like:

[10]:
```
class CIFARModule(pl.LightningModule):

    def __init__(self, model_name, model_hparams, optimizer_name, optimizer_hparams):
        """
        Inputs:
            model_name - Name of the model/CNN to run. Used for creating the model (see␣
↪function below)
```

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```
            model_hparams - Hyperparameters for the model, as dictionary.
            optimizer_name - Name of the optimizer to use. Currently supported: Adam, SGD
            optimizer_hparams - Hyperparameters for the optimizer, as dictionary. This␣
↪includes learning rate, weight decay, etc.
        """
        super().__init__()
        # Exports the hyperparameters to a YAML file, and create "self.hparams" namespace
        self.save_hyperparameters()
        # Create model
        self.model = create_model(model_name, model_hparams)
        # Create loss module
        self.loss_module = nn.CrossEntropyLoss()
        # Example input for visualizing the graph in Tensorboard
        self.example_input_array = torch.zeros((1, 3, 32, 32), dtype=torch.float32)

    def forward(self, imgs):
        # Forward function that is run when visualizing the graph
        return self.model(imgs)

    def configure_optimizers(self):
        # We will support Adam or SGD as optimizers.
        if self.hparams.optimizer_name == "Adam":
            # AdamW is Adam with a correct implementation of weight decay (see here for␣
↪details: https://arxiv.org/pdf/1711.05101.pdf)
            optimizer = optim.AdamW(
                self.parameters(), **self.hparams.optimizer_hparams)
        elif self.hparams.optimizer_name == "SGD":
            optimizer = optim.SGD(self.parameters(), **self.hparams.optimizer_hparams)
        else:
            assert False, f"Unknown optimizer: \"{self.hparams.optimizer_name}\""

        # We will reduce the learning rate by 0.1 after 100 and 150 epochs
        scheduler = optim.lr_scheduler.MultiStepLR(
            optimizer, milestones=[100, 150], gamma=0.1)
        return [optimizer], [scheduler]

    def training_step(self, batch, batch_idx):
        # "batch" is the output of the training data loader.
        imgs, labels = batch
        preds = self.model(imgs)
        loss = self.loss_module(preds, labels)
        acc = (preds.argmax(dim=-1) == labels).float().mean()

        # Logs the accuracy per epoch to tensorboard (weighted average over batches)
        self.log('train_acc', acc, on_step=False, on_epoch=True)
        self.log('train_loss', loss)
        return loss  # Return tensor to call ".backward" on

    def validation_step(self, batch, batch_idx):
        imgs, labels = batch
        preds = self.model(imgs).argmax(dim=-1)
        acc = (labels == preds).float().mean()
```

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```
        # By default logs it per epoch (weighted average over batches)
        self.log('val_acc', acc)

    def test_step(self, batch, batch_idx):
        imgs, labels = batch
        preds = self.model(imgs).argmax(dim=-1)
        acc = (labels == preds).float().mean()
        # By default logs it per epoch (weighted average over batches), and returns it␣
↪afterwards
        self.log('test_acc', acc)
```

We see that the code is organized and clear, which helps if someone else tries to understand your code.

Another important part of PyTorch Lightning is the concept of callbacks. Callbacks are self-contained functions that contain the non-essential logic of your Lightning Module. They are usually called after finishing a training epoch, but can also influence other parts of your training loop. For instance, we will use the following two pre-defined callbacks: `LearningRateMonitor` and `ModelCheckpoint`. The learning rate monitor adds the current learning rate to our TensorBoard, which helps to verify that our learning rate scheduler works correctly. The model checkpoint callback allows you to customize the saving routine of your checkpoints. For instance, how many checkpoints to keep, when to save, which metric to look out for, etc. We import them below:

[11]:
```
# Callbacks
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint
```

To allow running multiple different models with the same Lightning module, we define a function below that maps a model name to the model class. At this stage, the dictionary `model_dict` is empty, but we will fill it throughout the notebook with our new models.

[12]:
```
model_dict = {}

def create_model(model_name, model_hparams):
    if model_name in model_dict:
        return model_dict[model_name](**model_hparams)
    else:
        assert False, f"Unknown model name \"{model_name}\". Available models are:
↪{str(model_dict.keys())}"
```

Similarly, to use the activation function as another hyperparameter in our model, we define a "name to function" dict below:

[13]:
```
act_fn_by_name = {
    "tanh": nn.Tanh,
    "relu": nn.ReLU,
    "leakyrelu": nn.LeakyReLU,
    "gelu": nn.GELU
}
```

If we pass the classes or objects directly as an argument to the Lightning module, we couldn't take advantage of PyTorch Lightning's automatically hyperparameter saving and loading.

Besides the Lightning module, the second most important module in PyTorch Lightning is the `Trainer`. The trainer is responsible to execute the training steps defined in the Lightning module and completes the framework. Similar to the Lightning module, you can override any key part that you don't want to be automated, but the default settings are often the best practice to do. For a full overview, see the documentation. The most important functions we use below are:

- `trainer.fit`: Takes as input a lightning module, a training dataset, and an (optional) validation dataset. This function trains the given module on the training dataset with occasional validation (default once per epoch, can be changed)
- `trainer.test`: Takes as input a model and a dataset on which we want to test. It returns the test metric on the dataset.

For training and testing, we don't have to worry about things like setting the model to eval mode (`model.eval()`) as this is all done automatically. See below how we define a training function for our models:

[14]:
```
def train_model(model_name, save_name=None, **kwargs):
    """
    Inputs:
        model_name - Name of the model you want to run. Is used to look up the class in "model_dict"
        save_name (optional) - If specified, this name will be used for creating the checkpoint and logging directory.
    """
    if save_name is None:
        save_name = model_name

    # Create a PyTorch Lightning trainer with the generation callback
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, save_name),  # Where to save models
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",  # We run on a GPU (if possible)
                         devices=1,                                                      # How many GPUs/CPUs we want to use (1 is enough for the notebooks)
                         max_epochs=180,                                                 # How many epochs to train for if no patience is set
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max", monitor="val_acc"),  # Save the best checkpoint based on the maximum val_acc recorded. Saves only weights and not optimizer
                                    LearningRateMonitor("epoch")],                       # Log learning rate every epoch
                         enable_progress_bar=True)                                       # Set to False if you do not want a progress bar
    trainer.logger._log_graph = True         # If True, we plot the computation graph in tensorboard
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, save_name + ".ckpt")
    if os.path.isfile(pretrained_filename):
        print(f"Found pretrained model at {pretrained_filename}, loading...")
        model = CIFARModule.load_from_checkpoint(pretrained_filename) # Automatically loads the model with the saved hyperparameters
    else:
        pl.seed_everything(42) # To be reproducable
        model = CIFARModule(model_name=model_name, **kwargs)
        trainer.fit(model, train_loader, val_loader)
        model = CIFARModule.load_from_checkpoint(trainer.checkpoint_callback.best_model_path) # Load best checkpoint after training
```

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```
    # Test best model on validation and test set
    val_result = trainer.test(model, val_loader, verbose=False)
    test_result = trainer.test(model, test_loader, verbose=False)
    result = {"test": test_result[0]["test_acc"], "val": val_result[0]["test_acc"]}

    return model, result
```

Finally, we can focus on the Convolutional Neural Networks we want to implement today: GoogleNet, ResNet, and DenseNet.

4.19.2 Inception

The GoogleNet, proposed in 2014, won the ImageNet Challenge because of its usage of the Inception modules. In general, we will mainly focus on the concept of Inception in this tutorial instead of the specifics of the GoogleNet, as based on Inception, there have been many follow-up works (Inception-v2, Inception-v3, Inception-v4, Inception-ResNet,...). The follow-up works mainly focus on increasing efficiency and enabling very deep Inception networks. However, for a fundamental understanding, it is sufficient to look at the original Inception block.

An Inception block applies four convolution blocks separately on the same feature map: a 1x1, 3x3, and 5x5 convolution, and a max pool operation. This allows the network to look at the same data with different receptive fields. Of course, learning only 5x5 convolution would be theoretically more powerful. However, this is not only more computation and memory heavy but also tends to overfit much easier. The overall inception block looks like below (figure credit - Szegedy et al.):

The additional 1x1 convolutions before the 3x3 and 5x5 convolutions are used for dimensionality reduction. This is especially crucial as the feature maps of all branches are merged afterward, and we don't want any explosion of feature size. As 5x5 convolutions are 25 times more expensive than 1x1 convolutions, we can save a lot of computation and parameters by reducing the dimensionality before the large convolutions.

We can now try to implement the Inception Block ourselves:

[15]:
```
class InceptionBlock(nn.Module):

    def __init__(self, c_in, c_red : dict, c_out : dict, act_fn):
        """
        Inputs:
            c_in - Number of input feature maps from the previous layers
            c_red - Dictionary with keys "3x3" and "5x5" specifying the output of the␣
↪dimensionality reducing 1x1 convolutions
            c_out - Dictionary with keys "1x1", "3x3", "5x5", and "max"
            act_fn - Activation class constructor (e.g. nn.ReLU)
        """
        super().__init__()

        # 1x1 convolution branch
        self.conv_1x1 = nn.Sequential(
            nn.Conv2d(c_in, c_out["1x1"], kernel_size=1),
            nn.BatchNorm2d(c_out["1x1"]),
            act_fn()
        )
```

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```
        # 3x3 convolution branch
        self.conv_3x3 = nn.Sequential(
            nn.Conv2d(c_in, c_red["3x3"], kernel_size=1),
            nn.BatchNorm2d(c_red["3x3"]),
            act_fn(),
            nn.Conv2d(c_red["3x3"], c_out["3x3"], kernel_size=3, padding=1),
            nn.BatchNorm2d(c_out["3x3"]),
            act_fn()
        )

        # 5x5 convolution branch
        self.conv_5x5 = nn.Sequential(
            nn.Conv2d(c_in, c_red["5x5"], kernel_size=1),
            nn.BatchNorm2d(c_red["5x5"]),
            act_fn(),
            nn.Conv2d(c_red["5x5"], c_out["5x5"], kernel_size=5, padding=2),
            nn.BatchNorm2d(c_out["5x5"]),
            act_fn()
        )

        # Max-pool branch
        self.max_pool = nn.Sequential(
            nn.MaxPool2d(kernel_size=3, padding=1, stride=1),
            nn.Conv2d(c_in, c_out["max"], kernel_size=1),
            nn.BatchNorm2d(c_out["max"]),
            act_fn()
        )

    def forward(self, x):
        x_1x1 = self.conv_1x1(x)
        x_3x3 = self.conv_3x3(x)
        x_5x5 = self.conv_5x5(x)
        x_max = self.max_pool(x)
        x_out = torch.cat([x_1x1, x_3x3, x_5x5, x_max], dim=1)
        return x_out
```

The GoogleNet architecture consists of stacking multiple Inception blocks with occasional max pooling to reduce the height and width of the feature maps. The original GoogleNet was designed for image sizes of ImageNet (224x224 pixels) and had almost 7 million parameters. As we train on CIFAR10 with image sizes of 32x32, we don't require such a heavy architecture, and instead, apply a reduced version. The number of channels for dimensionality reduction and output per filter (1x1, 3x3, 5x5, and max pooling) need to be manually specified and can be changed if interested. The general intuition is to have the most filters for the 3x3 convolutions, as they are powerful enough to take the context into account while requiring almost a third of the parameters of the 5x5 convolution.

[16]:
```
class GoogleNet(nn.Module):

    def __init__(self, num_classes=10, act_fn_name="relu", **kwargs):
        super().__init__()
        self.hparams = SimpleNamespace(num_classes=num_classes,
                                       act_fn_name=act_fn_name,
                                       act_fn=act_fn_by_name[act_fn_name])
```

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```
        self._create_network()
        self._init_params()

    def _create_network(self):
        # A first convolution on the original image to scale up the channel size
        self.input_net = nn.Sequential(
            nn.Conv2d(3, 64, kernel_size=3, padding=1),
            nn.BatchNorm2d(64),
            self.hparams.act_fn()
        )
        # Stacking inception blocks
        self.inception_blocks = nn.Sequential(
            InceptionBlock(64, c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 16, "3x3": 32,
↪ "5x5": 8, "max": 8}, act_fn=self.hparams.act_fn),
            InceptionBlock(64, c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 24, "3x3": 48,
↪ "5x5": 12, "max": 12}, act_fn=self.hparams.act_fn),
            nn.MaxPool2d(3, stride=2, padding=1),  # 32x32 => 16x16
            InceptionBlock(96, c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 24, "3x3": 48,
↪ "5x5": 12, "max": 12}, act_fn=self.hparams.act_fn),
            InceptionBlock(96, c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 16, "3x3": 48,
↪ "5x5": 16, "max": 16}, act_fn=self.hparams.act_fn),
            InceptionBlock(96, c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 16, "3x3": 48,
↪ "5x5": 16, "max": 16}, act_fn=self.hparams.act_fn),
            InceptionBlock(96, c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 32, "3x3": 48,
↪ "5x5": 24, "max": 24}, act_fn=self.hparams.act_fn),
            nn.MaxPool2d(3, stride=2, padding=1),  # 16x16 => 8x8
            InceptionBlock(128, c_red={"3x3": 48, "5x5": 16}, c_out={"1x1": 32, "3x3":␣
↪64, "5x5": 16, "max": 16}, act_fn=self.hparams.act_fn),
            InceptionBlock(128, c_red={"3x3": 48, "5x5": 16}, c_out={"1x1": 32, "3x3":␣
↪64, "5x5": 16, "max": 16}, act_fn=self.hparams.act_fn)
        )
        # Mapping to classification output
        self.output_net = nn.Sequential(
            nn.AdaptiveAvgPool2d((1, 1)),
            nn.Flatten(),
            nn.Linear(128, self.hparams.num_classes)
        )

    def _init_params(self):
        # Based on our discussion in Tutorial 4, we should initialize the convolutions␣
↪according to the activation function
        for m in self.modules():
            if isinstance(m, nn.Conv2d):
                nn.init.kaiming_normal_(
                    m.weight, nonlinearity=self.hparams.act_fn_name)
            elif isinstance(m, nn.BatchNorm2d):
                nn.init.constant_(m.weight, 1)
                nn.init.constant_(m.bias, 0)

    def forward(self, x):
        x = self.input_net(x)
        x = self.inception_blocks(x)
```

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```
        x = self.output_net(x)
        return x
```

Now, we can integrate our model to the model dictionary we defined above:

[17]:
```
model_dict["GoogleNet"] = GoogleNet
```

The training of the model is handled by PyTorch Lightning, and we just have to define the command to start. Note that we train for almost 200 epochs, which takes less than an hour on Snellius's default GPUs (NVIDIA A100). We would recommend using the saved models and train your own model if you are interested.

[18]:
```
googlenet_model, googlenet_results = train_model(model_name="GoogleNet",
                                                 model_hparams={"num_classes": 10,
                                                                "act_fn_name": "relu"},
                                                 optimizer_name="Adam",
                                                 optimizer_hparams={"lr": 1e-3,
                                                                    "weight_decay": 1e-4}
↪)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
```

```
Found pretrained model at ../saved_models/tutorial5/GoogleNet.ckpt, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

We will compare the results later in the notebooks, but we can already print them here for a first glance:

[19]:
```
print("GoogleNet Results", googlenet_results)
```

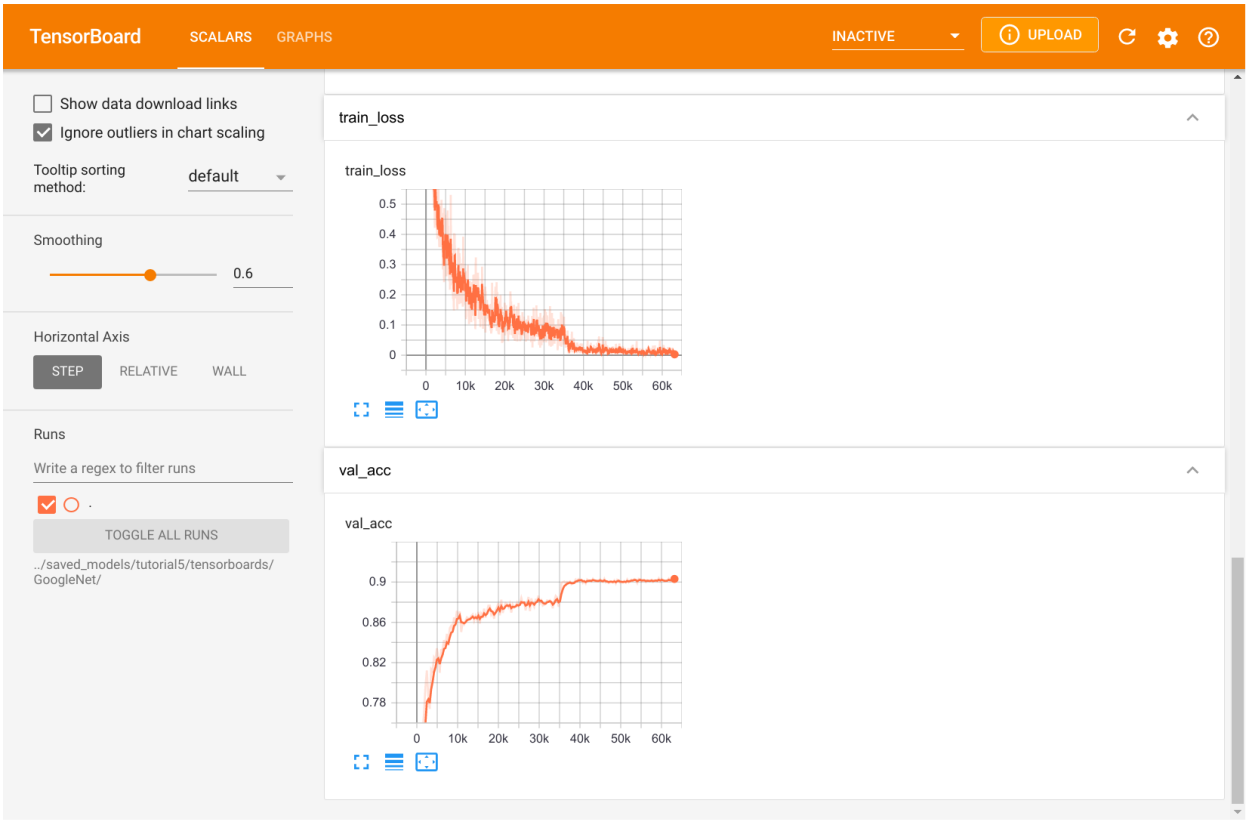
```
GoogleNet Results {'test': 0.8970000147819519, 'val': 0.9039999842643738}
```

Tensorboard log

A nice extra of PyTorch Lightning is the automatic logging into TensorBoard. To give you a better intuition of what TensorBoard can be used, we can look at the board that PyTorch Lightning has been generated when training the GoogleNet. TensorBoard provides an inline functionality for Jupyter notebooks, and we use it here:

[20]:
```
# Load tensorboard extension
%load_ext tensorboard
```

[21]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH!
%tensorboard --logdir ../saved_models/tutorial5/tensorboards/GoogleNet/
```



TensorBoard is organized in multiple tabs. The main tab is the scalar tab where we can log the development of single numbers. For example, we have plotted the training loss, accuracy, learning rate, etc. If we look at the training or validation accuracy, we can really see the impact of using a learning rate scheduler. Reducing the learning rate gives our model a nice increase in training performance. Similarly, when looking at the training loss, we see a sudden decrease at this point. However, the high numbers on the training set compared to validation indicate that our model was overfitting which is inevitable for such large networks.

Another interesting tab in TensorBoard is the graph tab. It shows us the network architecture organized by building blocks from the input to the output. It basically shows the operations taken in the forward step of `CIFARModule`. Double-click on a module to open it. Feel free to explore the architecture from a different perspective. The graph visualization can often help you to validate that your model is actually doing what it is supposed to do, and you don't miss any layers in the computation graph.

4.19.3 ResNet

The ResNet paper is one of the most cited AI papers, and has been the foundation for neural networks with more than 1,000 layers. Despite its simplicity, the idea of residual connections is highly effective as it supports stable gradient propagation through the network. Instead of modeling $x_{l+1} = F(x_l)$, we model $x_{l+1} = x_l + F(x_l)$ where F is a non-linear mapping (usually a sequence of NN modules likes convolutions, activation functions, and normalizations). If we do backpropagation on such residual connections, we obtain:

$$\frac{\partial x_{l+1}}{\partial x_l} = \mathbf{I} + \frac{\partial F(x_l)}{\partial x_l}$$

The bias towards the identity matrix guarantees a stable gradient propagation being less effected by F itself. There have been many variants of ResNet proposed, which mostly concern the function F, or operations applied on the sum. In this tutorial, we look at two of them: the original ResNet block, and the Pre-Activation ResNet block. We visually compare the blocks below (figure credit - He et al.):

The original ResNet block applies a non-linear activation function, usually ReLU, after the skip connection. In contrast, the pre-activation ResNet block applies the non-linearity at the beginning of F. Both have their advantages and disadvantages. For very deep network, however, the pre-activation ResNet has shown to perform better as the gradient flow is guaranteed to have the identity matrix as calculated above, and is not harmed by any non-linear activation applied to it. For comparison, in this notebook, we implement both ResNet types as shallow networks.

Let's start with the original ResNet block. The visualization above already shows what layers are included in F. One special case we have to handle is when we want to reduce the image dimensions in terms of width and height. The basic ResNet block requires $F(x_l)$ to be of the same shape as x_l. Thus, we need to change the dimensionality of x_l as well before adding to $F(x_l)$. The original implementation used an identity mapping with stride 2 and padded additional feature dimensions with 0. However, the more common implementation is to use a 1x1 convolution with stride 2 as it allows us to change the feature dimensionality while being efficient in parameter and computation cost. The code for the ResNet block is relatively simple, and shown below:

[22]:
```
class ResNetBlock(nn.Module):

    def __init__(self, c_in, act_fn, subsample=False, c_out=-1):
        """
        Inputs:
            c_in - Number of input features
            act_fn - Activation class constructor (e.g. nn.ReLU)
            subsample - If True, we want to apply a stride inside the block and reduce␣
↪the output shape by 2 in height and width
            c_out - Number of output features. Note that this is only relevant if␣
↪subsample is True, as otherwise, c_out = c_in
        """
        super().__init__()
        if not subsample:
            c_out = c_in

        # Network representing F
        self.net = nn.Sequential(
            nn.Conv2d(c_in, c_out, kernel_size=3, padding=1, stride=1 if not subsample␣
↪else 2, bias=False),  # No bias needed as the Batch Norm handles it
            nn.BatchNorm2d(c_out),
            act_fn(),
            nn.Conv2d(c_out, c_out, kernel_size=3, padding=1, bias=False),
            nn.BatchNorm2d(c_out)
        )

        # 1x1 convolution with stride 2 means we take the upper left value, and␣
↪transform it to new output size
        self.downsample = nn.Conv2d(c_in, c_out, kernel_size=1, stride=2) if subsample␣
↪else None
        self.act_fn = act_fn()

    def forward(self, x):
        z = self.net(x)
        if self.downsample is not None:
            x = self.downsample(x)
        out = z + x
        out = self.act_fn(out)
        return out
```

The second block we implement is the pre-activation ResNet block. For this, we have to change the order of layer in `self.net`, and do not apply an activation function on the output. Additionally, the downsampling operation has to apply a non-linearity as well as the input, x_l, has not been processed by a non-linearity yet. Hence, the block looks as follows:

[23]:
```
class PreActResNetBlock(nn.Module):

    def __init__(self, c_in, act_fn, subsample=False, c_out=-1):
        """
        Inputs:
            c_in - Number of input features
            act_fn - Activation class constructor (e.g. nn.ReLU)
            subsample - If True, we want to apply a stride inside the block and reduce␣
↪the output shape by 2 in height and width
            c_out - Number of output features. Note that this is only relevant if␣
↪subsample is True, as otherwise, c_out = c_in
        """
        super().__init__()
        if not subsample:
            c_out = c_in

        # Network representing F
        self.net = nn.Sequential(
            nn.BatchNorm2d(c_in),
            act_fn(),
            nn.Conv2d(c_in, c_out, kernel_size=3, padding=1, stride=1 if not subsample␣
↪else 2, bias=False),
            nn.BatchNorm2d(c_out),
            act_fn(),
            nn.Conv2d(c_out, c_out, kernel_size=3, padding=1, bias=False)
        )

        # 1x1 convolution can apply non-linearity as well, but not strictly necessary
        self.downsample = nn.Sequential(
            nn.BatchNorm2d(c_in),
            act_fn(),
            nn.Conv2d(c_in, c_out, kernel_size=1, stride=2, bias=False)
        ) if subsample else None

    def forward(self, x):
        z = self.net(x)
        if self.downsample is not None:
            x = self.downsample(x)
        out = z + x
        return out
```

Similarly to the model selection, we define a dictionary to create a mapping from string to block class. We will use the string name as hyperparameter value in our model to choose between the ResNet blocks. Feel free to implement any other ResNet block type and add it here as well.

[24]:
```
resnet_blocks_by_name = {
    "ResNetBlock": ResNetBlock,
    "PreActResNetBlock": PreActResNetBlock
}
```

The overall ResNet architecture consists of stacking multiple ResNet blocks, of which some are downsampling the input. When talking about ResNet blocks in the whole network, we usually group them by the same output shape. Hence, if we say the ResNet has `[3,3,3]` blocks, it means that we have 3 times a group of 3 ResNet blocks, where a subsampling is taking place in the fourth and seventh block. The ResNet with `[3,3,3]` blocks on CIFAR10 is visualized below.

The three groups operate on the resolutions 32×32, 16×16 and 8×8 respectively. The blocks in orange denote ResNet blocks with downsampling. The same notation is used by many other implementations such as in the torchvision library from PyTorch. Thus, our code looks as follows:

[25]:
```
class ResNet(nn.Module):

    def __init__(self, num_classes=10, num_blocks=[3,3,3], c_hidden=[16,32,64], act_fn_
↪name="relu", block_name="ResNetBlock", **kwargs):
        """
        Inputs:
            num_classes - Number of classification outputs (10 for CIFAR10)
            num_blocks - List with the number of ResNet blocks to use. The first block␣
↪of each group uses downsampling, except the first.
            c_hidden - List with the hidden dimensionalities in the different blocks.␣
↪Usually multiplied by 2 the deeper we go.
            act_fn_name - Name of the activation function to use, looked up in "act_fn_
↪by_name"
            block_name - Name of the ResNet block, looked up in "resnet_blocks_by_name"
        """
        super().__init__()
        assert block_name in resnet_blocks_by_name
        self.hparams = SimpleNamespace(num_classes=num_classes,
                                       c_hidden=c_hidden,
                                       num_blocks=num_blocks,
                                       act_fn_name=act_fn_name,
                                       act_fn=act_fn_by_name[act_fn_name],
                                       block_class=resnet_blocks_by_name[block_name])
        self._create_network()
        self._init_params()

    def _create_network(self):
        c_hidden = self.hparams.c_hidden

        # A first convolution on the original image to scale up the channel size
        if self.hparams.block_class == PreActResNetBlock: # => Don't apply non-linearity␣
↪on output
            self.input_net = nn.Sequential(
                nn.Conv2d(3, c_hidden[0], kernel_size=3, padding=1, bias=False)
            )
        else:
            self.input_net = nn.Sequential(
                nn.Conv2d(3, c_hidden[0], kernel_size=3, padding=1, bias=False),
                nn.BatchNorm2d(c_hidden[0]),
                self.hparams.act_fn()
            )

        # Creating the ResNet blocks
```

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```
        blocks = []
        for block_idx, block_count in enumerate(self.hparams.num_blocks):
            for bc in range(block_count):
                subsample = (bc == 0 and block_idx > 0) # Subsample the first block of␣
↪each group, except the very first one.
                blocks.append(
                    self.hparams.block_class(c_in=c_hidden[block_idx if not subsample␣
↪else (block_idx-1)],
                                             act_fn=self.hparams.act_fn,
                                             subsample=subsample,
                                             c_out=c_hidden[block_idx])
                )
        self.blocks = nn.Sequential(*blocks)

        # Mapping to classification output
        self.output_net = nn.Sequential(
            nn.AdaptiveAvgPool2d((1,1)),
            nn.Flatten(),
            nn.Linear(c_hidden[-1], self.hparams.num_classes)
        )

    def _init_params(self):
        # Based on our discussion in Tutorial 4, we should initialize the convolutions␣
↪according to the activation function
        # Fan-out focuses on the gradient distribution, and is commonly used in ResNets
        for m in self.modules():
            if isinstance(m, nn.Conv2d):
                nn.init.kaiming_normal_(m.weight, mode='fan_out', nonlinearity=self.
↪hparams.act_fn_name)
            elif isinstance(m, nn.BatchNorm2d):
                nn.init.constant_(m.weight, 1)
                nn.init.constant_(m.bias, 0)

    def forward(self, x):
        x = self.input_net(x)
        x = self.blocks(x)
        x = self.output_net(x)
        return x
```

We also need to add the new ResNet class to our model dictionary:

[26]:
```
model_dict["ResNet"] = ResNet
```

Finally, we can train our ResNet models. One difference to the GoogleNet training is that we explicitly use SGD with Momentum as optimizer instead of Adam. Adam often leads to a slightly worse accuracy on plain, shallow ResNets. It is not 100% clear why Adam performs worse in this context, but one possible explanation is related to ResNet's loss surface. ResNet has been shown to produce smoother loss surfaces than networks without skip connection (see Li et al., 2018 for details). A possible visualization of the loss surface with/out skip connections is below (figure credit - Li et al.):

The x and y axis shows a projection of the parameter space, and the z axis shows the loss values achieved by different parameter values. On smooth surfaces like the one on the right, we might not require an adaptive learning rate as Adam

provides. Instead, Adam can get stuck in local optima while SGD finds the wider minima that tend to generalize better. However, to answer this question in detail, we would need an extra tutorial because it is not easy to answer. For now, we conclude: for ResNet architectures, consider the optimizer to be an important hyperparameter, and try training with both Adam and SGD. Let's train the model below with SGD:

[27]:
```
resnet_model, resnet_results = train_model(model_name="ResNet",
                                           model_hparams={"num_classes": 10,
                                                          "c_hidden": [16,32,64],
                                                          "num_blocks": [3,3,3],
                                                          "act_fn_name": "relu"},
                                           optimizer_name="SGD",
                                           optimizer_hparams={"lr": 0.1,
                                                              "momentum": 0.9,
                                                              "weight_decay": 1e-4})
```

```
GPU available: True, used: True
WARNING: Logging before flag parsing goes to stderr.
I1109 15:33:03.301807 139927971620672 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1109 15:33:03.303210 139927971620672 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1109 15:33:03.304439 139927971620672 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model at ../saved_models/tutorial5/ResNet.ckpt, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

Let's also train the pre-activation ResNet as comparison:

[28]:
```
resnetpreact_model, resnetpreact_results = train_model(model_name="ResNet",
                                                       model_hparams={"num_classes": 10,
                                                                      "c_hidden": [16,32,
↪64],
                                                                      "num_blocks": [3,3,
↪3],
                                                                      "act_fn_name":
↪"relu",
                                                                      "block_name":
↪"PreActResNetBlock"},
                                                       optimizer_name="SGD",
                                                       optimizer_hparams={"lr": 0.1,
                                                                          "momentum": 0.
↪9,
                                                                          "weight_decay":
↪ 1e-4},
                                                       save_name="ResNetPreAct")
```

```
GPU available: True, used: True
I1109 15:33:06.813361 139927971620672 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1109 15:33:06.815118 139927971620672 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1109 15:33:06.816660 139927971620672 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model at ../saved_models/tutorial5/ResNetPreAct.ckpt, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

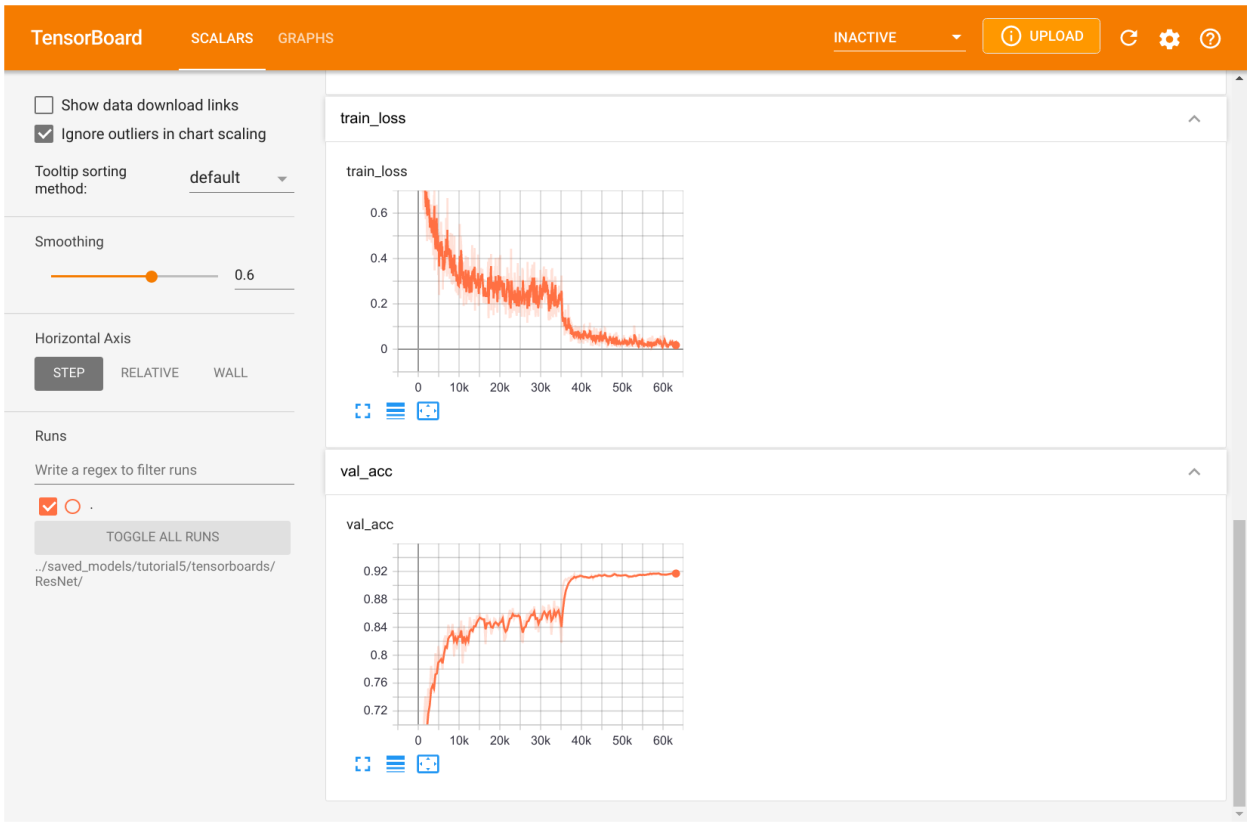
```

```

Tensorboard log

Similarly to our GoogleNet model, we also have a TensorBoard log for the ResNet model. We can open it below.

[29]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH! Feel free to␣
↪change "ResNet" to "ResNetPreAct"
%tensorboard --logdir ../saved_models/tutorial5/tensorboards/ResNet/
```



Feel free to explore the TensorBoard yourself, including the computation graph. In general, we can see that with SGD, the ResNet has a higher training loss than the GoogleNet in the first stage of the training. After reducing the learning rate however, the model achieves even higher validation accuracies. We compare the precise scores at the end of the notebook.

4.19.4 DenseNet

DenseNet is another architecture for enabling very deep neural networks and takes a slightly different perspective on residual connections. Instead of modeling the difference between layers, DenseNet considers residual connections as a possible way to reuse features across layers, removing any necessity to learn redundant feature maps. If we go deeper into the network, the model learns abstract features to recognize patterns. However, some complex patterns consist of a combination of abstract features (e.g. hand, face, etc.), and low-level features (e.g. edges, basic color, etc.). To find these low-level features in the deep layers, standard CNNs have to learn copy such feature maps, which wastes a lot of parameter complexity. DenseNet provides an efficient way of reusing features by having each convolution depends on all previous input features, but add only a small amount of filters to it. See the figure below for an illustration (figure credit - Hu et al.):

The last layer, called the transition layer, is responsible for reducing the dimensionality of the feature maps in height, width, and channel size. Although those technically break the identity backpropagation, there are only a few in a network so that it doesn't affect the gradient flow much.

We split the implementation of the layers in DenseNet into three parts: a `DenseLayer`, and a `DenseBlock`, and a `TransitionLayer`. The module `DenseLayer` implements a single layer inside a dense block. It applies a 1x1 convolution for dimensionality reduction with a subsequential 3x3 convolution. The output channels are concatenated to the originals and returned. Note that we apply the Batch Normalization as the first layer of each block. This allows slightly different activations for the same features to different layers, depending on what is needed. Overall, we can implement it as follows:

[30]:
```
class DenseLayer(nn.Module):

    def __init__(self, c_in, bn_size, growth_rate, act_fn):
        """
        Inputs:
            c_in - Number of input channels
            bn_size - Bottleneck size (factor of growth rate) for the output of the 1x1␣
↪convolution. Typically between 2 and 4.
            growth_rate - Number of output channels of the 3x3 convolution
            act_fn - Activation class constructor (e.g. nn.ReLU)
        """
        super().__init__()
        self.net = nn.Sequential(
            nn.BatchNorm2d(c_in),
            act_fn(),
            nn.Conv2d(c_in, bn_size * growth_rate, kernel_size=1, bias=False),
            nn.BatchNorm2d(bn_size * growth_rate),
            act_fn(),
            nn.Conv2d(bn_size * growth_rate, growth_rate, kernel_size=3, padding=1,␣
↪bias=False)
        )

    def forward(self, x):
        out = self.net(x)
```

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```
        out = torch.cat([out, x], dim=1)
        return out
```

The module DenseBlock summarizes multiple dense layers applied in sequence. Each dense layer takes as input the original input concatenated with all previous layers' feature maps:

[31]:
```
class DenseBlock(nn.Module):

    def __init__(self, c_in, num_layers, bn_size, growth_rate, act_fn):
        """
        Inputs:
            c_in - Number of input channels
            num_layers - Number of dense layers to apply in the block
            bn_size - Bottleneck size to use in the dense layers
            growth_rate - Growth rate to use in the dense layers
            act_fn - Activation function to use in the dense layers
        """
        super().__init__()
        layers = []
        for layer_idx in range(num_layers):
            layers.append(
                DenseLayer(c_in=c_in + layer_idx * growth_rate, # Input channels are␣
↪original plus the feature maps from previous layers
                           bn_size=bn_size,
                           growth_rate=growth_rate,
                           act_fn=act_fn)
            )
        self.block = nn.Sequential(*layers)

    def forward(self, x):
        out = self.block(x)
        return out
```

Finally, the TransitionLayer takes as input the final output of a dense block and reduces its channel dimensionality using a 1x1 convolution. To reduce the height and width dimension, we take a slightly different approach than in ResNet and apply an average pooling with kernel size 2 and stride 2. This is because we don't have an additional connection to the output that would consider the full 2x2 patch instead of a single value. Besides, it is more parameter efficient than using a 3x3 convolution with stride 2. Thus, the layer is implemented as follows:

[32]:
```
class TransitionLayer(nn.Module):

    def __init__(self, c_in, c_out, act_fn):
        super().__init__()
        self.transition = nn.Sequential(
            nn.BatchNorm2d(c_in),
            act_fn(),
            nn.Conv2d(c_in, c_out, kernel_size=1, bias=False),
            nn.AvgPool2d(kernel_size=2, stride=2) # Average the output for each 2x2␣
↪pixel group
        )

    def forward(self, x):
        return self.transition(x)
```

Now we can put everything together and create our DenseNet. To specify the number of layers, we use a similar notation as in ResNets and pass on a list of ints representing the number of layers per block. After each dense block except the last one, we apply a transition layer to reduce the dimensionality by 2.

[33]:
```
class DenseNet(nn.Module):

    def __init__(self, num_classes=10, num_layers=[6,6,6,6], bn_size=2, growth_rate=16,␣
↪act_fn_name="relu", **kwargs):
        super().__init__()
        self.hparams = SimpleNamespace(num_classes=num_classes,
                                       num_layers=num_layers,
                                       bn_size=bn_size,
                                       growth_rate=growth_rate,
                                       act_fn_name=act_fn_name,
                                       act_fn=act_fn_by_name[act_fn_name])
        self._create_network()
        self._init_params()

    def _create_network(self):
        c_hidden = self.hparams.growth_rate * self.hparams.bn_size # The start number of␣
↪hidden channels

        # A first convolution on the original image to scale up the channel size
        self.input_net = nn.Sequential(
            nn.Conv2d(3, c_hidden, kernel_size=3, padding=1) # No batch norm or␣
↪activation function as done inside the Dense layers
        )

        # Creating the dense blocks, eventually including transition layers
        blocks = []
        for block_idx, num_layers in enumerate(self.hparams.num_layers):
            blocks.append(
                DenseBlock(c_in=c_hidden,
                           num_layers=num_layers,
                           bn_size=self.hparams.bn_size,
                           growth_rate=self.hparams.growth_rate,
                           act_fn=self.hparams.act_fn)
            )
            c_hidden = c_hidden + num_layers * self.hparams.growth_rate # Overall output␣
↪of the dense block
            if block_idx < len(self.hparams.num_layers)-1: # Don't apply transition layer␣
↪on last block
                blocks.append(
                    TransitionLayer(c_in=c_hidden,
                                    c_out=c_hidden // 2,
                                    act_fn=self.hparams.act_fn))
                c_hidden = c_hidden // 2

        self.blocks = nn.Sequential(*blocks)

        # Mapping to classification output
        self.output_net = nn.Sequential(
            nn.BatchNorm2d(c_hidden), # The features have not passed a non-linearity␣
↪until here.
```

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```
            self.hparams.act_fn(),
            nn.AdaptiveAvgPool2d((1,1)),
            nn.Flatten(),
            nn.Linear(c_hidden, self.hparams.num_classes)
        )

    def _init_params(self):
        # Based on our discussion in Tutorial 4, we should initialize the convolutions␣
↪according to the activation function
        for m in self.modules():
            if isinstance(m, nn.Conv2d):
                nn.init.kaiming_normal_(m.weight, nonlinearity=self.hparams.act_fn_name)
            elif isinstance(m, nn.BatchNorm2d):
                nn.init.constant_(m.weight, 1)
                nn.init.constant_(m.bias, 0)

    def forward(self, x):
        x = self.input_net(x)
        x = self.blocks(x)
        x = self.output_net(x)
        return x
```

Let's also add the DenseNet to our model dictionary:

[34]:
```
model_dict["DenseNet"] = DenseNet
```

Lastly, we train our network. In contrast to ResNet, DenseNet does not show any issues with Adam, and hence we train it with this optimizer. The other hyperparameters are chosen to result in a network with a similar parameter size as the ResNet and GoogleNet. Commonly, when designing very deep networks, DenseNet is more parameter efficient than ResNet while achieving a similar or even better performance.

[35]:
```
densenet_model, densenet_results = train_model(model_name="DenseNet",
                                               model_hparams={"num_classes": 10,
                                                              "num_layers": [6,6,6,6],
                                                              "bn_size": 2,
                                                              "growth_rate": 16,
                                                              "act_fn_name": "relu"},
                                               optimizer_name="Adam",
                                               optimizer_hparams={"lr": 1e-3,
                                                                  "weight_decay": 1e-4})
```

```
GPU available: True, used: True
I1109 15:33:10.534986 139927971620672 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1109 15:33:10.536422 139927971620672 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1109 15:33:10.538130 139927971620672 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model at ../saved_models/tutorial5/DenseNet.ckpt, loading...
```

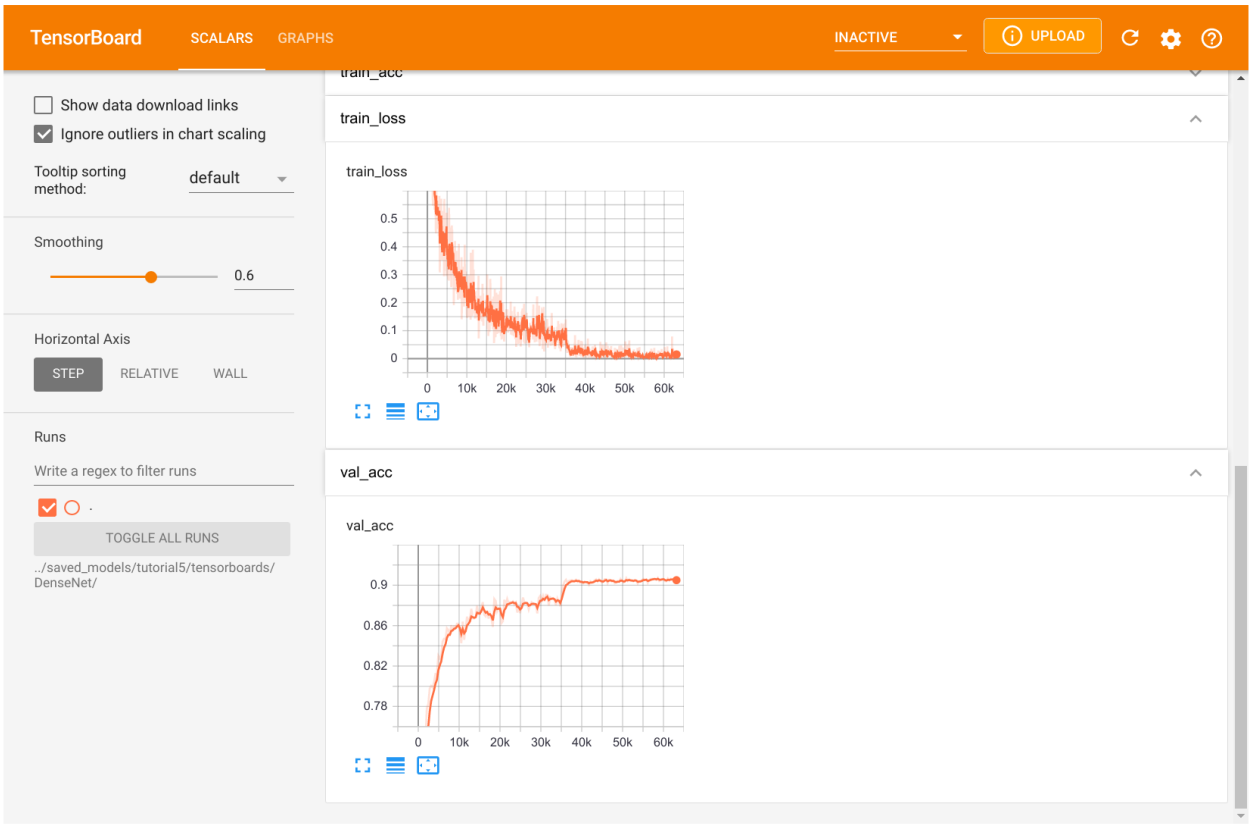
```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

Tensorboard log

Finally, we also have another TensorBoard for the DenseNet training. We take a look at it below:

[36]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH!
%tensorboard --logdir ../saved_models/tutorial5/tensorboards/DenseNet/
```



The overall course of the validation accuracy and training loss resemble the training of GoogleNet, which is also related to training the network with Adam. Feel free to explore the training metrics yourself.

4.19.5 Conclusion and Comparison

After discussing each model separately, and training all of them, we can finally compare them. First, let's organize the results of all models in a table:

[37]:
```
%%html
<!-- Some HTML code to increase font size in the following table -->
<style>
th {font-size: 120%;}
td {font-size: 120%;}
</style>
```

```
<IPython.core.display.HTML object>
```

[38]:
```
import tabulate
from IPython.display import display, HTML
all_models = [
    ("GoogleNet", googlenet_results, googlenet_model),
    ("ResNet", resnet_results, resnet_model),
    ("ResNetPreAct", resnetpreact_results, resnetpreact_model),
    ("DenseNet", densenet_results, densenet_model)
]
table = [[model_name,
          f"{100.0*model_results['val']:4.2f}%",
          f"{100.0*model_results['test']:4.2f}%",
          "{:,}".format(sum([np.prod(p.shape) for p in model.parameters()]))]
         for model_name, model_results, model in all_models]
display(HTML(tabulate.tabulate(table, tablefmt='html', headers=["Model", "Val Accuracy",
↪"Test Accuracy", "Num Parameters"])))
```

```
<IPython.core.display.HTML object>
```

First of all, we see that all models are performing reasonably well. Simple models as you have implemented them in the practical achieve considerably lower performance, which is beside the lower number of parameters also attributed to the architecture design choice. GoogleNet is the model to obtain the lowest performance on the validation and test set, although it is very close to DenseNet. A proper hyperparameter search over all the channel sizes in GoogleNet would likely improve the accuracy of the model to a similar level, but this is also expensive given a large number of hyperparameters. ResNet outperforms both DenseNet and GoogleNet by more than 1% on the validation set, while there is a minor difference between both versions, original and pre-activation. We can conclude that for shallow networks, the place of the activation function does not seem to be crucial, although papers have reported the contrary for very deep networks (e.g. He et al.).

In general, we can conclude that ResNet is a simple, but powerful architecture. If we would apply the models on more complex tasks with larger images and more layers inside the networks, we would likely see a bigger gap between GoogleNet and skip-connection architectures like ResNet and DenseNet. A comparison with deeper models on CIFAR10 can be for example found here. Interestingly, DenseNet outperforms the original ResNet on their setup but comes closely behind the Pre-Activation ResNet. The best model, a Dual Path Network (Chen et. al), is actually a combination of ResNet and DenseNet showing that both offer different advantages.

Which model should I choose for my task?

We have reviewed four different models. So, which one should we choose if have given a new task? Usually, starting with a ResNet is a good idea given the superior performance of the CIFAR dataset and its simple implementation. Besides, for the parameter number we have chosen here, ResNet is the fastest as DenseNet and GoogleNet have many more layers that are applied in sequence in our primitive implementation. However, if you have a really difficult task, such as semantic segmentation on HD images, more complex variants of ResNet and DenseNet are recommended.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.20 Tutorial 6: Transformers and Multi-Head Attention

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will discuss one of the most impactful architectures of the last 2 years: the Transformer model. Since the paper Attention Is All You Need by Vaswani et al. had been published in 2017, the Transformer architecture has continued to beat benchmarks in many domains, most importantly in Natural Language Processing. Transformers with an incredible amount of parameters can generate long, convincing essays, and opened up new application fields of AI. As the hype of the Transformer architecture seems not to come to an end in the next years, it is important to understand how it works, and have implemented it yourself, which we will do in this notebook.

Despite the huge success of Transformers in NLP, we will *not* include the NLP domain in our notebook here. Why? Firstly, the Master AI at UvA offers many great NLP courses that will take a closer look at the application of the Transformer architecture in NLP (NLP2, Advanced Topics in Computational Semantics). Secondly, assignment 2 takes already a closer look at language generation on character level, on which you could easily apply our transformer architecture. Finally, and most importantly, there is so much more to the Transformer architecture. NLP is the domain the Transformer architecture has been originally proposed for and had the greatest impact on, but it also accelerated research in other domains, recently even Computer Vision. Thus, we focus here on what makes the Transformer and self-attention so powerful in general. In Tutorial 15, we will discuss the application of Transformers in Computer Vision.

Below, we import our standard libraries. Similarly as in Tutorial 5, we will use PyTorch Lightning as an additional framework. If you are not familiar with PyTorch Lightning, please make sure to have read Tutorial 5 carefully.

[1]:
```
## Standard libraries
import os
import numpy as np
import random
import math
import json
from functools import partial

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## tqdm for loading bars
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim

## Torchvision
import torchvision
from torchvision.datasets import CIFAR100
from torchvision import transforms

# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial6"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
```

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```
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)
```

```
Device: cuda:0
```

Two pre-trained models are downloaded below. Make sure to have adjusted your `CHECKPOINT_PATH` before running this code if not already done.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial6/"
# Files to download
pretrained_files = ["ReverseTask.ckpt", "SetAnomalyTask.ckpt"]

# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.20.1 The Transformer architecture

In the first part of this notebook, we will implement the Transformer architecture by hand. As the architecture is so popular, there already exists a Pytorch module `nn.Transformer` (documentation) and a tutorial on how to use it for next token prediction. However, we will implement it here ourselves, to get through to the smallest details.

There are of course many more tutorials out there about attention and Transformers. Below, we list a few that are worth exploring if you are interested in the topic and might want yet another perspective on the topic after this one:

- Transformer: A Novel Neural Network Architecture for Language Understanding (Jakob Uszkoreit, 2017) - The original Google blog post about the Transformer paper, focusing on the application in machine translation.
- The Illustrated Transformer (Jay Alammar, 2018) - A very popular and great blog post intuitively explaining the Transformer architecture with many nice visualizations. The focus is on NLP.
- Attention? Attention! (Lilian Weng, 2018) - A nice blog post summarizing attention mechanisms in many domains including vision.

- Illustrated: Self-Attention (Raimi Karim, 2019) - A nice visualization of the steps of self-attention. Recommended going through if the explanation below is too abstract for you.
- The Transformer family (Lilian Weng, 2020) - A very detailed blog post reviewing more variants of Transformers besides the original one.

What is Attention?

The attention mechanism describes a recent new group of layers in neural networks that has attracted a lot of interest in the past few years, especially in sequence tasks. There are a lot of different possible definitions of "attention" in the literature, but the one we will use here is the following: *the attention mechanism describes a weighted average of (sequence) elements with the weights dynamically computed based on an input query and elements' keys*. So what does this exactly mean? The goal is to take an average over the features of multiple elements. However, instead of weighting each element equally, we want to weight them depending on their actual values. In other words, we want to dynamically decide on which inputs we want to "attend" more than others. In particular, an attention mechanism has usually four parts we need to specify:

- **Query**: The query is a feature vector that describes what we are looking for in the sequence, i.e. what would we maybe want to pay attention to.
- **Keys**: For each input element, we have a key which is again a feature vector. This feature vector roughly describes what the element is "offering", or when it might be important. The keys should be designed such that we can identify the elements we want to pay attention to based on the query.
- **Values**: For each input element, we also have a value vector. This feature vector is the one we want to average over.
- **Score function**: To rate which elements we want to pay attention to, we need to specify a score function f_{attn}. The score function takes the query and a key as input, and output the score/attention weight of the query-key pair. It is usually implemented by simple similarity metrics like a dot product, or a small MLP.

The weights of the average are calculated by a softmax over all score function outputs. Hence, we assign those value vectors a higher weight whose corresponding key is most similar to the query. If we try to describe it with pseudo-math, we can write:

$$\alpha_i = \frac{\exp\left(f_{attn}\left(\text{key}_i, \text{query}\right)\right)}{\sum_j \exp\left(f_{attn}\left(\text{key}_j, \text{query}\right)\right)}, \qquad \text{out} = \sum_i \alpha_i \cdot \text{value}_i$$

Visually, we can show the attention over a sequence of words as follows:

For every word, we have one key and one value vector. The query is compared to all keys with a score function (in this case the dot product) to determine the weights. The softmax is not visualized for simplicity. Finally, the value vectors of all words are averaged using the attention weights.

Most attention mechanisms differ in terms of what queries they use, how the key and value vectors are defined, and what score function is used. The attention applied inside the Transformer architecture is called **self-attention**. In self-attention, each sequence element provides a key, value, and query. For each element, we perform an attention layer where based on its query, we check the similarity of the all sequence elements' keys, and returned a different, averaged value vector for each element. We will now go into a bit more detail by first looking at the specific implementation of the attention mechanism which is in the Transformer case the scaled dot product attention.

Scaled Dot Product Attention

The core concept behind self-attention is the scaled dot product attention. Our goal is to have an attention mechanism with which any element in a sequence can attend to any other while still being efficient to compute. The dot product attention takes as input a set of queries $Q \in \mathbb{R}^{T \times d_k}$, keys $K \in \mathbb{R}^{T \times d_k}$ and values $V \in \mathbb{R}^{T \times d_v}$ where T is the sequence length, and d_k and d_v are the hidden dimensionality for queries/keys and values respectively. For simplicity, we neglect the batch dimension for now. The attention value from element i to j is based on its similarity of the query Q_i and key K_j, using the dot product as the similarity metric. In math, we calculate the dot product attention as follows:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

The matrix multiplication QK^T performs the dot product for every possible pair of queries and keys, resulting in a matrix of the shape $T \times T$. Each row represents the attention logits for a specific element i to all other elements in the sequence. On these, we apply a softmax and multiply with the value vector to obtain a weighted mean (the weights being determined by the attention). Another perspective on this attention mechanism offers the computation graph which is visualized below (figure credit - Vaswani et al., 2017).

One aspect we haven't discussed yet is the scaling factor of $1/\sqrt{d_k}$. This scaling factor is crucial to maintain an appropriate variance of attention values after initialization. Remember that we intialize our layers with the intention of having equal variance throughout the model, and hence, Q and K might also have a variance close to 1. However, performing a dot product over two vectors with a variance σ^2 results in a scalar having d_k-times higher variance:

$$q_i \sim \mathcal{N}(0, \sigma^2), k_i \sim \mathcal{N}(0, \sigma^2) \rightarrow \text{Var}\left(\sum_{i=1}^{d_k} q_i \cdot k_i\right) = \sigma^4 \cdot d_k$$

If we do not scale down the variance back to $\sim \sigma^2$, the softmax over the logits will already saturate to 1 for one random element and 0 for all others. The gradients through the softmax will be close to zero so that we can't learn the parameters appropriately. Note that the extra factor of σ^2, i.e., having σ^4 instead of σ^2, is usually not an issue, since we keep the original variance σ^2 close to 1 anyways.

The block `Mask (opt.)` in the diagram above represents the optional masking of specific entries in the attention matrix. This is for instance used if we stack multiple sequences with different lengths into a batch. To still benefit from parallelization in PyTorch, we pad the sentences to the same length and mask out the padding tokens during the calculation of the attention values. This is usually done by setting the respective attention logits to a very low value.

After we have discussed the details of the scaled dot product attention block, we can write a function below which computes the output features given the triple of queries, keys, and values:

[3]:
```
def scaled_dot_product(q, k, v, mask=None):
    d_k = q.size()[-1]
    attn_logits = torch.matmul(q, k.transpose(-2, -1))
    attn_logits = attn_logits / math.sqrt(d_k)
    if mask is not None:
        attn_logits = attn_logits.masked_fill(mask == 0, -9e15)
    attention = F.softmax(attn_logits, dim=-1)
    values = torch.matmul(attention, v)
    return values, attention
```

Note that our code above supports any additional dimensionality in front of the sequence length so that we can also use it for batches. However, for a better understanding, let's generate a few random queries, keys, and value vectors, and calculate the attention outputs:

[4]:
```
seq_len, d_k = 3, 2
pl.seed_everything(42)
q = torch.randn(seq_len, d_k)
k = torch.randn(seq_len, d_k)
v = torch.randn(seq_len, d_k)
values, attention = scaled_dot_product(q, k, v)
print("Q\n", q)
print("K\n", k)
print("V\n", v)
print("Values\n", values)
print("Attention\n", attention)
```

```
Q
 tensor([[ 0.3367,  0.1288],
        [ 0.2345,  0.2303],
        [-1.1229, -0.1863]])
K
 tensor([[ 2.2082, -0.6380],
        [ 0.4617,  0.2674],
        [ 0.5349,  0.8094]])
V
 tensor([[ 1.1103, -1.6898],
        [-0.9890,  0.9580],
        [ 1.3221,  0.8172]])
Values
 tensor([[ 0.5698, -0.1520],
        [ 0.5379, -0.0265],
        [ 0.2246,  0.5556]])
Attention
 tensor([[0.4028, 0.2886, 0.3086],
        [0.3538, 0.3069, 0.3393],
        [0.1303, 0.4630, 0.4067]])
```

Before continuing, make sure you can follow the calculation of the specific values here, and also check it by hand. It is important to fully understand how the scaled dot product attention is calculated.

Multi-Head Attention

The scaled dot product attention allows a network to attend over a sequence. However, often there are multiple different aspects a sequence element wants to attend to, and a single weighted average is not a good option for it. This is why we extend the attention mechanisms to multiple heads, i.e. multiple different query-key-value triplets on the same features. Specifically, given a query, key, and value matrix, we transform those into h sub-queries, sub-keys, and sub-values, which we pass through the scaled dot product attention independently. Afterward, we concatenate the heads and combine them with a final weight matrix. Mathematically, we can express this operation as:

$$\text{Multihead}(Q, K, V) = \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O$$
$$\text{where head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

We refer to this as Multi-Head Attention layer with the learnable parameters $W^Q_{1...h} \in \mathbb{R}^{D\times d_k}$, $W^K_{1...h} \in \mathbb{R}^{D\times d_k}$, $W^V_{1...h} \in \mathbb{R}^{D\times d_v}$, and $W^O \in \mathbb{R}^{h\cdot d_v \times d_{out}}$ (D being the input dimensionality). Expressed in a computational graph, we can visualize it as below (figure credit - Vaswani et al., 2017).

How are we applying a Multi-Head Attention layer in a neural network, where we don't have an arbitrary query, key, and value vector as input? Looking at the computation graph above, a simple but effective implementation is to set the current feature map in a NN, $X \in \mathbb{R}^{B \times T \times d_{\text{model}}}$, as Q, K and V (B being the batch size, T the sequence length, d_{model} the hidden dimensionality of X). The consecutive weight matrices W^Q, W^K, and W^V can transform X to the corresponding feature vectors that represent the queries, keys, and values of the input. Using this approach, we can implement the Multi-Head Attention module below.

[ ]:
```
# Helper function to support different mask shapes.
# Output shape supports (batch_size, number of heads, seq length, seq length)
# If 2D: broadcasted over batch size and number of heads
# If 3D: broadcasted over number of heads
# If 4D: leave as is
def expand_mask(mask):
    assert mask.ndim >= 2, "Mask must be at least 2-dimensional with seq_length x seq_
↪length"
    if mask.ndim == 3:
        mask = mask.unsqueeze(1)
    while mask.ndim < 4:
        mask = mask.unsqueeze(0)
    return mask
```

[5]:
```
class MultiheadAttention(nn.Module):

    def __init__(self, input_dim, embed_dim, num_heads):
        super().__init__()
        assert embed_dim % num_heads == 0, "Embedding dimension must be 0 modulo number␣
↪of heads."

        self.embed_dim = embed_dim
        self.num_heads = num_heads
        self.head_dim = embed_dim // num_heads

        # Stack all weight matrices 1...h together for efficiency
        # Note that in many implementations you see "bias=False" which is optional
        self.qkv_proj = nn.Linear(input_dim, 3*embed_dim)
        self.o_proj = nn.Linear(embed_dim, embed_dim)

        self._reset_parameters()

    def _reset_parameters(self):
        # Original Transformer initialization, see PyTorch documentation
        nn.init.xavier_uniform_(self.qkv_proj.weight)
        self.qkv_proj.bias.data.fill_(0)
        nn.init.xavier_uniform_(self.o_proj.weight)
        self.o_proj.bias.data.fill_(0)

    def forward(self, x, mask=None, return_attention=False):
        batch_size, seq_length, _ = x.size()
        if mask is not None:
            mask = expand_mask(mask)
        qkv = self.qkv_proj(x)

        # Separate Q, K, V from linear output
```

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```
        qkv = qkv.reshape(batch_size, seq_length, self.num_heads, 3*self.head_dim)
        qkv = qkv.permute(0, 2, 1, 3) # [Batch, Head, SeqLen, Dims]
        q, k, v = qkv.chunk(3, dim=-1)

        # Determine value outputs
        values, attention = scaled_dot_product(q, k, v, mask=mask)
        values = values.permute(0, 2, 1, 3) # [Batch, SeqLen, Head, Dims]
        values = values.reshape(batch_size, seq_length, self.embed_dim)
        o = self.o_proj(values)

        if return_attention:
            return o, attention
        else:
            return o
```

One crucial characteristic of the multi-head attention is that it is permutation-equivariant with respect to its inputs. This means that if we switch two input elements in the sequence, e.g. $X_1 \leftrightarrow X_2$ (neglecting the batch dimension for now), the output is exactly the same besides the elements 1 and 2 switched. Hence, the multi-head attention is actually looking at the input not as a sequence, but as a set of elements. This property makes the multi-head attention block and the Transformer architecture so powerful and widely applicable! But what if the order of the input is actually important for solving the task, like language modeling? The answer is to encode the position in the input features, which we will take a closer look at later (topic *Positional encodings* below).

Before moving on to creating the Transformer architecture, we can compare the self-attention operation with our other common layer competitors for sequence data: convolutions and recurrent neural networks. Below you can find a table by Vaswani et al. (2017) on the complexity per layer, the number of sequential operations, and maximum path length. The complexity is measured by the upper bound of the number of operations to perform, while the maximum path length represents the maximum number of steps a forward or backward signal has to traverse to reach any other position. The lower this length, the better gradient signals can backpropagate for long-range dependencies. Let's take a look at the table below:

n is the sequence length, d is the representation dimension and k is the kernel size of convolutions. In contrast to recurrent networks, the self-attention layer can parallelize all its operations making it much faster to execute for smaller sequence lengths. However, when the sequence length exceeds the hidden dimensionality, self-attention becomes more expensive than RNNs. One way of reducing the computational cost for long sequences is by restricting the self-attention to a neighborhood of inputs to attend over, denoted by r. Nevertheless, there has been recently a lot of work on more efficient Transformer architectures that still allow long dependencies, of which you can find an overview in the paper by Tay et al. (2020) if interested.

Transformer Encoder

Next, we will look at how to apply the multi-head attention block inside the Transformer architecture. Originally, the Transformer model was designed for machine translation. Hence, it got an encoder-decoder structure where the encoder takes as input the sentence in the original language and generates an attention-based representation. On the other hand, the decoder attends over the encoded information and generates the translated sentence in an autoregressive manner, as in a standard RNN. While this structure is extremely useful for Sequence-to-Sequence tasks with the necessity of autoregressive decoding, we will focus here on the encoder part. Many advances in NLP have been made using pure encoder-based Transformer models (if interested, models include the BERT-family, the Vision Transformer, and more), and in our tutorial, we will also mainly focus on the encoder part. If you have understood the encoder architecture, the decoder is a very small step to implement as well. The full Transformer architecture looks as follows (figure credit - Vaswani et al., 2017).:

The encoder consists of N identical blocks that are applied in sequence. Taking as input x, it is first passed through a Multi-Head Attention block as we have implemented above. The output is added to the original input using a residual connection, and we apply a consecutive Layer Normalization on the sum. Overall, it calculates $\text{LayerNorm}(x + \text{Multihead}(x, x, x))$ (x being Q, K and V input to the attention layer). The residual connection is crucial in the Transformer architecture for two reasons:

1. Similar to ResNets, Transformers are designed to be very deep. Some models contain more than 24 blocks in the encoder. Hence, the residual connections are crucial for enabling a smooth gradient flow through the model.
2. Without the residual connection, the information about the original sequence is lost. Remember that the Multi-Head Attention layer ignores the position of elements in a sequence, and can only learn it based on the input features. Removing the residual connections would mean that this information is lost after the first attention layer (after initialization), and with a randomly initialized query and key vector, the output vectors for position i has no relation to its original input. All outputs of the attention are likely to represent similar/same information, and there is no chance for the model to distinguish which information came from which input element. An alternative option to residual connection would be to fix at least one head to focus on its original input, but this is very inefficient and does not have the benefit of the improved gradient flow.

The Layer Normalization also plays an important role in the Transformer architecture as it enables faster training and provides small regularization. Additionally, it ensures that the features are in a similar magnitude among the elements in the sequence. We are not using Batch Normalization because it depends on the batch size which is often small with Transformers (they require a lot of GPU memory), and BatchNorm has shown to perform particularly bad in language as the features of words tend to have a much higher variance (there are many, very rare words which need to be considered for a good distribution estimate).

Additionally to the Multi-Head Attention, a small fully connected feed-forward network is added to the model, which is applied to each position separately and identically. Specifically, the model uses a Linear→ReLU→Linear MLP. The full transformation including the residual connection can be expressed as:

$$\text{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$
$$x = \text{LayerNorm}(x + \text{FFN}(x))$$

This MLP adds extra complexity to the model and allows transformations on each sequence element separately. You can imagine as this allows the model to "post-process" the new information added by the previous Multi-Head Attention, and prepare it for the next attention block. Usually, the inner dimensionality of the MLP is 2-8$\times$ larger than d_{model}, i.e. the dimensionality of the original input x. The general advantage of a wider layer instead of a narrow, multi-layer MLP is the faster, parallelizable execution.

Finally, after looking at all parts of the encoder architecture, we can start implementing it below. We first start by implementing a single encoder block. Additionally to the layers described above, we will add dropout layers in the MLP and on the output of the MLP and Multi-Head Attention for regularization.

[6]:
```
class EncoderBlock(nn.Module):

    def __init__(self, input_dim, num_heads, dim_feedforward, dropout=0.0):
        """
        Inputs:
            input_dim - Dimensionality of the input
            num_heads - Number of heads to use in the attention block
            dim_feedforward - Dimensionality of the hidden layer in the MLP
            dropout - Dropout probability to use in the dropout layers
        """
        super().__init__()

        # Attention layer
```

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```
        self.self_attn = MultiheadAttention(input_dim, input_dim, num_heads)

        # Two-layer MLP
        self.linear_net = nn.Sequential(
            nn.Linear(input_dim, dim_feedforward),
            nn.Dropout(dropout),
            nn.ReLU(inplace=True),
            nn.Linear(dim_feedforward, input_dim)
        )

        # Layers to apply in between the main layers
        self.norm1 = nn.LayerNorm(input_dim)
        self.norm2 = nn.LayerNorm(input_dim)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x, mask=None):
        # Attention part
        attn_out = self.self_attn(x, mask=mask)
        x = x + self.dropout(attn_out)
        x = self.norm1(x)

        # MLP part
        linear_out = self.linear_net(x)
        x = x + self.dropout(linear_out)
        x = self.norm2(x)

        return x
```

Based on this block, we can implement a module for the full Transformer encoder. Additionally to a forward function that iterates through the sequence of encoder blocks, we also provide a function called `get_attention_maps`. The idea of this function is to return the attention probabilities for all Multi-Head Attention blocks in the encoder. This helps us in understanding, and in a sense, explaining the model. However, the attention probabilities should be interpreted with a grain of salt as it does not necessarily reflect the true interpretation of the model (there is a series of papers about this, including Attention is not Explanation and Attention is not not Explanation).

[7]:
```
class TransformerEncoder(nn.Module):

    def __init__(self, num_layers, **block_args):
        super().__init__()
        self.layers = nn.ModuleList([EncoderBlock(**block_args) for _ in range(num_
↪layers)])

    def forward(self, x, mask=None):
        for l in self.layers:
            x = l(x, mask=mask)
        return x

    def get_attention_maps(self, x, mask=None):
        attention_maps = []
        for l in self.layers:
            _, attn_map = l.self_attn(x, mask=mask, return_attention=True)
            attention_maps.append(attn_map)
```

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```
            x = l(x)
        return attention_maps
```

Positional encoding

We have discussed before that the Multi-Head Attention block is permutation-equivariant, and cannot distinguish whether an input comes before another one in the sequence or not. In tasks like language understanding, however, the position is important for interpreting the input words. The position information can therefore be added via the input features. We could learn a embedding for every possible position, but this would not generalize to a dynamical input sequence length. Hence, the better option is to use feature patterns that the network can identify from the features and potentially generalize to larger sequences. The specific pattern chosen by Vaswani et al. are sine and cosine functions of different frequencies, as follows:

$$PE_{(pos,i)} = \begin{cases} \sin\left(\frac{pos}{10000^{i/d_{\text{model}}}}\right) & \text{if} \quad i \bmod 2 = 0 \\ \cos\left(\frac{pos}{10000^{(i-1)/d_{\text{model}}}}\right) & \text{otherwise} \end{cases}$$

$PE_{(pos,i)}$ represents the position encoding at position pos in the sequence, and hidden dimensionality i. These values, concatenated for all hidden dimensions, are added to the original input features (in the Transformer visualization above, see "Positional encoding"), and constitute the position information. We distinguish between even ($i \bmod 2 = 0$) and uneven ($i \bmod 2 = 1$) hidden dimensionalities where we apply a sine/cosine respectively. The intuition behind this encoding is that you can represent $PE_{(pos+k,:)}$ as a linear function of $PE_{(pos,:)}$, which might allow the model to easily attend to relative positions. The wavelengths in different dimensions range from 2π to $10000 \cdot 2\pi$.

The positional encoding is implemented below. The code is taken from the PyTorch tutorial about Transformers on NLP and adjusted for our purposes.

[8]:
```
class PositionalEncoding(nn.Module):

    def __init__(self, d_model, max_len=5000):
        """
        Inputs
            d_model - Hidden dimensionality of the input.
            max_len - Maximum length of a sequence to expect.
        """
        super().__init__()

        # Create matrix of [SeqLen, HiddenDim] representing the positional encoding for␣
↪max_len inputs
        pe = torch.zeros(max_len, d_model)
        position = torch.arange(0, max_len, dtype=torch.float).unsqueeze(1)
        div_term = torch.exp(torch.arange(0, d_model, 2).float() * (-math.log(10000.0) /␣
↪d_model))
        pe[:, 0::2] = torch.sin(position * div_term)
        pe[:, 1::2] = torch.cos(position * div_term)
        pe = pe.unsqueeze(0)

        # register_buffer => Tensor which is not a parameter, but should be part of the␣
↪modules state.
        # Used for tensors that need to be on the same device as the module.
        # persistent=False tells PyTorch to not add the buffer to the state dict (e.g.␣
↪when we save the model)
```

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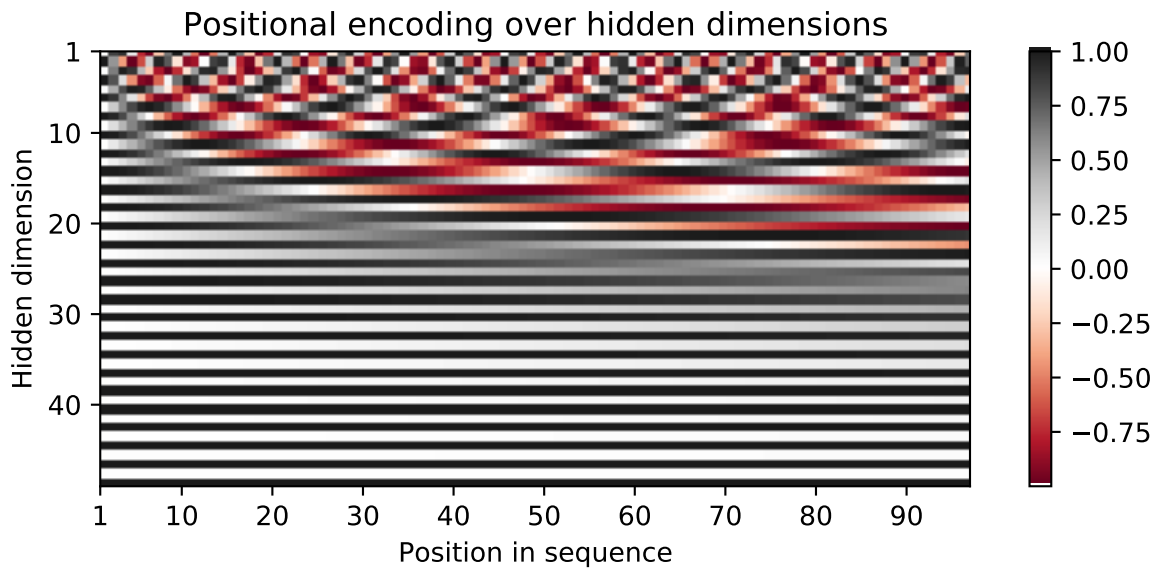
```
        self.register_buffer('pe', pe, persistent=False)

    def forward(self, x):
        x = x + self.pe[:, :x.size(1)]
        return x
```

To understand the positional encoding, we can visualize it below. We will generate an image of the positional encoding over hidden dimensionality and position in a sequence. Each pixel, therefore, represents the change of the input feature we perform to encode the specific position. Let's do it below.

[9]:
```
encod_block = PositionalEncoding(d_model=48, max_len=96)
pe = encod_block.pe.squeeze().T.cpu().numpy()

fig, ax = plt.subplots(nrows=1, ncols=1, figsize=(8,3))
pos = ax.imshow(pe, cmap="RdGy", extent=(1,pe.shape[1]+1,pe.shape[0]+1,1))
fig.colorbar(pos, ax=ax)
ax.set_xlabel("Position in sequence")
ax.set_ylabel("Hidden dimension")
ax.set_title("Positional encoding over hidden dimensions")
ax.set_xticks([1]+[i*10 for i in range(1,1+pe.shape[1]//10)])
ax.set_yticks([1]+[i*10 for i in range(1,1+pe.shape[0]//10)])
plt.show()
```



You can clearly see the sine and cosine waves with different wavelengths that encode the position in the hidden dimensions. Specifically, we can look at the sine/cosine wave for each hidden dimension separately, to get a better intuition of the pattern. Below we visualize the positional encoding for the hidden dimensions 1, 2, 3 and 4.

[10]:
```
sns.set_theme()
fig, ax = plt.subplots(2, 2, figsize=(12,4))
ax = [a for a_list in ax for a in a_list]
for i in range(len(ax)):
    ax[i].plot(np.arange(1,17), pe[i,:16], color=f'C{i}', marker="o", markersize=6,␣
↪markeredgecolor="black")
```

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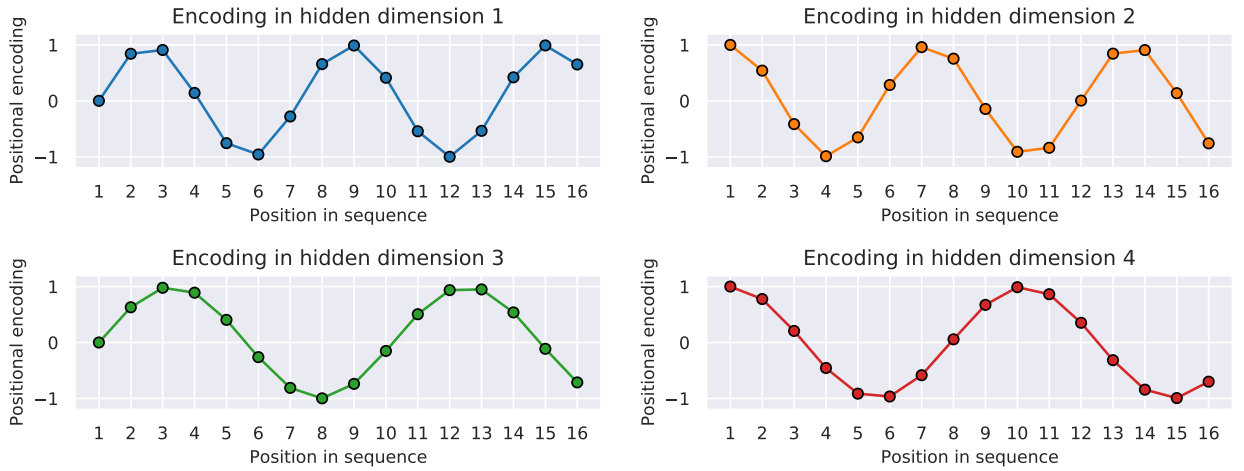
```
    ax[i].set_title(f"Encoding in hidden dimension {i+1}")
    ax[i].set_xlabel("Position in sequence", fontsize=10)
    ax[i].set_ylabel("Positional encoding", fontsize=10)
    ax[i].set_xticks(np.arange(1,17))
    ax[i].tick_params(axis='both', which='major', labelsize=10)
    ax[i].tick_params(axis='both', which='minor', labelsize=8)
    ax[i].set_ylim(-1.2, 1.2)
fig.subplots_adjust(hspace=0.8)
sns.reset_orig()
plt.show()
```



As we can see, the patterns between the hidden dimension 1 and 2 only differ in the starting angle. The wavelength is 2π, hence the repetition after position 6. The hidden dimensions 2 and 3 have about twice the wavelength.

Learning rate warm-up

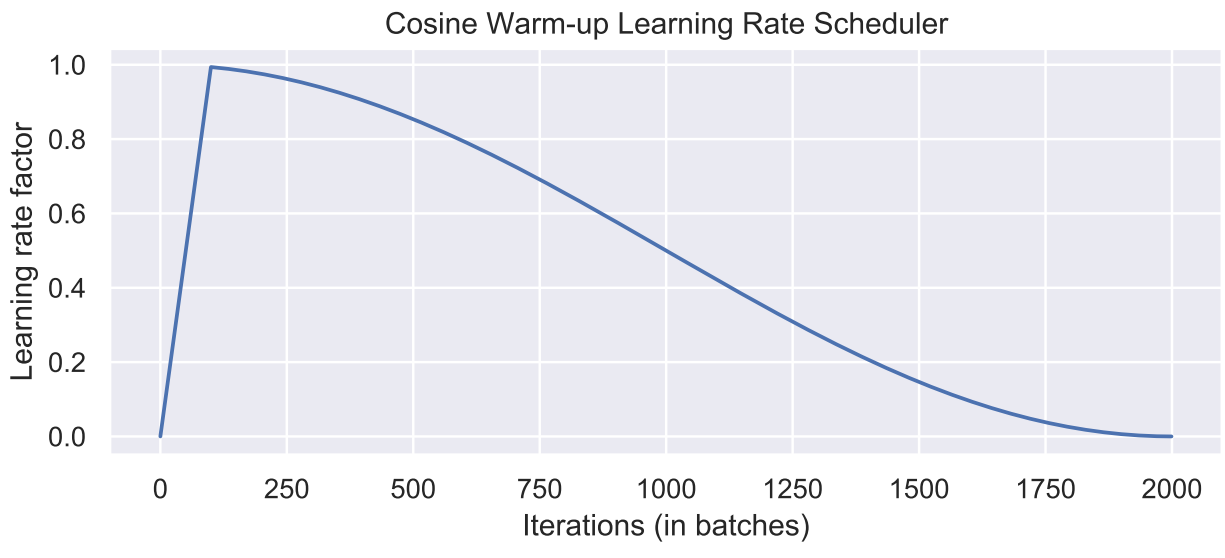
One commonly used technique for training a Transformer is learning rate warm-up. This means that we gradually increase the learning rate from 0 on to our originally specified learning rate in the first few iterations. Thus, we slowly start learning instead of taking very large steps from the beginning. In fact, training a deep Transformer without learning rate warm-up can make the model diverge and achieve a much worse performance on training and testing. Take for instance the following plot by Liu et al. (2019) comparing Adam-vanilla (i.e. Adam without warm-up) vs Adam with a warm-up:

Clearly, the warm-up is a crucial hyperparameter in the Transformer architecture. Why is it so important? There are currently two common explanations. Firstly, Adam uses the bias correction factors which however can lead to a higher variance in the adaptive learning rate during the first iterations. Improved optimizers like RAdam have been shown to overcome this issue, not requiring warm-up for training Transformers. Secondly, the iteratively applied Layer Normalization across layers can lead to very high gradients during the first iterations, which can be solved by using Pre-Layer Normalization (similar to Pre-Activation ResNet), or replacing Layer Normalization by other techniques (Adaptive Normalization, Power Normalization).

Nevertheless, many applications and papers still use the original Transformer architecture with Adam, because warm-up is a simple, yet effective way of solving the gradient problem in the first iterations. There are many different schedulers we could use. For instance, the original Transformer paper used an exponential decay scheduler with a warm-up. However, the currently most popular scheduler is the cosine warm-up scheduler, which combines warm-up with a cosine-shaped learning rate decay. We can implement it below, and visualize the learning rate factor over epochs.

[11]:
```
class CosineWarmupScheduler(optim.lr_scheduler._LRScheduler):

    def __init__(self, optimizer, warmup, max_iters):
        self.warmup = warmup
        self.max_num_iters = max_iters
        super().__init__(optimizer)

    def get_lr(self):
        lr_factor = self.get_lr_factor(epoch=self.last_epoch)
        return [base_lr * lr_factor for base_lr in self.base_lrs]

    def get_lr_factor(self, epoch):
        lr_factor = 0.5 * (1 + np.cos(np.pi * epoch / self.max_num_iters))
        if epoch <= self.warmup:
            lr_factor *= epoch * 1.0 / self.warmup
        return lr_factor
```

[12]:
```
# Needed for initializing the lr scheduler
p = nn.Parameter(torch.empty(4,4))
optimizer = optim.Adam([p], lr=1e-3)
lr_scheduler = CosineWarmupScheduler(optimizer=optimizer, warmup=100, max_iters=2000)

# Plotting
epochs = list(range(2000))
sns.set()
plt.figure(figsize=(8,3))
plt.plot(epochs, [lr_scheduler.get_lr_factor(e) for e in epochs])
plt.ylabel("Learning rate factor")
plt.xlabel("Iterations (in batches)")
plt.title("Cosine Warm-up Learning Rate Scheduler")
plt.show()
sns.reset_orig()
```



In the first 100 iterations, we increase the learning rate factor from 0 to 1, whereas for all later iterations, we decay it using the cosine wave. Pre-implementations of this scheduler can be found in the popular NLP Transformer library

huggingface.

PyTorch Lightning Module

Finally, we can embed the Transformer architecture into a PyTorch lightning module. From Tutorial 5, you know that PyTorch Lightning simplifies our training and test code, as well as structures the code nicely in separate functions. We will implement a template for a classifier based on the Transformer encoder. Thereby, we have a prediction output per sequence element. If we would need a classifier over the whole sequence, the common approach is to add an additional `[CLS]` token to the sequence, representing the classifier token. However, here we focus on tasks where we have an output per element.

Additionally to the Transformer architecture, we add a small input network (maps input dimensions to model dimensions), the positional encoding, and an output network (transforms output encodings to predictions). We also add the learning rate scheduler, which takes a step each iteration instead of once per epoch. This is needed for the warmup and the smooth cosine decay. The training, validation, and test step is left empty for now and will be filled for our task-specific models.

[13]:
```
class TransformerPredictor(pl.LightningModule):

    def __init__(self, input_dim, model_dim, num_classes, num_heads, num_layers, lr,␣
↪warmup, max_iters, dropout=0.0, input_dropout=0.0):
        """
        Inputs:
            input_dim - Hidden dimensionality of the input
            model_dim - Hidden dimensionality to use inside the Transformer
            num_classes - Number of classes to predict per sequence element
            num_heads - Number of heads to use in the Multi-Head Attention blocks
            num_layers - Number of encoder blocks to use.
            lr - Learning rate in the optimizer
            warmup - Number of warmup steps. Usually between 50 and 500
            max_iters - Number of maximum iterations the model is trained for. This is␣
↪needed for the CosineWarmup scheduler
            dropout - Dropout to apply inside the model
            input_dropout - Dropout to apply on the input features
        """
        super().__init__()
        self.save_hyperparameters()
        self._create_model()

    def _create_model(self):
        # Input dim -> Model dim
        self.input_net = nn.Sequential(
            nn.Dropout(self.hparams.input_dropout),
            nn.Linear(self.hparams.input_dim, self.hparams.model_dim)
        )
        # Positional encoding for sequences
        self.positional_encoding = PositionalEncoding(d_model=self.hparams.model_dim)
        # Transformer
        self.transformer = TransformerEncoder(num_layers=self.hparams.num_layers,
                                              input_dim=self.hparams.model_dim,
                                              dim_feedforward=2*self.hparams.model_dim,
                                              num_heads=self.hparams.num_heads,
                                              dropout=self.hparams.dropout)
```

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```
        # Output classifier per sequence lement
        self.output_net = nn.Sequential(
            nn.Linear(self.hparams.model_dim, self.hparams.model_dim),
            nn.LayerNorm(self.hparams.model_dim),
            nn.ReLU(inplace=True),
            nn.Dropout(self.hparams.dropout),
            nn.Linear(self.hparams.model_dim, self.hparams.num_classes)
        )

    def forward(self, x, mask=None, add_positional_encoding=True):
        """
        Inputs:
            x - Input features of shape [Batch, SeqLen, input_dim]
            mask - Mask to apply on the attention outputs (optional)
            add_positional_encoding - If True, we add the positional encoding to the␣
↪input.
                                      Might not be desired for some tasks.
        """
        x = self.input_net(x)
        if add_positional_encoding:
            x = self.positional_encoding(x)
        x = self.transformer(x, mask=mask)
        x = self.output_net(x)
        return x

    @torch.no_grad()
    def get_attention_maps(self, x, mask=None, add_positional_encoding=True):
        """
        Function for extracting the attention matrices of the whole Transformer for a␣
↪single batch.
        Input arguments same as the forward pass.
        """
        x = self.input_net(x)
        if add_positional_encoding:
            x = self.positional_encoding(x)
        attention_maps = self.transformer.get_attention_maps(x, mask=mask)
        return attention_maps

    def configure_optimizers(self):
        optimizer = optim.Adam(self.parameters(), lr=self.hparams.lr)

        # Apply lr scheduler per step
        lr_scheduler = CosineWarmupScheduler(optimizer,
                                             warmup=self.hparams.warmup,
                                             max_iters=self.hparams.max_iters)
        return [optimizer], [{'scheduler': lr_scheduler, 'interval': 'step'}]

    def training_step(self, batch, batch_idx):
        raise NotImplementedError

    def validation_step(self, batch, batch_idx):
        raise NotImplementedError
```

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```
    def test_step(self, batch, batch_idx):
        raise NotImplementedError
```

4.20.2 Experiments

After having finished the implementation of the Transformer architecture, we can start experimenting and apply it to various tasks. In this notebook, we will focus on two tasks: parallel Sequence-to-Sequence, and set anomaly detection. The two tasks focus on different properties of the Transformer architecture, and we go through them below.

Sequence to Sequence

A Sequence-to-Sequence task represents a task where the input *and* the output is a sequence, not necessarily of the same length. Popular tasks in this domain include machine translation and summarization. For this, we usually have a Transformer encoder for interpreting the input sequence, and a decoder for generating the output in an autoregressive manner. Here, however, we will go back to a much simpler example task and use only the encoder. Given a sequence of N numbers between 0 and M, the task is to reverse the input sequence. In Numpy notation, if our input is x, the output should be x[::-1]. Although this task sounds very simple, RNNs can have issues with such because the task requires long-term dependencies. Transformers are built to support such, and hence, we expect it to perform very well.

First, let's create a dataset class below.

[14]:
```
class ReverseDataset(data.Dataset):

    def __init__(self, num_categories, seq_len, size):
        super().__init__()
        self.num_categories = num_categories
        self.seq_len = seq_len
        self.size = size

        self.data = torch.randint(self.num_categories, size=(self.size, self.seq_len))

    def __len__(self):
        return self.size

    def __getitem__(self, idx):
        inp_data = self.data[idx]
        labels = torch.flip(inp_data, dims=(0,))
        return inp_data, labels
```

We create an arbitrary number of random sequences of numbers between 0 and `num_categories-1`. The label is simply the tensor flipped over the sequence dimension. We can create the corresponding data loaders below.

[15]:
```
dataset = partial(ReverseDataset, 10, 16)
train_loader = data.DataLoader(dataset(50000), batch_size=128, shuffle=True, drop_
↪last=True, pin_memory=True)
val_loader   = data.DataLoader(dataset(1000), batch_size=128)
test_loader  = data.DataLoader(dataset(10000), batch_size=128)
```

Let's look at an arbitrary sample of the dataset:

[16]:
```
inp_data, labels = train_loader.dataset[0]
print("Input data:", inp_data)
print("Labels:    ", labels)
```

```
Input data: tensor([9, 6, 2, 0, 6, 2, 7, 9, 7, 3, 3, 4, 3, 7, 0, 9])
Labels:     tensor([9, 0, 7, 3, 4, 3, 3, 7, 9, 7, 2, 6, 0, 2, 6, 9])
```

During training, we pass the input sequence through the Transformer encoder and predict the output for each input token. We use the standard Cross-Entropy loss to perform this. Every number is represented as a one-hot vector. Remember that representing the categories as single scalars decreases the expressiveness of the model extremely as 0 and 1 are not closer related than 0 and 9 in our example. An alternative to a one-hot vector is using a learned embedding vector as it is provided by the PyTorch module `nn.Embedding`. However, using a one-hot vector with an additional linear layer as in our case has the same effect as an embedding layer (`self.input_net` maps one-hot vector to a dense vector, where each row of the weight matrix represents the embedding for a specific category).

To implement the training dynamic, we create a new class inheriting from `TransformerPredictor` and overwriting the training, validation and test step functions.

[17]:
```
class ReversePredictor(TransformerPredictor):

    def _calculate_loss(self, batch, mode="train"):
        # Fetch data and transform categories to one-hot vectors
        inp_data, labels = batch
        inp_data = F.one_hot(inp_data, num_classes=self.hparams.num_classes).float()

        # Perform prediction and calculate loss and accuracy
        preds = self.forward(inp_data, add_positional_encoding=True)
        loss = F.cross_entropy(preds.view(-1,preds.size(-1)), labels.view(-1))
        acc = (preds.argmax(dim=-1) == labels).float().mean()

        # Logging
        self.log(f"{mode}_loss", loss)
        self.log(f"{mode}_acc", acc)
        return loss, acc

    def training_step(self, batch, batch_idx):
        loss, _ = self._calculate_loss(batch, mode="train")
        return loss

    def validation_step(self, batch, batch_idx):
        _ = self._calculate_loss(batch, mode="val")

    def test_step(self, batch, batch_idx):
        _ = self._calculate_loss(batch, mode="test")
```

Finally, we can create a training function similar to the one we have seen in Tutorial 5 for PyTorch Lightning. We create a `pl.Trainer` object, running for N epochs, logging in TensorBoard, and saving our best model based on the validation. Afterward, we test our models on the test set. An additional parameter we pass to the trainer here is `gradient_clip_val`. This clips the norm of the gradients for all parameters before taking an optimizer step and prevents the model from diverging if we obtain very high gradients at, for instance, sharp loss surfaces (see many good blog posts on gradient clipping, like DeepAI glossary). For Transformers, gradient clipping can help to further stabilize the training during the first few iterations, and also afterward. In plain PyTorch, you can apply gradient clipping via `torch.nn.utils.clip_grad_norm_(...)` (see documentation). The clip value is usually between 0.5 and 10, depending on how harsh you want to clip large gradients. After having explained this, let's implement the training function:

[18]:
```
def train_reverse(**kwargs):
    # Create a PyTorch Lightning trainer with the generation callback
    root_dir = os.path.join(CHECKPOINT_PATH, "ReverseTask")
    os.makedirs(root_dir, exist_ok=True)
    trainer = pl.Trainer(default_root_dir=root_dir,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc")],
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=10,
                         gradient_clip_val=5)
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, "ReverseTask.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = ReversePredictor.load_from_checkpoint(pretrained_filename)
    else:
        model = ReversePredictor(max_iters=trainer.max_epochs*len(train_loader),␣
↪**kwargs)
        trainer.fit(model, train_loader, val_loader)

    # Test best model on validation and test set
    val_result = trainer.test(model, val_loader, verbose=False)
    test_result = trainer.test(model, test_loader, verbose=False)
    result = {"test_acc": test_result[0]["test_acc"], "val_acc": val_result[0]["test_acc
↪"]}

    model = model.to(device)
    return model, result
```

Finally, we can train the model. In this setup, we will use a single encoder block and a single head in the Multi-Head Attention. This is chosen because of the simplicity of the task, and in this case, the attention can actually be interpreted as an "explanation" of the predictions (compared to the other papers above dealing with deep Transformers).

[19]:
```
reverse_model, reverse_result = train_reverse(input_dim=train_loader.dataset.num_
↪categories,
                                              model_dim=32,
                                              num_heads=1,
                                              num_classes=train_loader.dataset.num_
↪categories,
                                              num_layers=1,
                                              dropout=0.0,
                                              lr=5e-4,
                                              warmup=50)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

```
/home/phillip/anaconda3/envs/nlp1/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:45: UserWarning: The dataloader, test dataloader 0, does not␣
↪have many workers which may be a bottleneck. Consider increasing the value of the `num_
↪workers` argument` (try 16 which is the number of cpus on this machine) in the␣
↪`DataLoader` init to improve performance.
  warnings.warn(*args, **kwargs)
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

The warning of PyTorch Lightning regarding the number of workers can be ignored for now. As the data set is so simple and the `__getitem__` finishes a neglectable time, we don't need subprocesses to provide us the data (in fact, more workers can slow down the training as we have communication overhead among processes/threads). First, let's print the results:

[20]:
```
print(f"Val accuracy:  {(100.0 * reverse_result['val_acc']):4.2f}%")
print(f"Test accuracy: {(100.0 * reverse_result['test_acc']):4.2f}%")
```

```
Val accuracy:  100.00%
Test accuracy: 100.00%
```

As we would have expected, the Transformer can correctly solve the task. However, how does the attention in the Multi-Head Attention block looks like for an arbitrary input? Let's try to visualize it below.

[21]:
```
data_input, labels = next(iter(val_loader))
inp_data = F.one_hot(data_input, num_classes=reverse_model.hparams.num_classes).float()
inp_data = inp_data.to(device)
attention_maps = reverse_model.get_attention_maps(inp_data)
```

The object `attention_maps` is a list of length N where N is the number of layers. Each element is a tensor of shape [Batch, Heads, SeqLen, SeqLen], which we can verify below.

[22]:
```
attention_maps[0].shape
```

[22]:
```
torch.Size([128, 1, 16, 16])
```

Next, we will write a plotting function that takes as input the sequences, attention maps, and an index indicating for which batch element we want to visualize the attention map. We will create a plot where over rows, we have different layers, while over columns, we show the different heads. Remember that the softmax has been applied for each row separately.

[23]:
```
def plot_attention_maps(input_data, attn_maps, idx=0):
    if input_data is not None:
        input_data = input_data[idx].detach().cpu().numpy()
    else:
        input_data = np.arange(attn_maps[0][idx].shape[-1])
    attn_maps = [m[idx].detach().cpu().numpy() for m in attn_maps]

    num_heads = attn_maps[0].shape[0]
```

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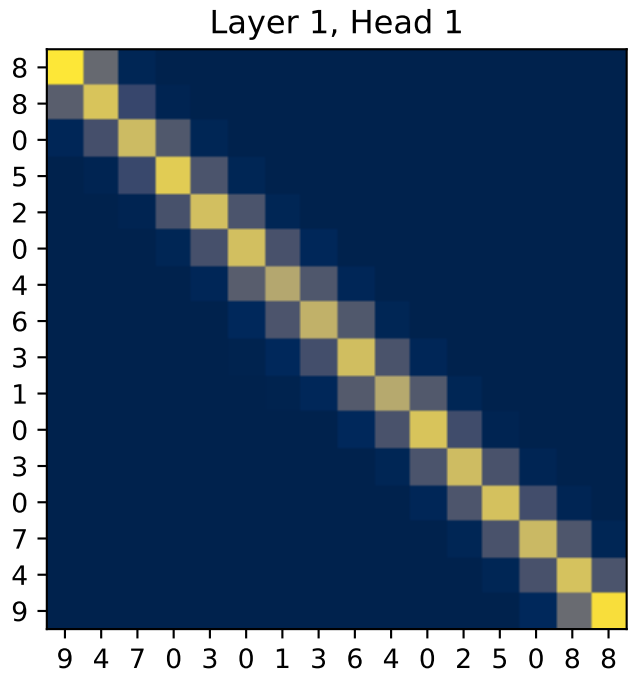
```
    num_layers = len(attn_maps)
    seq_len = input_data.shape[0]
    fig_size = 4 if num_heads == 1 else 3
    fig, ax = plt.subplots(num_layers, num_heads, figsize=(num_heads*fig_size, num_
↪layers*fig_size))
    if num_layers == 1:
        ax = [ax]
    if num_heads == 1:
        ax = [[a] for a in ax]
    for row in range(num_layers):
        for column in range(num_heads):
            ax[row][column].imshow(attn_maps[row][column], origin='lower', vmin=0)
            ax[row][column].set_xticks(list(range(seq_len)))
            ax[row][column].set_xticklabels(input_data.tolist())
            ax[row][column].set_yticks(list(range(seq_len)))
            ax[row][column].set_yticklabels(input_data.tolist())
            ax[row][column].set_title(f"Layer {row+1}, Head {column+1}")
    fig.subplots_adjust(hspace=0.5)
    plt.show()
```

Finally, we can plot the attention map of our trained Transformer on the reverse task:

[24]:
```
plot_attention_maps(data_input, attention_maps, idx=0)
```

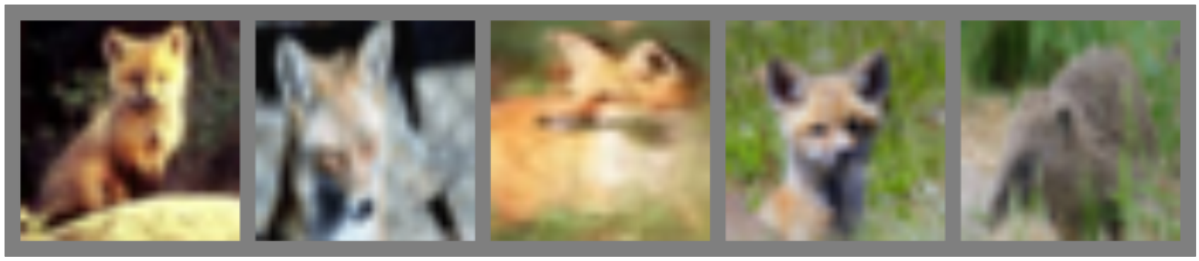


The model has learned to attend to the token that is on the flipped index of itself. Hence, it actually does what we intended it to do. We see that it however also pays some attention to values close to the flipped index. This is because the model doesn't need the perfect, hard attention to solve this problem, but is fine with this approximate, noisy attention map. The close-by indices are caused by the similarity of the positional encoding, which we also intended with the positional encoding.

Set Anomaly Detection

Besides sequences, sets are another data structure that is relevant for many applications. In contrast to sequences, elements are unordered in a set. RNNs can only be applied on sets by assuming an order in the data, which however biases the model towards a non-existing order in the data. Vinyals et al. (2015) and other papers have shown that the assumed order can have a significant impact on the model's performance, and hence, we should try to not use RNNs on sets. Ideally, our model should be permutation-equivariant/invariant such that the output is the same no matter how we sort the elements in a set.

Transformers offer the perfect architecture for this as the Multi-Head Attention is permutation-equivariant, and thus, outputs the same values no matter in what order we enter the inputs (inputs and outputs are permuted equally). The task we are looking at for sets is *Set Anomaly Detection* which means that we try to find the element(s) in a set that does not fit the others. In the research community, the common application of anomaly detection is performed on a set of images, where $N - 1$ images belong to the same category/have the same high-level features while one belongs to another category. Note that category does not necessarily have to relate to a class in a standard classification problem, but could be the combination of multiple features. For instance, on a face dataset, this could be people with glasses, male, beard, etc. An example of distinguishing different animals can be seen below. The first four images show foxes, while the last represents a different animal. We want to recognize that the last image shows a different animal, but it is not relevant which class of animal it is.



In this tutorial, we will use the CIFAR100 dataset. CIFAR100 has 600 images for 100 classes each with a resolution of 32x32, similar to CIFAR10. The larger amount of classes requires the model to attend to specific features in the images instead of coarse features as in CIFAR10, therefore making the task harder. We will show the model a set of 9 images of one class, and 1 image from another class. The task is to find the image that is from a different class than the other images. Using the raw images directly as input to the Transformer is not a good idea, because it is not translation invariant as a CNN, and would need to learn to detect image features from high-dimensional input first of all. Instead, we will use a pre-trained ResNet34 model from the torchvision package to obtain high-level, low-dimensional features of the images. The ResNet model has been pre-trained on the ImageNet dataset which contains 1 million images of 1k classes and varying resolutions. However, during training and testing, the images are usually scaled to a resolution of 224x224, and hence we rescale our CIFAR images to this resolution as well. Below, we will load the dataset, and prepare the data for being processed by the ResNet model.

[25]:
```
# ImageNet statistics
DATA_MEANS = np.array([0.485, 0.456, 0.406])
DATA_STD = np.array([0.229, 0.224, 0.225])
# As torch tensors for later preprocessing
TORCH_DATA_MEANS = torch.from_numpy(DATA_MEANS).view(1,3,1,1)
TORCH_DATA_STD = torch.from_numpy(DATA_STD).view(1,3,1,1)

# Resize to 224x224, and normalize to ImageNet statistic
transform = transforms.Compose([transforms.Resize((224,224)),
                                transforms.ToTensor(),
                                transforms.Normalize(DATA_MEANS, DATA_STD)
                                ])
# Loading the training dataset.
train_set = CIFAR100(root=DATASET_PATH, train=True, transform=transform, download=True)
```

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```
# Loading the test set
test_set = CIFAR100(root=DATASET_PATH, train=False, transform=transform, download=True)
```

```
Files already downloaded and verified
Files already downloaded and verified
```

Next, we want to run the pre-trained ResNet model on the images, and extract the features before the classification layer. These are the most high-level features, and should sufficiently describe the images. CIFAR100 has some similarity to ImageNet, and thus we are not retraining the ResNet model in any form. However, if you would want to get the best performance and have a very large dataset, it would be better to add the ResNet to the computation graph during training and finetune its parameters as well. As we don't have a large enough dataset and want to train our model efficiently, we will extract the features beforehand. Let's load and prepare the model below.

[26]:
```
import os
os.environ["TORCH_HOME"] = CHECKPOINT_PATH
pretrained_model = torchvision.models.resnet34(weights='IMAGENET1K_V1')
# Remove classification layer
# In some models, it is called "fc", others have "classifier"
# Setting both to an empty sequential represents an identity map of the final features.
pretrained_model.fc = nn.Sequential()
pretrained_model.classifier = nn.Sequential()
# To GPU
pretrained_model = pretrained_model.to(device)

# Only eval, no gradient required
pretrained_model.eval()
for p in pretrained_model.parameters():
    p.requires_grad = False
```

We will now write a extraction function for the features below. This cell requires access to a GPU, as the model is rather deep and the images relatively large. The GPUs on GoogleColab are sufficient, but running this cell can take 2-3 minutes. Once it is run, the features are exported on disk so they don't have to be recalculated every time you run the notebook. However, this requires >150MB free disk space. So it is recommended to run this only on a local computer if you have enough free disk and a GPU (GoogleColab is fine for this). If you do not have a GPU, you can download the features from the GoogleDrive folder.

[27]:
```
@torch.no_grad()
def extract_features(dataset, save_file):
    if not os.path.isfile(save_file):
        data_loader = data.DataLoader(dataset, batch_size=128, shuffle=False, drop_
↪last=False, num_workers=4)
        extracted_features = []
        for imgs, _ in tqdm(data_loader):
            imgs = imgs.to(device)
            feats = pretrained_model(imgs)
            extracted_features.append(feats)
        extracted_features = torch.cat(extracted_features, dim=0)
        extracted_features = extracted_features.detach().cpu()
        torch.save(extracted_features, save_file)
    else:
        extracted_features = torch.load(save_file)
    return extracted_features
```

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```
train_feat_file = os.path.join(CHECKPOINT_PATH, "train_set_features.tar")
train_set_feats = extract_features(train_set, train_feat_file)

test_feat_file = os.path.join(CHECKPOINT_PATH, "test_set_features.tar")
test_feats = extract_features(test_set, test_feat_file)
```

Let's verify the feature shapes below. The training should have 50k elements, and the test 10k images. The feature dimension is 512 for the ResNet34. If you experiment with other models, you likely see a different feature dimension.

[28]:
```
print("Train:", train_set_feats.shape)
print("Test: ", test_feats.shape)
```

```
Train: torch.Size([50000, 512])
Test:  torch.Size([10000, 512])
```

As usual, we want to create a validation set to detect when we should stop training. In this case, we will split the training set into 90% training, 10% validation. However, the difficulty is here that we need to ensure that the validation set has the same number of images for all 100 labels. Otherwise, we have a class imbalance which is not good for creating the image sets. Hence, we take 10% of the images for each class, and move them into the validation set. The code below does exactly this.

[29]:
```
## Split train into train+val
# Get labels from train set
labels = train_set.targets

# Get indices of images per class
labels = torch.LongTensor(labels)
num_labels = labels.max()+1
sorted_indices = torch.argsort(labels).reshape(num_labels, -1) # [classes, num_imgs per␣
↪class]

# Determine number of validation images per class
num_val_exmps = sorted_indices.shape[1] // 10

# Get image indices for validation and training
val_indices   = sorted_indices[:,:num_val_exmps].reshape(-1)
train_indices = sorted_indices[:,num_val_exmps:].reshape(-1)

# Group corresponding image features and labels
train_feats, train_labels = train_set_feats[train_indices], labels[train_indices]
val_feats,   val_labels   = train_set_feats[val_indices],   labels[val_indices]
```

Now we can prepare a dataset class for the set anomaly task. We define an epoch to be the sequence in which each image has been exactly once as an "anomaly". Hence, the length of the dataset is the number of images in it. For the training set, each time we access an item with `__getitem__`, we sample a random, different class than the image at the corresponding index `idx` has. In a second step, we sample $N-1$ images of this sampled class. The set of 10 images is finally returned. The randomness in the `__getitem__` allows us to see a slightly different set during each iteration. However, we can't use the same strategy for the test set as we want the test dataset to be the same every time we iterate over it. Hence, we sample the sets in the `__init__` method, and return those in `__getitem__`. The code below implements exactly this dynamic.

[30]:
```
class SetAnomalyDataset(data.Dataset):
```

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```
    def __init__(self, img_feats, labels, set_size=10, train=True):
        """
        Inputs:
            img_feats - Tensor of shape [num_imgs, img_dim]. Represents the high-level␣
↪features.
            labels - Tensor of shape [num_imgs], containing the class labels for the␣
↪images
            set_size - Number of elements in a set. N-1 are sampled from one class, and␣
↪one from another one.
            train - If True, a new set will be sampled every time __getitem__ is called.
        """
        super().__init__()
        self.img_feats = img_feats
        self.labels = labels
        self.set_size = set_size-1 # The set size is here the size of correct images
        self.train = train

        # Tensors with indices of the images per class
        self.num_labels = labels.max()+1
        self.img_idx_by_label = torch.argsort(self.labels).reshape(self.num_labels, -1)

        if not train:
            self.test_sets = self._create_test_sets()


    def _create_test_sets(self):
        # Pre-generates the sets for each image for the test set
        test_sets = []
        num_imgs = self.img_feats.shape[0]
        np.random.seed(42)
        test_sets = [self.sample_img_set(self.labels[idx]) for idx in range(num_imgs)]
        test_sets = torch.stack(test_sets, dim=0)
        return test_sets


    def sample_img_set(self, anomaly_label):
        """
        Samples a new set of images, given the label of the anomaly.
        The sampled images come from a different class than anomaly_label
        """
        # Sample class from 0,...,num_classes-1 while skipping anomaly_label as class
        set_label = np.random.randint(self.num_labels-1)
        if set_label >= anomaly_label:
            set_label += 1

        # Sample images from the class determined above
        img_indices = np.random.choice(self.img_idx_by_label.shape[1], size=self.set_
↪size, replace=False)
        img_indices = self.img_idx_by_label[set_label, img_indices]
        return img_indices
```

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```
    def __len__(self):
        return self.img_feats.shape[0]


    def __getitem__(self, idx):
        anomaly = self.img_feats[idx]
        if self.train: # If train => sample
            img_indices = self.sample_img_set(self.labels[idx])
        else: # If test => use pre-generated ones
            img_indices = self.test_sets[idx]

        # Concatenate images. The anomaly is always the last image for simplicity
        img_set = torch.cat([self.img_feats[img_indices], anomaly[None]], dim=0)
        indices = torch.cat([img_indices, torch.LongTensor([idx])], dim=0)
        label = img_set.shape[0]-1

        # We return the indices of the images for visualization purpose. "Label" is the␣
↪index of the anomaly
        return img_set, indices, label
```

Next, we can setup our datasets and data loaders below. Here, we will use a set size of 10, i.e. 9 images from one category + 1 anomaly. Feel free to change it if you want to experiment with the sizes.

[31]:
```
SET_SIZE = 10
test_labels = torch.LongTensor(test_set.targets)

train_anom_dataset = SetAnomalyDataset(train_feats, train_labels, set_size=SET_SIZE,␣
↪train=True)
val_anom_dataset   = SetAnomalyDataset(val_feats,   val_labels,   set_size=SET_SIZE,␣
↪train=False)
test_anom_dataset  = SetAnomalyDataset(test_feats,  test_labels,  set_size=SET_SIZE,␣
↪train=False)

train_anom_loader = data.DataLoader(train_anom_dataset, batch_size=64, shuffle=True, ␣
↪drop_last=True,  num_workers=4, pin_memory=True)
val_anom_loader   = data.DataLoader(val_anom_dataset,   batch_size=64, shuffle=False,␣
↪drop_last=False, num_workers=4)
test_anom_loader  = data.DataLoader(test_anom_dataset,  batch_size=64, shuffle=False,␣
↪drop_last=False, num_workers=4)
```

To understand the dataset a little better, we can plot below a few sets from the test dataset. Each row shows a different input set, where the first 9 are from the same class.

[32]:
```
def visualize_exmp(indices, orig_dataset):
    images = [orig_dataset[idx][0] for idx in indices.reshape(-1)]
    images = torch.stack(images, dim=0)
    images = images * TORCH_DATA_STD + TORCH_DATA_MEANS

    img_grid = torchvision.utils.make_grid(images, nrow=SET_SIZE, normalize=True, pad_
↪value=0.5, padding=16)
    img_grid = img_grid.permute(1, 2, 0)
```

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```
    plt.figure(figsize=(12,8))
    plt.title("Anomaly examples on CIFAR100")
    plt.imshow(img_grid)
    plt.axis('off')
    plt.show()
    plt.close()

_, indices, _ = next(iter(test_anom_loader))
visualize_exmp(indices[:4], test_set)
```

We can already see that for some sets the task might be easier than for others. Difficulties can especially arise if the anomaly is in a different, but yet visually similar class (e.g. train vs bus, flour vs worm, etc.).

After having prepared the data, we can look closer at the model. Here, we have a classification of the whole set. For the prediction to be permutation-equivariant, we will output one logit for each image. Over these logits, we apply a softmax and train the anomaly image to have the highest score/probability. This is a bit different than a standard classification layer as the softmax is applied over images, not over output classes in the classical sense. However, if we swap two images in their position, we effectively swap their position in the output softmax. Hence, the prediction is equivariant with respect to the input. We implement this idea below in the subclass of the Transformer Lightning module.

[33]:
```
class AnomalyPredictor(TransformerPredictor):

    def _calculate_loss(self, batch, mode="train"):
        img_sets, _, labels = batch
        preds = self.forward(img_sets, add_positional_encoding=False) # No positional␣
↪encodings as it is a set, not a sequence!
        preds = preds.squeeze(dim=-1) # Shape: [Batch_size, set_size]
        loss = F.cross_entropy(preds, labels) # Softmax/CE over set dimension
        acc = (preds.argmax(dim=-1) == labels).float().mean()
        self.log(f"{mode}_loss", loss)
        self.log(f"{mode}_acc", acc, on_step=False, on_epoch=True)
        return loss, acc

    def training_step(self, batch, batch_idx):
```

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```
        loss, _ = self._calculate_loss(batch, mode="train")
        return loss

    def validation_step(self, batch, batch_idx):
        _ = self._calculate_loss(batch, mode="val")

    def test_step(self, batch, batch_idx):
        _ = self._calculate_loss(batch, mode="test")
```

Finally, we write our train function below. It has the exact same structure as the reverse task one, hence not much of an explanation is needed here.

[34]:
```
def train_anomaly(**kwargs):
    # Create a PyTorch Lightning trainer with the generation callback
    root_dir = os.path.join(CHECKPOINT_PATH, "SetAnomalyTask")
    os.makedirs(root_dir, exist_ok=True)
    trainer = pl.Trainer(default_root_dir=root_dir,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc")],
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=100,
                         gradient_clip_val=2)
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, "SetAnomalyTask.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = AnomalyPredictor.load_from_checkpoint(pretrained_filename)
    else:
        model = AnomalyPredictor(max_iters=trainer.max_epochs*len(train_anom_loader),␣
↪**kwargs)
        trainer.fit(model, train_anom_loader, val_anom_loader)
        model = AnomalyPredictor.load_from_checkpoint(trainer.checkpoint_callback.best_
↪model_path)

    # Test best model on validation and test set
    train_result = trainer.test(model, train_anom_loader, verbose=False)
    val_result = trainer.test(model, val_anom_loader, verbose=False)
    test_result = trainer.test(model, test_anom_loader, verbose=False)
    result = {"test_acc": test_result[0]["test_acc"], "val_acc": val_result[0]["test_acc
↪"], "train_acc": train_result[0]["test_acc"]}

    model = model.to(device)
    return model, result
```

Let's finally train our model. We will use 4 layers with 4 attention heads each. The hidden dimensionality of the model is 256, and we use a dropout of 0.1 throughout the model for good regularization. Note that we also apply the dropout on the input features, as this makes the model more robust against image noise and generalizes better. Again, we use warmup to slowly start our model training.

[35]:
```
anomaly_model, anomaly_result = train_anomaly(input_dim=train_anom_dataset.img_feats.
↪shape[-1],
                                              model_dim=256,
                                              num_heads=4,
                                              num_classes=1,
                                              num_layers=4,
                                              dropout=0.1,
                                              input_dropout=0.1,
                                              lr=5e-4,
                                              warmup=100)
```

```
GPU available: True, used: True
WARNING: Logging before flag parsing goes to stderr.
I1109 10:43:31.036801 139648634296128 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1109 10:43:31.038146 139648634296128 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1109 10:43:31.039162 139648634296128 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

```
/home/phillip/anaconda3/envs/nlp1/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:45: UserWarning: Your test_dataloader has `shuffle=True`, it␣
↪is best practice to turn this off for validation and test dataloaders.
  warnings.warn(*args, **kwargs)
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

We can print the achieved accuracy below.

[36]:
```
print(f"Train accuracy: {(100.0*anomaly_result['train_acc']):4.2f}%")
print(f"Val accuracy:   {(100.0*anomaly_result['val_acc']):4.2f}%")
print(f"Test accuracy:  {(100.0*anomaly_result['test_acc']):4.2f}%")
```

```
Train accuracy: 97.77%
Val accuracy:   94.38%
Test accuracy:  94.30%
```

With ~94% validation and test accuracy, the model generalizes quite well. It should be noted that you might see slightly different scores depending on what computer/device you are running this notebook. This is because despite setting the seed before generating the test dataset, it is not the same across platforms and numpy versions. Nevertheless, we can conclude that the model performs quite well and can solve the task for most sets. Before trying to interpret the model, let's verify that our model is permutation-equivariant, and assigns the same predictions for different permutations of the input set. For this, we sample a batch from the test set and run it through the model to obtain the probabilities.

[37]:
```
inp_data, indices, labels = next(iter(test_anom_loader))
inp_data = inp_data.to(device)

anomaly_model.eval()

with torch.no_grad():
    preds = anomaly_model.forward(inp_data, add_positional_encoding=False)
    preds = F.softmax(preds.squeeze(dim=-1), dim=-1)

    # Permut input data
    permut = np.random.permutation(inp_data.shape[1])
    perm_inp_data = inp_data[:,permut]
    perm_preds = anomaly_model.forward(perm_inp_data, add_positional_encoding=False)
    perm_preds = F.softmax(perm_preds.squeeze(dim=-1), dim=-1)

assert (preds[:,permut] - perm_preds).abs().max() < 1e-5, "Predictions are not␣
↪permutation equivariant"

print("Preds\n", preds[0,permut].cpu().numpy())
print("Permuted preds\n", perm_preds[0].cpu().numpy())
```

```
Preds
 [5.4543594e-05 1.4208173e-04 6.6922468e-05 7.6413504e-05 7.7112330e-05
 8.7848457e-05 6.6820685e-05 9.9929154e-01 7.3219831e-05 6.3545609e-05]
Permuted preds
 [5.4543532e-05 1.4208158e-04 6.6922395e-05 7.6413417e-05 7.7112243e-05
 8.7848362e-05 6.6820678e-05 9.9929142e-01 7.3219751e-05 6.3545544e-05]
```

You can see that the predictions are almost exactly the same, and only differ because of slight numerical differences inside the network operation.

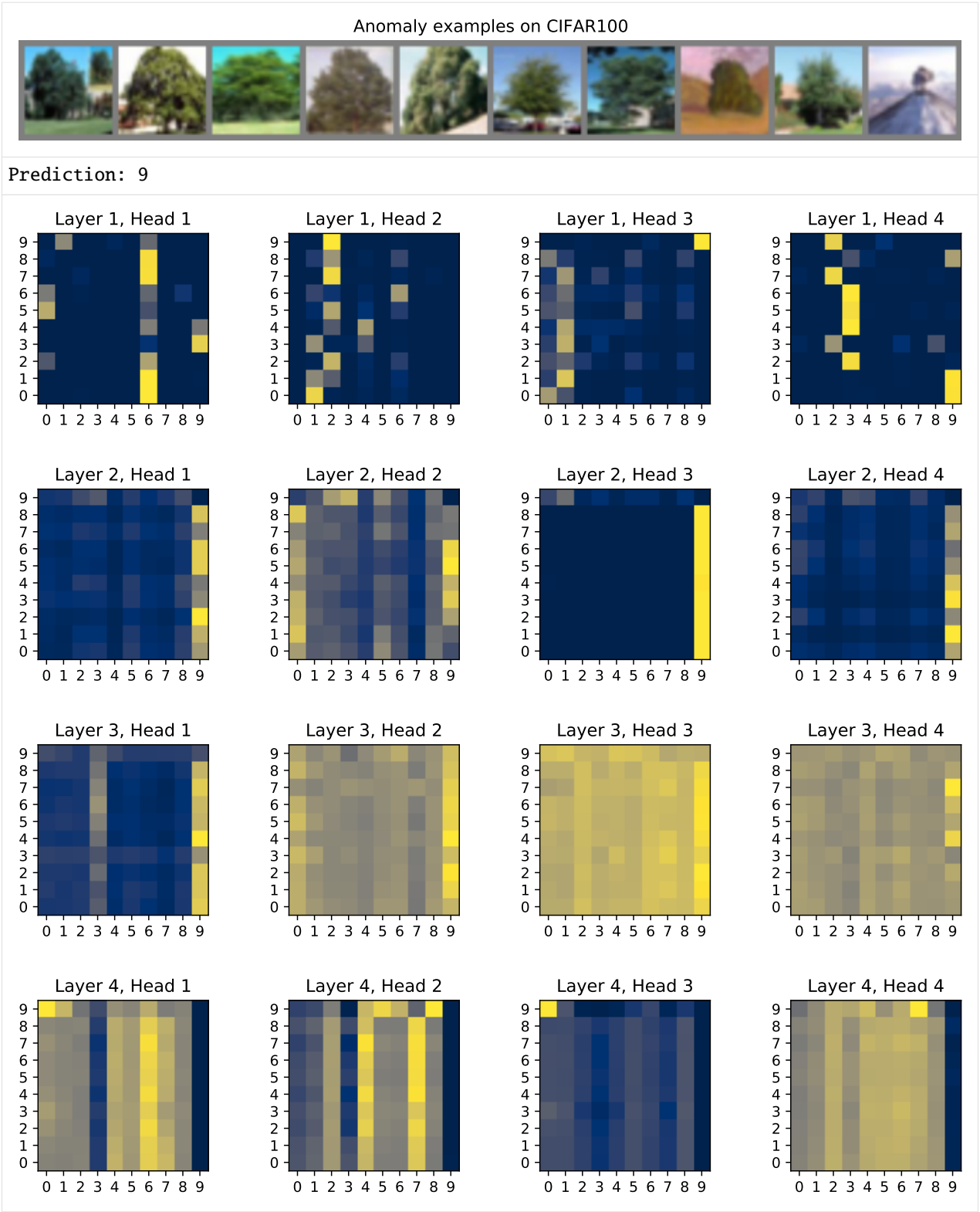
To interpret the model a little more, we can plot the attention maps inside the model. This will give us an idea of what information the model is sharing/communicating between images, and what each head might represent. First, we need to extract the attention maps for the test batch above, and determine the discrete predictions for simplicity.

[38]:
```
attention_maps = anomaly_model.get_attention_maps(inp_data, add_positional_
↪encoding=False)
predictions = preds.argmax(dim=-1)
```

Below we write a plot function which plots the images in the input set, the prediction of the model, and the attention maps of the different heads on layers of the transformer. Feel free to explore the attention maps for different input examples as well.

[39]:
```
def visualize_prediction(idx):
    visualize_exmp(indices[idx:idx+1], test_set)
    print("Prediction:", predictions[idx].item())
    plot_attention_maps(input_data=None, attn_maps=attention_maps, idx=idx)

visualize_prediction(0)
```



Depending on the random seed, you might see a slightly different input set. For the version on the website, we compare 9 tree images with a volcano. We see that multiple heads, for instance, Layer 2 Head 1, Layer 2 Head 3, and Layer 3 Head 1 focus on the last image. Additionally, the heads in Layer 4 all seem to ignore the last image and assign a very low attention probability to it. This shows that the model has indeed recognized that the image doesn't fit the setting,

and hence predicted it to be the anomaly. Layer 3 Head 2-4 seems to take a slightly weighted average of all images. That might indicate that the model extracts the "average" information of all images, to compare it to the image features itself.

Let's try to find where the model actually makes a mistake. We can do this by identifying the sets where the model predicts something else than 9, as in the dataset, we ensured that the anomaly is always at the last position in the set.

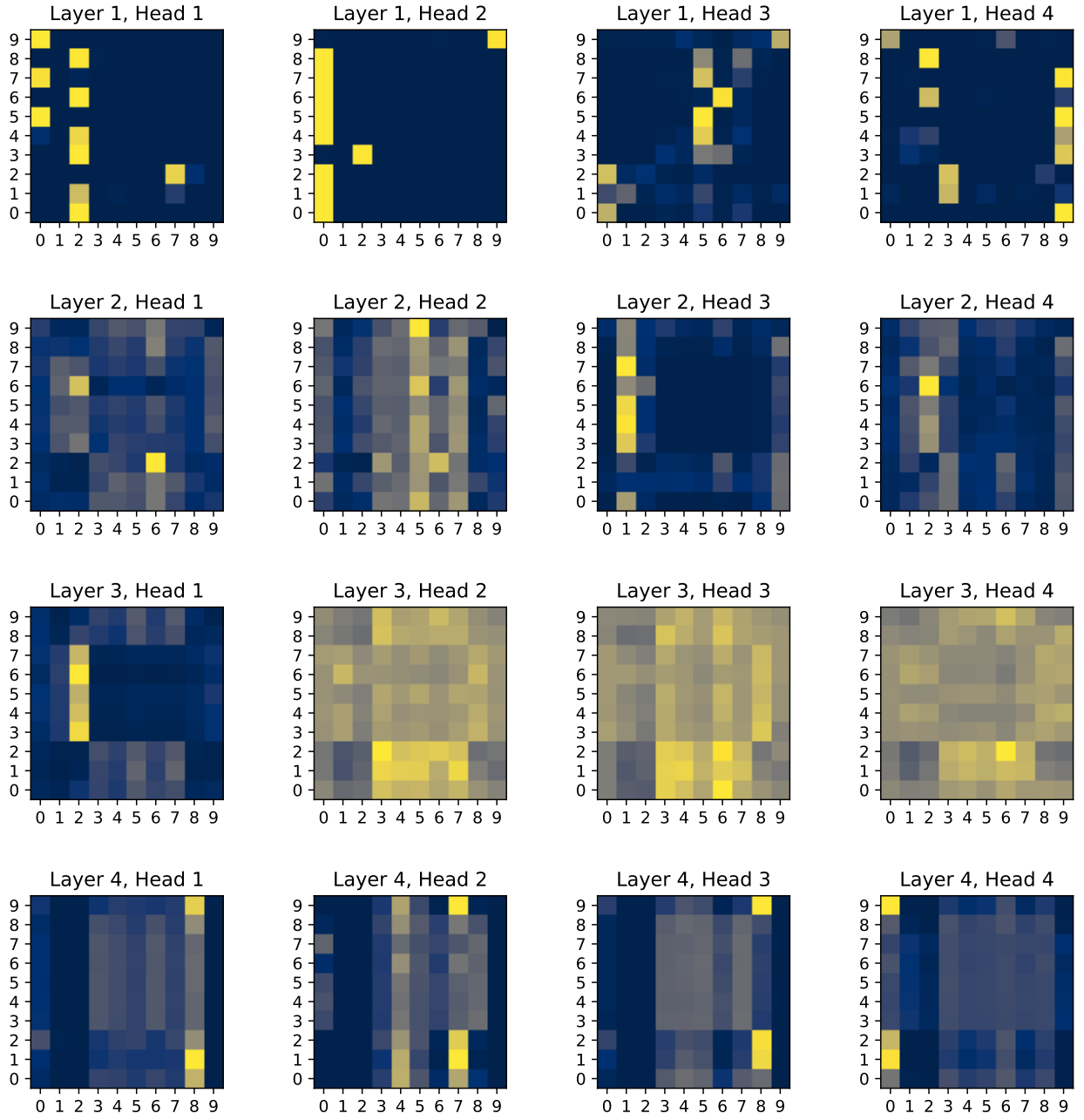
[40]:
```
mistakes = torch.where(predictions != 9)[0].cpu().numpy()
print("Indices with mistake:", mistakes)
```

```
Indices with mistake: [36 49]
```

As our model achieves ~94% accuracy, we only have very little number of mistakes in a batch of 64 sets. Still, let's visualize one of them, for example the last one:

[41]:
```
visualize_prediction(mistakes[-1])
print("Probabilities:")
for i, p in enumerate(preds[mistakes[-1]].cpu().numpy()):
    print(f"Image {i}: {100.0*p:4.2f}%")
```


```
Prediction: 2
```




```
Probabilities:
Image 0: 0.06%
Image 1: 1.63%
Image 2: 89.63%
Image 3: 0.01%
Image 4: 0.01%
Image 5: 0.01%
Image 6: 0.01%
Image 7: 0.01%
Image 8: 0.01%
Image 9: 8.63%
```

In this example, the model confuses a palm tree with a building, giving a probability of ~90% to image 2, and 8% to the actual anomaly. However, the difficulty here is that the picture of the building has been taken at a similar angle as the palms. Meanwhile, image 2 shows a rather unusual palm with a different color palette, which is why the model fails here. Nevertheless, in general, the model performs quite well.

4.20.3 Conclusion

In this tutorial, we took a closer look at the Multi-Head Attention layer which uses a scaled dot product between queries and keys to find correlations and similarities between input elements. The Transformer architecture is based on the Multi-Head Attention layer and applies multiple of them in a ResNet-like block. The Transformer is a very important, recent architecture that can be applied to many tasks and datasets. Although it is best known for its success in NLP, there is so much more to it. We have seen its application on sequence-to-sequence tasks and set anomaly detection. Its property of being permutation-equivariant if we do not provide any positional encodings, allows it to generalize to many settings. Hence, it is important to know the architecture, but also its possible issues such as the gradient problem during the first iterations solved by learning rate warm-up. If you are interested in continuing with the study of the Transformer architecture, please have a look at the blog posts listed at the beginning of the tutorial notebook.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.21 Tutorial 7: Graph Neural Networks

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will discuss the application of neural networks on graphs. Graph Neural Networks (GNNs) have recently gained increasing popularity in both applications and research, including domains such as social networks, knowledge graphs, recommender systems, and bioinformatics. While the theory and math behind GNNs might first seem complicated, the implementation of those models is quite simple and helps in understanding the methodology. Therefore, we will discuss the implementation of basic network layers of a GNN, namely graph convolutions, and attention layers. Finally, we will apply a GNN on a node-level, edge-level, and graph-level tasks.

Below, we will start by importing our standard libraries. We will use PyTorch Lightning as already done in Tutorial 5 and 6.

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
import time

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()
sns.set()

## Progress bar
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import CIFAR10
from torchvision import transforms
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial7"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False
```

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```
device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print(device)
```

```
cuda:0
```

We also have a few pre-trained models we download below.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial7/"
# Files to download
pretrained_files = ["NodeLevelMLP.ckpt", "NodeLevelGNN.ckpt", "GraphLevelGraphConv.ckpt"]

# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.21.1 Graph Neural Networks

Graph representation

Before starting the discussion of specific neural network operations on graphs, we should consider how to represent a graph. Mathematically, a graph $\mathcal{G}$ is defined as a tuple of a set of nodes/vertices V, and a set of edges/links E: $\mathcal{G} = (V, E)$. Each edge is a pair of two vertices, and represents a connection between them. For instance, let's look at the following graph:

The vertices are $V = \{1, 2, 3, 4\}$, and edges $E = \{(1, 2), (2, 3), (2, 4), (3, 4)\}$. Note that for simplicity, we assume the graph to be undirected and hence don't add mirrored pairs like $(2, 1)$. In application, vertices and edge can often have specific attributes, and edges can even be directed. The question is how we could represent this diversity in an efficient way for matrix operations. Usually, for the edges, we decide between two variants: an adjacency matrix, or a list of paired vertex indices.

The **adjacency matrix** A is a square matrix whose elements indicate whether pairs of vertices are adjacent, i.e. connected, or not. In the simplest case, A_{ij} is 1 if there is a connection from node i to j, and otherwise 0. If we have edge attributes or different categories of edges in a graph, this information can be added to the matrix as well. For an undirected graph, keep in mind that A is a symmetric matrix ($A_{ij} = A_{ji}$). For the example graph above, we have the

following adjacency matrix:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

While expressing a graph as a list of edges is more efficient in terms of memory and (possibly) computation, using an adjacency matrix is more intuitive and simpler to implement. In our implementations below, we will rely on the adjacency matrix to keep the code simple. However, common libraries use edge lists, which we will discuss later more. Alternatively, we could also use the list of edges to define a sparse adjacency matrix with which we can work as if it was a dense matrix, but allows more memory-efficient operations. PyTorch supports this with the sub-package `torch.sparse` (documentation) which is however still in a beta-stage (API might change in future).

Graph Convolutions

Graph Convolutional Networks have been introduced by Kipf et al. in 2016 at the University of Amsterdam. He also wrote a great blog post about this topic, which is recommended if you want to read about GCNs from a different perspective. GCNs are similar to convolutions in images in the sense that the "filter" parameters are typically shared over all locations in the graph. At the same time, GCNs rely on message passing methods, which means that vertices exchange information with the neighbors, and send "messages" to each other. Before looking at the math, we can try to visually understand how GCNs work. The first step is that each node creates a feature vector that represents the message it wants to send to all its neighbors. In the second step, the messages are sent to the neighbors, so that a node receives one message per adjacent node. Below we have visualized the two steps for our example graph.

If we want to formulate that in more mathematical terms, we need to first decide how to combine all the messages a node receives. As the number of messages vary across nodes, we need an operation that works for any number. Hence, the usual way to go is to sum or take the mean. Given the previous features of nodes $H^{(l)}$, the GCN layer is defined as follows:

$$H^{(l+1)} = \sigma\left(\hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}H^{(l)}W^{(l)}\right)$$

$W^{(l)}$ is the weight parameters with which we transform the input features into messages ($H^{(l)}W^{(l)}$). To the adjacency matrix A we add the identity matrix so that each node sends its own message also to itself: $\hat{A} = A + I$. Finally, to take the average instead of summing, we calculate the matrix $\hat{D}$ which is a diagonal matrix with D_{ii} denoting the number of neighbors node i has. σ represents an arbitrary activation function, and not necessarily the sigmoid (usually a ReLU-based activation function is used in GNNs).

When implementing the GCN layer in PyTorch, we can take advantage of the flexible operations on tensors. Instead of defining a matrix $\hat{D}$, we can simply divide the summed messages by the number of neighbors afterward. Additionally, we replace the weight matrix with a linear layer, which additionally allows us to add a bias. Written as a PyTorch module, the GCN layer is defined as follows:

[3]:
```
class GCNLayer(nn.Module):

    def __init__(self, c_in, c_out):
        super().__init__()
        self.projection = nn.Linear(c_in, c_out)

    def forward(self, node_feats, adj_matrix):
        """
        Inputs:
            node_feats - Tensor with node features of shape [batch_size, num_nodes, c_in]
```

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```
            adj_matrix - Batch of adjacency matrices of the graph. If there is an edge␣
↪from i to j, adj_matrix[b,i,j]=1 else 0.
                         Supports directed edges by non-symmetric matrices. Assumes to␣
↪already have added the identity connections.
                         Shape: [batch_size, num_nodes, num_nodes]
        """
        # Num neighbours = number of incoming edges
        num_neighbours = adj_matrix.sum(dim=-1, keepdims=True)
        node_feats = self.projection(node_feats)
        node_feats = torch.bmm(adj_matrix, node_feats)
        node_feats = node_feats / num_neighbours
        return node_feats
```

To further understand the GCN layer, we can apply it to our example graph above. First, let's specify some node features and the adjacency matrix with added self-connections:

[4]:
```
node_feats = torch.arange(8, dtype=torch.float32).view(1, 4, 2)
adj_matrix = torch.Tensor([[[1, 1, 0, 0],
                            [1, 1, 1, 1],
                            [0, 1, 1, 1],
                            [0, 1, 1, 1]]])

print("Node features:\n", node_feats)
print("\nAdjacency matrix:\n", adj_matrix)
```

```
Node features:
 tensor([[[0., 1.],
         [2., 3.],
         [4., 5.],
         [6., 7.]]])

Adjacency matrix:
 tensor([[[1., 1., 0., 0.],
         [1., 1., 1., 1.],
         [0., 1., 1., 1.],
         [0., 1., 1., 1.]]])
```

Next, let's apply a GCN layer to it. For simplicity, we initialize the linear weight matrix as an identity matrix so that the input features are equal to the messages. This makes it easier for us to verify the message passing operation.

[5]:
```
layer = GCNLayer(c_in=2, c_out=2)
layer.projection.weight.data = torch.Tensor([[1., 0.], [0., 1.]])
layer.projection.bias.data = torch.Tensor([0., 0.])

with torch.no_grad():
    out_feats = layer(node_feats, adj_matrix)

print("Adjacency matrix", adj_matrix)
print("Input features", node_feats)
print("Output features", out_feats)
```

```
Adjacency matrix tensor([[[1., 1., 0., 0.],
         [1., 1., 1., 1.],
```

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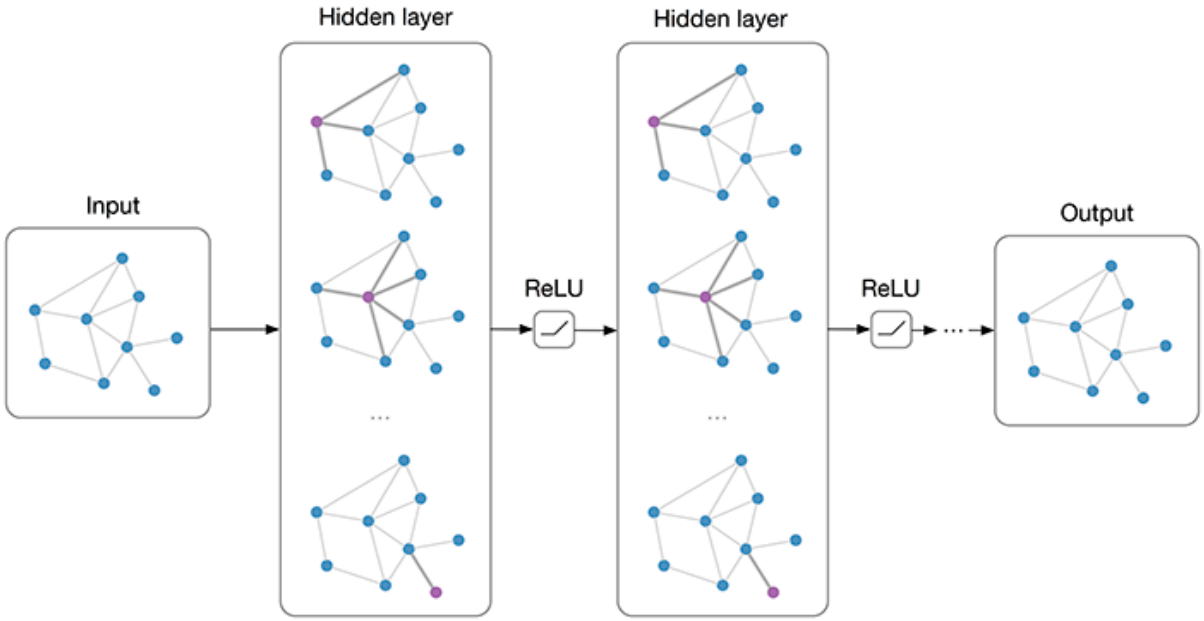
```
        [0., 1., 1., 1.],
        [0., 1., 1., 1.]]])
Input features tensor([[[0., 1.],
        [2., 3.],
        [4., 5.],
        [6., 7.]]])
Output features tensor([[[1., 2.],
        [3., 4.],
        [4., 5.],
        [4., 5.]]])
```

As we can see, the first node's output values are the average of itself and the second node. Similarly, we can verify all other nodes. However, in a GNN, we would also want to allow feature exchange between nodes beyond its neighbors. This can be achieved by applying multiple GCN layers, which gives us the final layout of a GNN. The GNN can be build up by a sequence of GCN layers and non-linearities such as ReLU. For a visualization, see below (figure credit - Thomas Kipf, 2016).



However, one issue we can see from looking at the example above is that the output features for nodes 3 and 4 are the same because they have the same adjacent nodes (including itself). Therefore, GCN layers can make the network forget node-specific information if we just take a mean over all messages. Multiple possible improvements have been proposed. While the simplest option might be using residual connections, the more common approach is to either weigh the self-connections higher or define a separate weight matrix for the self-connections. Alternatively, we can re-visit a concept from the last tutorial: attention.

Graph Attention

If you remember from the last tutorial, attention describes a weighted average of multiple elements with the weights dynamically computed based on an input query and elements' keys (if you haven't read Tutorial 6 yet, it is recommended to at least go through the very first section called What is Attention?). This concept can be similarly applied to graphs, one of such is the Graph Attention Network (called GAT, proposed by Velickovic et al., 2017). Similarly to the GCN, the graph attention layer creates a message for each node using a linear layer/weight matrix. For the attention part, it uses the message from the node itself as a query, and the messages to average as both keys and values (note that this also includes the message to itself). The score function f_{attn} is implemented as a one-layer MLP which maps the query and key to a single value. The MLP looks as follows (figure credit - Velickovic et al.):

h_i and h_j are the original features from node i and j respectively, and represent the messages of the layer with $\mathbf{W}$ as weight matrix. $\mathbf{a}$ is the weight matrix of the MLP, which has the shape $[1, 2 \times d_{\text{message}}]$, and α_{ij} the final attention weight from node i to j. The calculation can be described as follows:

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_j\right]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_k\right]\right)\right)}$$

The operator $||$ represents the concatenation, and $\mathcal{N}_i$ the indices of the neighbors of node i. Note that in contrast to usual practice, we apply a non-linearity (here LeakyReLU) before the softmax over elements. Although it seems like a minor change at first, it is crucial for the attention to depend on the original input. Specifically, let's remove the non-linearity for a second, and try to simplify the expression:

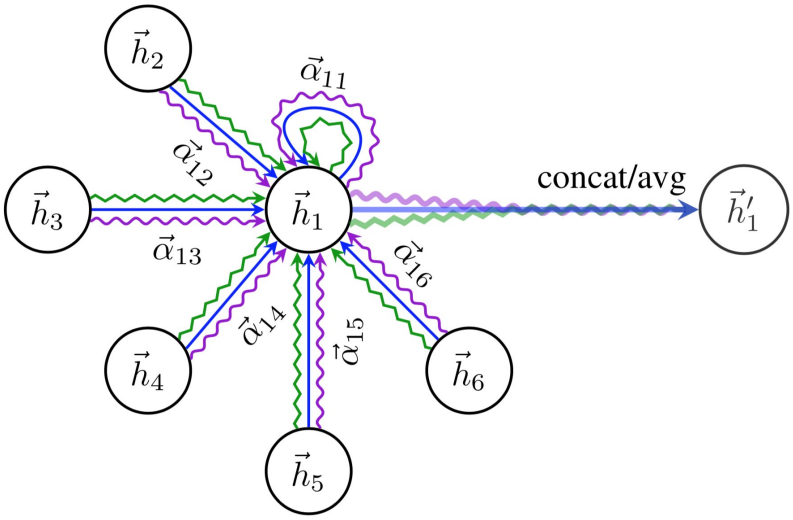
$$\begin{aligned}
\alpha_{ij} &= \frac{\exp\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_j\right]\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_k\right]\right)}\\
&= \frac{\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i + \mathbf{a}_{:,d/2:}\mathbf{W}h_j\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i + \mathbf{a}_{:,d/2:}\mathbf{W}h_k\right)}\\
&= \frac{\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i\right)\cdot\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_j\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i\right)\cdot\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_k\right)}\\
&= \frac{\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_j\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_k\right)}
\end{aligned}$$

We can see that without the non-linearity, the attention term with h_i actually cancels itself out, resulting in the attention being independent of the node itself. Hence, we would have the same issue as the GCN of creating the same output features for nodes with the same neighbors. This is why the LeakyReLU is crucial and adds some dependency on h_i to the attention.

Once we obtain all attention factors, we can calculate the output features for each node by performing the weighted average:

$$h_i' = \sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}\mathbf{W}h_j\right)$$

σ is yet another non-linearity, as in the GCN layer. Visually, we can represent the full message passing in an attention layer as follows (figure credit - Velickovic et al.):



To increase the expressiveness of the graph attention network, Velickovic et al. proposed to extend it to multiple heads similar to the Multi-Head Attention block in Transformers. This results in N attention layers being applied in parallel. In the image above, it is visualized as three different colors of arrows (green, blue, and purple) that are afterward concatenated. The average is only applied for the very final prediction layer in a network.

After having discussed the graph attention layer in detail, we can implement it below:

[6]:
```
class GATLayer(nn.Module):

    def __init__(self, c_in, c_out, num_heads=1, concat_heads=True, alpha=0.2):
        """
        Inputs:
            c_in - Dimensionality of input features
            c_out - Dimensionality of output features
            num_heads - Number of heads, i.e. attention mechanisms to apply in parallel. The
                        output features are equally split up over the heads if concat_heads=True.
            concat_heads - If True, the output of the different heads is concatenated instead of averaged.
            alpha - Negative slope of the LeakyReLU activation.
        """
        super().__init__()
        self.num_heads = num_heads
        self.concat_heads = concat_heads
        if self.concat_heads:
            assert c_out % num_heads == 0, "Number of output features must be a multiple of the count of heads."
            c_out = c_out // num_heads

        # Sub-modules and parameters needed in the layer
        self.projection = nn.Linear(c_in, c_out * num_heads)
        self.a = nn.Parameter(torch.Tensor(num_heads, 2 * c_out)) # One per head
        self.leakyrelu = nn.LeakyReLU(alpha)

        # Initialization from the original implementation
        nn.init.xavier_uniform_(self.projection.weight.data, gain=1.414)
```

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```
        nn.init.xavier_uniform_(self.a.data, gain=1.414)

    def forward(self, node_feats, adj_matrix, print_attn_probs=False):
        """
        Inputs:
            node_feats - Input features of the node. Shape: [batch_size, c_in]
            adj_matrix - Adjacency matrix including self-connections. Shape: [batch_size,
↪ num_nodes, num_nodes]
            print_attn_probs - If True, the attention weights are printed during the␣
↪forward pass (for debugging purposes)
        """
        batch_size, num_nodes = node_feats.size(0), node_feats.size(1)

        # Apply linear layer and sort nodes by head
        node_feats = self.projection(node_feats)
        node_feats = node_feats.view(batch_size, num_nodes, self.num_heads, -1)

        # We need to calculate the attention logits for every edge in the adjacency␣
↪matrix
        # Doing this on all possible combinations of nodes is very expensive
        # => Create a tensor of [W*h_i||W*h_j] with i and j being the indices of all␣
↪edges
        edges = adj_matrix.nonzero(as_tuple=False) # Returns indices where the adjacency␣
↪matrix is not 0 => edges
        node_feats_flat = node_feats.view(batch_size * num_nodes, self.num_heads, -1)
        edge_indices_row = edges[:,0] * num_nodes + edges[:,1]
        edge_indices_col = edges[:,0] * num_nodes + edges[:,2]
        a_input = torch.cat([
            torch.index_select(input=node_feats_flat, index=edge_indices_row, dim=0),
            torch.index_select(input=node_feats_flat, index=edge_indices_col, dim=0)
        ], dim=-1) # Index select returns a tensor with node_feats_flat being indexed at␣
↪the desired positions along dim=0

        # Calculate attention MLP output (independent for each head)
        attn_logits = torch.einsum('bhc,hc->bh', a_input, self.a)
        attn_logits = self.leakyrelu(attn_logits)

        # Map list of attention values back into a matrix
        attn_matrix = attn_logits.new_zeros(adj_matrix.shape+(self.num_heads,)).fill_(-
↪9e15)
        attn_matrix[adj_matrix[...,None].repeat(1,1,1,self.num_heads) == 1] = attn_
↪logits.reshape(-1)

        # Weighted average of attention
        attn_probs = F.softmax(attn_matrix, dim=2)
        if print_attn_probs:
            print("Attention probs\n", attn_probs.permute(0, 3, 1, 2))
        node_feats = torch.einsum('bijh,bjhc->bihc', attn_probs, node_feats)

        # If heads should be concatenated, we can do this by reshaping. Otherwise, take␣
↪mean
        if self.concat_heads:
```

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```
            node_feats = node_feats.reshape(batch_size, num_nodes, -1)
        else:
            node_feats = node_feats.mean(dim=2)

        return node_feats
```

Again, we can apply the graph attention layer on our example graph above to understand the dynamics better. As before, the input layer is initialized as an identity matrix, but we set $\mathbf{a}$ to be a vector of arbitrary numbers to obtain different attention values. We use two heads to show the parallel, independent attention mechanisms working in the layer.

[7]:
```
layer = GATLayer(2, 2, num_heads=2)
layer.projection.weight.data = torch.Tensor([[1., 0.], [0., 1.]])
layer.projection.bias.data = torch.Tensor([0., 0.])
layer.a.data = torch.Tensor([[-0.2, 0.3], [0.1, -0.1]])

with torch.no_grad():
    out_feats = layer(node_feats, adj_matrix, print_attn_probs=True)

print("Adjacency matrix", adj_matrix)
print("Input features", node_feats)
print("Output features", out_feats)
```

```
Attention probs
 tensor([[[[0.3543, 0.6457, 0.0000, 0.0000],
          [0.1096, 0.1450, 0.2642, 0.4813],
          [0.0000, 0.1858, 0.2885, 0.5257],
          [0.0000, 0.2391, 0.2696, 0.4913]],

         [[0.5100, 0.4900, 0.0000, 0.0000],
          [0.2975, 0.2436, 0.2340, 0.2249],
          [0.0000, 0.3838, 0.3142, 0.3019],
          [0.0000, 0.4018, 0.3289, 0.2693]]]])
Adjacency matrix tensor([[[1., 1., 0., 0.],
         [1., 1., 1., 1.],
         [0., 1., 1., 1.],
         [0., 1., 1., 1.]]])
Input features tensor([[[0., 1.],
         [2., 3.],
         [4., 5.],
         [6., 7.]]])
Output features tensor([[[1.2913, 1.9800],
         [4.2344, 3.7725],
         [4.6798, 4.8362],
         [4.5043, 4.7351]]])
```

We recommend that you try to calculate the attention matrix at least for one head and one node for yourself. The entries are 0 where there does not exist an edge between i and j. For the others, we see a diverse set of attention probabilities. Moreover, the output features of node 3 and 4 are now different although they have the same neighbors.

4.21.2 PyTorch Geometric

We had mentioned before that implementing graph networks with adjacency matrix is simple and straight-forward but can be computationally expensive for large graphs. Many real-world graphs can reach over 200k nodes, for which adjacency matrix-based implementations fail. There are a lot of optimizations possible when implementing GNNs, and luckily, there exist packages that provide such layers. The most popular packages for PyTorch are PyTorch Geometric and the Deep Graph Library (the latter being actually framework agnostic). Which one to use depends on the project you are planning to do and personal taste. In this tutorial, we will look at PyTorch Geometric as part of the PyTorch family. Similar to PyTorch Lightning, PyTorch Geometric is not installed by default on GoogleColab (and actually also not in our `dl2021` environment due to many dependencies that would be unnecessary for the practicals). Hence, let's import and/or install it below:

[8]:
```
# torch geometric
try:
    import torch_geometric
except ModuleNotFoundError:
    # Installing torch geometric packages with specific CUDA+PyTorch version.
    # See https://pytorch-geometric.readthedocs.io/en/latest/notes/installation.html for␣
↪details
    TORCH = torch.__version__.split('+')[0]
    CUDA = 'cu' + torch.version.cuda.replace('.','')

    !pip install torch-scatter     -f https://pytorch-geometric.com/whl/torch-{TORCH}+
↪{CUDA}.html
    !pip install torch-sparse      -f https://pytorch-geometric.com/whl/torch-{TORCH}+
↪{CUDA}.html
    !pip install torch-cluster     -f https://pytorch-geometric.com/whl/torch-{TORCH}+
↪{CUDA}.html
    !pip install torch-spline-conv -f https://pytorch-geometric.com/whl/torch-{TORCH}+
↪{CUDA}.html
    !pip install torch-geometric
    import torch_geometric
import torch_geometric.nn as geom_nn
import torch_geometric.data as geom_data
```

```
RDKit WARNING: [19:12:50] Enabling RDKit 2019.09.3 jupyter extensions
```

PyTorch Geometric provides us a set of common graph layers, including the GCN and GAT layer we implemented above. Additionally, similar to PyTorch's torchvision, it provides the common graph datasets and transformations on those to simplify training. Compared to our implementation above, PyTorch Geometric uses a list of index pairs to represent the edges. The details of this library will be explored further in our experiments.

In our tasks below, we want to allow us to pick from a multitude of graph layers. Thus, we define again below a dictionary to access those using a string:

[9]:
```
gnn_layer_by_name = {
    "GCN": geom_nn.GCNConv,
    "GAT": geom_nn.GATConv,
    "GraphConv": geom_nn.GraphConv
}
```

Additionally to GCN and GAT, we added the layer `geom_nn.GraphConv` (documentation). GraphConv is a GCN with a separate weight matrix for the self-connections. Mathematically, this would be:

$$\mathbf{x}_i^{(l+1)} = \mathbf{W}_1^{(l+1)}\mathbf{x}_i^{(l)} + \mathbf{W}_2^{(\ell+1)}\sum_{j\in\mathcal{N}_i}\mathbf{x}_j^{(l)}$$

In this formula, the neighbor's messages are added instead of averaged. However, PyTorch Geometric provides the argument `aggr` to switch between summing, averaging, and max pooling.

4.21.3 Experiments on graph structures

Tasks on graph-structured data can be grouped into three groups: node-level, edge-level and graph-level. The different levels describe on which level we want to perform classification/regression. We will discuss all three types in more detail below.

Node-level tasks: Semi-supervised node classification

Node-level tasks have the goal to classify nodes in a graph. Usually, we have given a single, large graph with >1000 nodes of which a certain amount of nodes are labeled. We learn to classify those labeled examples during training and try to generalize to the unlabeled nodes.

A popular example that we will use in this tutorial is the Cora dataset, a citation network among papers. The Cora consists of 2708 scientific publications with links between each other representing the citation of one paper by another. The task is to classify each publication into one of seven classes. Each publication is represented by a bag-of-words vector. This means that we have a vector of 1433 elements for each publication, where a 1 at feature i indicates that the i-th word of a pre-defined dictionary is in the article. Binary bag-of-words representations are commonly used when we need very simple encodings, and already have an intuition of what words to expect in a network. There exist much better approaches, but we will leave this to the NLP courses to discuss.

We will load the dataset below:

[10]:
```
cora_dataset = torch_geometric.datasets.Planetoid(root=DATASET_PATH, name="Cora")
```

Let's look at how PyTorch Geometric represents the graph data. Note that although we have a single graph, PyTorch Geometric returns a dataset for compatibility to other datasets.

[11]:
```
cora_dataset[0]
```

[11]:
```
Data(edge_index=[2, 10556], test_mask=[2708], train_mask=[2708], val_mask=[2708],␣
↪x=[2708, 1433], y=[2708])
```

The graph is represented by a `Data` object (documentation) which we can access as a standard Python namespace. The edge index tensor is the list of edges in the graph and contains the mirrored version of each edge for undirected graphs. The `train_mask`, `val_mask`, and `test_mask` are boolean masks that indicate which nodes we should use for training, validation, and testing. The `x` tensor is the feature tensor of our 2708 publications, and `y` the labels for all nodes.

After having seen the data, we can implement a simple graph neural network. The GNN applies a sequence of graph layers (GCN, GAT, or GraphConv), ReLU as activation function, and dropout for regularization. See below for the specific implementation.

[12]:
```
class GNNModel(nn.Module):

    def __init__(self, c_in, c_hidden, c_out, num_layers=2, layer_name="GCN", dp_rate=0.
↪1, **kwargs):
        """
        Inputs:
            c_in - Dimension of input features
            c_hidden - Dimension of hidden features
            c_out - Dimension of the output features. Usually number of classes in␣
↪classification
```

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```
            num_layers - Number of "hidden" graph layers
            layer_name - String of the graph layer to use
            dp_rate - Dropout rate to apply throughout the network
            kwargs - Additional arguments for the graph layer (e.g. number of heads for␣
↪GAT)
        """
        super().__init__()
        gnn_layer = gnn_layer_by_name[layer_name]

        layers = []
        in_channels, out_channels = c_in, c_hidden
        for l_idx in range(num_layers-1):
            layers += [
                gnn_layer(in_channels=in_channels,
                          out_channels=out_channels,
                          **kwargs),
                nn.ReLU(inplace=True),
                nn.Dropout(dp_rate)
            ]
            in_channels = c_hidden
        layers += [gnn_layer(in_channels=in_channels,
                             out_channels=c_out,
                             **kwargs)]
        self.layers = nn.ModuleList(layers)

    def forward(self, x, edge_index):
        """
        Inputs:
            x - Input features per node
            edge_index - List of vertex index pairs representing the edges in the graph␣
↪(PyTorch geometric notation)
        """
        for l in self.layers:
            # For graph layers, we need to add the "edge_index" tensor as additional␣
↪input
            # All PyTorch Geometric graph layer inherit the class "MessagePassing", hence
            # we can simply check the class type.
            if isinstance(l, geom_nn.MessagePassing):
                x = l(x, edge_index)
            else:
                x = l(x)
        return x
```

Good practice in node-level tasks is to create an MLP baseline that is applied to each node independently. This way we can verify whether adding the graph information to the model indeed improves the prediction, or not. It might also be that the features per node are already expressive enough to clearly point towards a specific class. To check this, we implement a simple MLP below.

[13]:
```
class MLPModel(nn.Module):

    def __init__(self, c_in, c_hidden, c_out, num_layers=2, dp_rate=0.1):
        """
```

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```
        Inputs:
            c_in - Dimension of input features
            c_hidden - Dimension of hidden features
            c_out - Dimension of the output features. Usually number of classes in␣
↪classification
            num_layers - Number of hidden layers
            dp_rate - Dropout rate to apply throughout the network
        """
        super().__init__()
        layers = []
        in_channels, out_channels = c_in, c_hidden
        for l_idx in range(num_layers-1):
            layers += [
                nn.Linear(in_channels, out_channels),
                nn.ReLU(inplace=True),
                nn.Dropout(dp_rate)
            ]
            in_channels = c_hidden
        layers += [nn.Linear(in_channels, c_out)]
        self.layers = nn.Sequential(*layers)

    def forward(self, x, *args, **kwargs):
        """
        Inputs:
            x - Input features per node
        """
        return self.layers(x)
```

Finally, we can merge the models into a PyTorch Lightning module which handles the training, validation, and testing for us.

[14]:
```
class NodeLevelGNN(pl.LightningModule):

    def __init__(self, model_name, **model_kwargs):
        super().__init__()
        # Saving hyperparameters
        self.save_hyperparameters()

        if model_name == "MLP":
            self.model = MLPModel(**model_kwargs)
        else:
            self.model = GNNModel(**model_kwargs)
        self.loss_module = nn.CrossEntropyLoss()

    def forward(self, data, mode="train"):
        x, edge_index = data.x, data.edge_index
        x = self.model(x, edge_index)

        # Only calculate the loss on the nodes corresponding to the mask
        if mode == "train":
            mask = data.train_mask
        elif mode == "val":
```

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```
            mask = data.val_mask
        elif mode == "test":
            mask = data.test_mask
        else:
            assert False, f"Unknown forward mode: {mode}"

        loss = self.loss_module(x[mask], data.y[mask])
        acc = (x[mask].argmax(dim=-1) == data.y[mask]).sum().float() / mask.sum()
        return loss, acc

    def configure_optimizers(self):
        # We use SGD here, but Adam works as well
        optimizer = optim.SGD(self.parameters(), lr=0.1, momentum=0.9, weight_decay=2e-3)
        return optimizer

    def training_step(self, batch, batch_idx):
        loss, acc = self.forward(batch, mode="train")
        self.log('train_loss', loss)
        self.log('train_acc', acc)
        return loss

    def validation_step(self, batch, batch_idx):
        _, acc = self.forward(batch, mode="val")
        self.log('val_acc', acc)

    def test_step(self, batch, batch_idx):
        _, acc = self.forward(batch, mode="test")
        self.log('test_acc', acc)
```

Additionally to the Lightning module, we define a training function below. As we have a single graph, we use a batch size of 1 for the data loader and share the same data loader for the train, validation, and test set (the mask is picked inside the Lightning module). Besides, we set the argument `enable_progress_bar` to False as it usually shows the progress per epoch, but an epoch only consists of a single step. The rest of the code is very similar to what we have seen in Tutorial 5 and 6 already.

[15]:
```
def train_node_classifier(model_name, dataset, **model_kwargs):
    pl.seed_everything(42)
    node_data_loader = geom_data.DataLoader(dataset, batch_size=1)

    # Create a PyTorch Lightning trainer with the generation callback
    root_dir = os.path.join(CHECKPOINT_PATH, "NodeLevel" + model_name)
    os.makedirs(root_dir, exist_ok=True)
    trainer = pl.Trainer(default_root_dir=root_dir,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc")],
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=200,
                         enable_progress_bar=False) # False because epoch size is 1
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need
```

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```
    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, f"NodeLevel{model_name}.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = NodeLevelGNN.load_from_checkpoint(pretrained_filename)
    else:
        pl.seed_everything()
        model = NodeLevelGNN(model_name=model_name, c_in=dataset.num_node_features, c_
↪out=dataset.num_classes, **model_kwargs)
        trainer.fit(model, node_data_loader, node_data_loader)
        model = NodeLevelGNN.load_from_checkpoint(trainer.checkpoint_callback.best_model_
↪path)

    # Test best model on the test set
    test_result = trainer.test(model, node_data_loader, verbose=False)
    batch = next(iter(node_data_loader))
    batch = batch.to(model.device)
    _, train_acc = model.forward(batch, mode="train")
    _, val_acc = model.forward(batch, mode="val")
    result = {"train": train_acc,
              "val": val_acc,
              "test": test_result[0]['test_acc']}
    return model, result
```

Finally, we can train our models. First, let's train the simple MLP:

[16]:
```
# Small function for printing the test scores
def print_results(result_dict):
    if "train" in result_dict:
        print(f"Train accuracy: {(100.0*result_dict['train']):4.2f}%")
    if "val" in result_dict:
        print(f"Val accuracy:   {(100.0*result_dict['val']):4.2f}%")
    print(f"Test accuracy:  {(100.0*result_dict['test']):4.2f}%")
```

[17]:
```
node_mlp_model, node_mlp_result = train_node_classifier(model_name="MLP",
                                                        dataset=cora_dataset,
                                                        c_hidden=16,
                                                        num_layers=2,
                                                        dp_rate=0.1)

print_results(node_mlp_result)
```

```
GPU available: True, used: True
WARNING: Logging before flag parsing goes to stderr.
I1113 19:12:52.401648 139969460983616 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1113 19:12:52.403518 139969460983616 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1113 19:12:52.404974 139969460983616 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
Train accuracy: 96.43%
Val accuracy:   52.60%
Test accuracy:  60.60%
```

```
/home/phillip/anaconda3/envs/nlp1/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:45: UserWarning: The dataloader, test dataloader 0, does not␣
↪have many workers which may be a bottleneck. Consider increasing the value of the `num_
↪workers` argument` (try 16 which is the number of cpus on this machine) in the␣
↪`DataLoader` init to improve performance.
  warnings.warn(*args, **kwargs)
```

Although the MLP can overfit on the training dataset because of the high-dimensional input features, it does not perform too well on the test set. Let's see if we can beat this score with our graph networks:

[18]:
```
node_gnn_model, node_gnn_result = train_node_classifier(model_name="GNN",
                                                        layer_name="GCN",
                                                        dataset=cora_dataset,
                                                        c_hidden=16,
                                                        num_layers=2,
                                                        dp_rate=0.1)
print_results(node_gnn_result)
```

```
GPU available: True, used: True
I1113 19:12:53.906714 139969460983616 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1113 19:12:53.907762 139969460983616 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1113 19:12:53.909639 139969460983616 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
Train accuracy: 100.00%
Val accuracy:   77.20%
Test accuracy:  82.40%
```

As we would have hoped for, the GNN model outperforms the MLP by quite a margin. This shows that using the graph information indeed improves our predictions and lets us generalizes better.

The hyperparameters in the model have been chosen to create a relatively small network. This is because the first layer with an input dimension of 1433 can be relatively expensive to perform for large graphs. In general, GNNs can become relatively expensive for very big graphs. This is why such GNNs either have a small hidden size or use a special batching strategy where we sample a connected subgraph of the big, original graph.

Edge-level tasks: Link prediction

In some applications, we might have to predict on an edge-level instead of node-level. The most common edge-level task in GNN is link prediction. Link prediction means that given a graph, we want to predict whether there will be/should be an edge between two nodes or not. For example, in a social network, this is used by Facebook and co to propose new friends to you. Again, graph level information can be crucial to perform this task. The output prediction is usually done by performing a similarity metric on the pair of node features, which should be 1 if there should be a link, and otherwise close to 0. To keep the tutorial short, we will not implement this task ourselves. Nevertheless, there are many good resources out there if you are interested in looking closer at this task. Tutorials and papers for this topic include:

- PyTorch Geometric example
- Graph Neural Networks: A Review of Methods and Applications, Zhou et al. 2019
- Link Prediction Based on Graph Neural Networks, Zhang and Chen, 2018.

Graph-level tasks: Graph classification

Finally, in this part of the tutorial, we will have a closer look at how to apply GNNs to the task of graph classification. The goal is to classify an entire graph instead of single nodes or edges. Therefore, we are also given a dataset of multiple graphs that we need to classify based on some structural graph properties. The most common task for graph classification is molecular property prediction, in which molecules are represented as graphs. Each atom is linked to a node, and edges in the graph are the bonds between atoms. For example, look at the figure below.

On the left, we have an arbitrary, small molecule with different atoms, whereas the right part of the image shows the graph representation. The atom types are abstracted as node features (e.g. a one-hot vector), and the different bond types are used as edge features. For simplicity, we will neglect the edge attributes in this tutorial, but you can include by using methods like the Relational Graph Convolution that uses a different weight matrix for each edge type.

The dataset we will use below is called the MUTAG dataset. It is a common small benchmark for graph classification algorithms, and contain 188 graphs with 18 nodes and 20 edges on average for each graph. The graph nodes have 7 different labels/atom types, and the binary graph labels represent "their mutagenic effect on a specific gram negative bacterium" (the specific meaning of the labels are not too important here). The dataset is part of a large collection of different graph classification datasets, known as the TUDatasets, which is directly accessible via `torch_geometric.datasets.TUDataset` (documentation) in PyTorch Geometric. We can load the dataset below.

[19]:
```
tu_dataset = torch_geometric.datasets.TUDataset(root=DATASET_PATH, name="MUTAG")
```

Let's look at some statistics for the dataset:

[20]:
```
print("Data object:", tu_dataset.data)
print("Length:", len(tu_dataset))
print(f"Average label: {tu_dataset.data.y.float().mean().item():4.2f}")
```

```
Data object: Data(edge_attr=[7442, 4], edge_index=[2, 7442], x=[3371, 7], y=[188])
Length: 188
Average label: 0.66
```

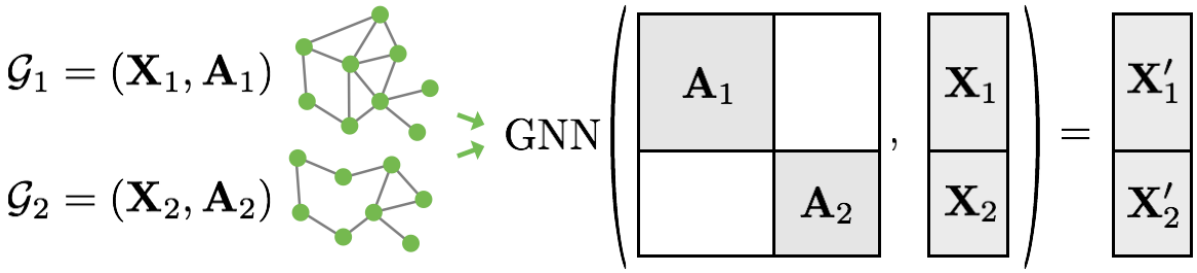
The first line shows how the dataset stores different graphs. The nodes, edges, and labels of each graph are concatenated to one tensor, and the dataset stores the indices where to split the tensors correspondingly. The length of the dataset is the number of graphs we have, and the "average label" denotes the percentage of the graph with label 1. As long as the percentage is in the range of 0.5, we have a relatively balanced dataset. It happens quite often that graph datasets are very imbalanced, hence checking the class balance is always a good thing to do.

Next, we will split our dataset into a training and test part. Note that we do not use a validation set this time because of the small size of the dataset. Therefore, our model might overfit slightly on the validation set due to the noise of the evaluation, but we still get an estimate of the performance on untrained data.

[21]:
```
torch.manual_seed(42)
tu_dataset.shuffle()
train_dataset = tu_dataset[:150]
test_dataset = tu_dataset[150:]
```

When using a data loader, we encounter a problem with batching N graphs. Each graph in the batch can have a different number of nodes and edges, and hence we would require a lot of padding to obtain a single tensor. Torch geometric

uses a different, more efficient approach: we can view the N graphs in a batch as a single large graph with concatenated node and edge list. As there is no edge between the N graphs, running GNN layers on the large graph gives us the same output as running the GNN on each graph separately. Visually, this batching strategy is visualized below (figure credit - PyTorch Geometric team, tutorial here).



The adjacency matrix is zero for any nodes that come from two different graphs, and otherwise according to the adjacency matrix of the individual graph. Luckily, this strategy is already implemented in torch geometric, and hence we can use the corresponding data loader:

[22]:
```
graph_train_loader = geom_data.DataLoader(train_dataset, batch_size=64, shuffle=True)
graph_val_loader = geom_data.DataLoader(test_dataset, batch_size=64) # Additional loader␣
↪if you want to change to a larger dataset
graph_test_loader = geom_data.DataLoader(test_dataset, batch_size=64)
```

Let's load a batch below to see the batching in action:

[23]:
```
batch = next(iter(graph_test_loader))
print("Batch:", batch)
print("Labels:", batch.y[:10])
print("Batch indices:", batch.batch[:40])
```

```
Batch: Batch(batch=[687], edge_attr=[1512, 4], edge_index=[2, 1512], x=[687, 7], y=[38])
Labels: tensor([1, 1, 1, 0, 0, 0, 1, 1, 1, 0])
Batch indices: tensor([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,␣
↪1, 1,
        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2])
```

We have 38 graphs stacked together for the test dataset. The batch indices, stored in `batch`, show that the first 12 nodes belong to the first graph, the next 22 to the second graph, and so on. These indices are important for performing the final prediction. To perform a prediction over a whole graph, we usually perform a pooling operation over all nodes after running the GNN model. In this case, we will use the average pooling. Hence, we need to know which nodes should be included in which average pool. Using this pooling, we can already create our graph network below. Specifically, we re-use our class `GNNModel` from before, and simply add an average pool and single linear layer for the graph prediction task.

[24]:
```
class GraphGNNModel(nn.Module):

    def __init__(self, c_in, c_hidden, c_out, dp_rate_linear=0.5, **kwargs):
        """
        Inputs:
            c_in - Dimension of input features
            c_hidden - Dimension of hidden features
            c_out - Dimension of output features (usually number of classes)
            dp_rate_linear - Dropout rate before the linear layer (usually much higher␣
↪than inside the GNN)
            kwargs - Additional arguments for the GNNModel object
```

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```
        """
        super().__init__()
        self.GNN = GNNModel(c_in=c_in,
                            c_hidden=c_hidden,
                            c_out=c_hidden, # Not our prediction output yet!
                            **kwargs)
        self.head = nn.Sequential(
            nn.Dropout(dp_rate_linear),
            nn.Linear(c_hidden, c_out)
        )

    def forward(self, x, edge_index, batch_idx):
        """
        Inputs:
            x - Input features per node
            edge_index - List of vertex index pairs representing the edges in the graph␣
↪(PyTorch geometric notation)
            batch_idx - Index of batch element for each node
        """
        x = self.GNN(x, edge_index)
        x = geom_nn.global_mean_pool(x, batch_idx) # Average pooling
        x = self.head(x)
        return x
```

Finally, we can create a PyTorch Lightning module to handle the training. It is similar to the modules we have seen before and does nothing surprising in terms of training. As we have a binary classification task, we use the Binary Cross Entropy loss.

[25]:
```
class GraphLevelGNN(pl.LightningModule):

    def __init__(self, **model_kwargs):
        super().__init__()
        # Saving hyperparameters
        self.save_hyperparameters()

        self.model = GraphGNNModel(**model_kwargs)
        self.loss_module = nn.BCEWithLogitsLoss() if self.hparams.c_out == 1 else nn.
↪CrossEntropyLoss()

    def forward(self, data, mode="train"):
        x, edge_index, batch_idx = data.x, data.edge_index, data.batch
        x = self.model(x, edge_index, batch_idx)
        x = x.squeeze(dim=-1)

        if self.hparams.c_out == 1:
            preds = (x > 0).float()
            data.y = data.y.float()
        else:
            preds = x.argmax(dim=-1)
        loss = self.loss_module(x, data.y)
        acc = (preds == data.y).sum().float() / preds.shape[0]
        return loss, acc
```

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```
    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(), lr=1e-2, weight_decay=0.0) # High lr␣
↪because of small dataset and small model
        return optimizer

    def training_step(self, batch, batch_idx):
        loss, acc = self.forward(batch, mode="train")
        self.log('train_loss', loss)
        self.log('train_acc', acc)
        return loss

    def validation_step(self, batch, batch_idx):
        _, acc = self.forward(batch, mode="val")
        self.log('val_acc', acc)

    def test_step(self, batch, batch_idx):
        _, acc = self.forward(batch, mode="test")
        self.log('test_acc', acc)
```

Below we train the model on our dataset. It resembles the typical training functions we have seen so far.

[26]:
```
def train_graph_classifier(model_name, **model_kwargs):
    pl.seed_everything(42)

    # Create a PyTorch Lightning trainer with the generation callback
    root_dir = os.path.join(CHECKPOINT_PATH, "GraphLevel" + model_name)
    os.makedirs(root_dir, exist_ok=True)
    trainer = pl.Trainer(default_root_dir=root_dir,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc")],
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=500,
                         enable_progress_bar=False)
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, f"GraphLevel{model_name}.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = GraphLevelGNN.load_from_checkpoint(pretrained_filename)
    else:
        pl.seed_everything(42)
        model = GraphLevelGNN(c_in=tu_dataset.num_node_features,
                              c_out=1 if tu_dataset.num_classes==2 else tu_dataset.num_
↪classes,
                              **model_kwargs)
        trainer.fit(model, graph_train_loader, graph_val_loader)
        model = GraphLevelGNN.load_from_checkpoint(trainer.checkpoint_callback.best_
↪model_path)
```

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```
    # Test best model on validation and test set
    train_result = trainer.test(model, graph_train_loader, verbose=False)
    test_result = trainer.test(model, graph_test_loader, verbose=False)
    result = {"test": test_result[0]['test_acc'], "train": train_result[0]['test_acc']}
    return model, result
```

Finally, let's perform the training and testing. Feel free to experiment with different GNN layers, hyperparameters, etc.

[27]:
```
model, result = train_graph_classifier(model_name="GraphConv",
                                       c_hidden=256,
                                       layer_name="GraphConv",
                                       num_layers=3,
                                       dp_rate_linear=0.5,
                                       dp_rate=0.0)
```

```
GPU available: True, used: True
I1113 19:12:54.045717 139969460983616 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1113 19:12:54.047091 139969460983616 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1113 19:12:54.048336 139969460983616 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
/home/phillip/anaconda3/envs/nlp1/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:45: UserWarning: Your test_dataloader has `shuffle=True`, it␣
↪is best practice to turn this off for validation and test dataloaders.
  warnings.warn(*args, **kwargs)
```

```
Found pretrained model, loading...
```

[28]:
```
print(f"Train performance: {100.0*result['train']:4.2f}%")
print(f"Test performance:  {100.0*result['test']:4.2f}%")
```

```
Train performance: 94.27%
Test performance:  92.11%
```

The test performance shows that we obtain quite good scores on an unseen part of the dataset. It should be noted that as we have been using the test set for validation as well, we might have overfitted slightly to this set. Nevertheless, the experiment shows us that GNNs can be indeed powerful to predict the properties of graphs and/or molecules.

4.21.4 Conclusion

In this tutorial, we have seen the application of neural networks to graph structures. We looked at how a graph can be represented (adjacency matrix or edge list), and discussed the implementation of common graph layers: GCN and GAT. The implementations showed the practical side of the layers, which is often easier than the theory. Finally, we experimented with different tasks, on node-, edge- and graph-level. Overall, we have seen that including graph information in the predictions can be crucial for achieving high performance. There are a lot of applications that benefit from GNNs, and the importance of these networks will likely increase over the next years.

If you found this tutorial helpful, consider -ing our repository.

For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.22 Tutorial 8: Deep Energy-Based Generative Models

Filled notebook:
Pre-trained models:
Recordings:
Author: Phillip Lippe

In this tutorial, we will look at energy-based deep learning models, and focus on their application as generative models. Energy models have been a popular tool before the huge deep learning hype around 2012 hit. However, in recent years, energy-based models have gained increasing attention because of improved training methods and tricks being proposed. Although they are still in a research stage, they have shown to outperform strong Generative Adversarial Networks (Lecture/Tutorial 10) in certain cases which have been the state of the art of generating images (blog post about strong energy-based models, blog post about the power of GANs). Hence, it is important to be aware of energy-based models, and as the theory can be abstract sometimes, we will show the idea of energy-based models with a lot of examples.

First, let's import our standard libraries below.

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
import random

## Imports for plotting
import matplotlib.pyplot as plt
from matplotlib import cm
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
from mpl_toolkits.mplot3d.axes3d import Axes3D
from mpl_toolkits.mplot3d import proj3d
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
```

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```
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import MNIST
from torchvision import transforms
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial8"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)
```

We also have pre-trained models that we download below.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial8/"
# Files to download
pretrained_files = ["MNIST.ckpt", "tensorboards/events.out.tfevents.MNIST"]

# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
```

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```
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.22.1 Energy Models

In the first part of this tutorial, we will review the theory of the energy-based models (the same theory has been discussed in Lecture 8). While most of the previous models had the goal of classification or regression, energy-based models are motivated from a different perspective: density estimation. Given a dataset with a lot of elements, we want to estimate the probability distribution over the whole data space. As an example, if we model images from CIFAR10, our goal would be to have a probability distribution over all possible images of size $32 \times 32 \times 3$ where those images have a high likelihood that look realistic and are one of the 10 CIFAR classes. Simple methods like interpolation between images don't work because images are extremely high-dimensional (especially for large HD images). Hence, we turn to deep learning methods that have performed well on complex data.

However, how do we predict a probability distribution $p(\mathbf{x})$ over so many dimensions using a simple neural network? The problem is that we cannot just predict a score between 0 and 1, because a probability distribution over data needs to fulfill two properties:

1. The probability distribution needs to assign any possible value of $\mathbf{x}$ a non-negative value: $p(\mathbf{x}) \geq 0$.
2. The probability density must sum/integrate to 1 over **all** possible inputs: $\int_{\mathbf{x}} p(\mathbf{x}) d\mathbf{x} = 1$.

Luckily, there are actually many approaches for this, and one of them are energy-based models. The fundamental idea of energy-based models is that you can turn any function that predicts values larger than zero into a probability distribution by dividing by its volume. Imagine we have a neural network, which has as output a single neuron, like in regression. We can call this network $E_\theta(\mathbf{x})$, where θ are our parameters of the network, and $\mathbf{x}$ the input data (e.g. an image). The output of E_θ is a scalar value between $-\infty$ and ∞. Now, we can use basic probability theory to *normalize* the scores of all possible inputs:

$$q_\theta(\mathbf{x}) = \frac{\exp\left(-E_\theta(\mathbf{x})\right)}{Z_\theta} \qquad \text{where} \qquad Z_\theta = \begin{cases} \int_{\mathbf{x}} \exp\left(-E_\theta(\mathbf{x})\right) d\mathbf{x} & \text{if } x \text{ is continuous} \\ \sum_{\mathbf{x}} \exp\left(-E_\theta(\mathbf{x})\right) & \text{if } x \text{ is discrete} \end{cases}$$

The $\exp$-function ensures that we assign a probability greater than zero to any possible input. We use a negative sign in front of E because we call E_θ to be the energy function: data points with high likelihood have a low energy, while data points with low likelihood have a high energy. Z_θ is our normalization terms that ensures that the density integrates/sums to 1. We can show this by integrating over $q_\theta(\mathbf{x})$:

$$\int_{\mathbf{x}} q_\theta(\mathbf{x}) d\mathbf{x} = \int_{\mathbf{x}} \frac{\exp\left(-E_\theta(\mathbf{x})\right)}{\int_{\tilde{\mathbf{x}}} \exp\left(-E_\theta(\tilde{\mathbf{x}})\right) d\tilde{\mathbf{x}}} d\mathbf{x} = \frac{\int_{\mathbf{x}} \exp\left(-E_\theta(\mathbf{x})\right) d\mathbf{x}}{\int_{\tilde{\mathbf{x}}} \exp\left(-E_\theta(\tilde{\mathbf{x}})\right) d\tilde{\mathbf{x}}} = 1$$

Note that we call the probability distribution $q_\theta(\mathbf{x})$ because this is the learned distribution by the model, and is trained to be as close as possible to the *true*, unknown distribution $p(\mathbf{x})$.

The main benefit of this formulation of the probability distribution is its great flexibility as we can choose E_θ in whatever way we like, without any constraints. Nevertheless, when looking at the equation above, we can see a fundamental issue: How do we calculate Z_θ? There is no chance that we can calculate Z_θ analytically for high-dimensional input and/or larger neural networks, but the task requires us to know Z_θ. Although we can't determine the exact likelihood of a point, there exist methods with which we can train energy-based models. Thus, we will look next at "Contrastive Divergence" for training the model.

Contrastive Divergence

When we train a model on generative modeling, it is usually done by maximum likelihood estimation. In other words, we try to maximize the likelihood of the examples in the training set. As the exact likelihood of a point cannot be determined due to the unknown normalization constant Z_θ, we need to train energy-based models slightly different. We cannot just maximize the un-normalized probability $\exp(-E_\theta(\mathbf{x}_{\text{train}}))$ because there is no guarantee that Z_θ stays constant, or that $\mathbf{x}_{\text{train}}$ is becoming more likely than the others. However, if we base our training on comparing the likelihood of points, we can create a stable objective. Namely, we can re-write our maximum likelihood objective where we maximize the probability of $\mathbf{x}_{\text{train}}$ compared to a randomly sampled data point of our model:

$$\begin{aligned}\nabla_\theta \mathcal{L}_{\text{MLE}}(\theta; p) &= -\mathbb{E}_{p(\mathbf{x})}\left[\nabla_\theta \log q_\theta(\mathbf{x})\right] \\ &= \mathbb{E}_{p(\mathbf{x})}\left[\nabla_\theta E_\theta(\mathbf{x})\right] - \mathbb{E}_{q_\theta(\mathbf{x})}\left[\nabla_\theta E_\theta(\mathbf{x})\right]\end{aligned}$$

Note that the loss is still an objective we want to minimize. Thus, we try to minimize the energy for data points from the dataset, while maximizing the energy for randomly sampled data points from our model (how we sample will be explained below). Although this objective sounds intuitive, how is it actually derived from our original distribution $q_\theta(\mathbf{x})$? The trick is that we approximate Z_θ by a single Monte-Carlo sample. This gives us the exact same objective as written above.

Visually, we can look at the objective as follows (figure credit - Stefano Ermon and Aditya Grover):

f_θ represents $\exp(-E_\theta(\mathbf{x}))$ in our case. The point on the right, called "correct answer", represents a data point from the dataset (i.e. x_{train}), and the left point, "wrong answer", a sample from our model (i.e. x_{sample}). Thus, we try to "pull up" the probability of the data points in the dataset, while "pushing down" randomly sampled points. The two forces for pulling and pushing are in balance iff $q_\theta(\mathbf{x}) = p(\mathbf{x})$.

Sampling from Energy-Based Models

For sampling from an energy-based model, we can apply a Markov Chain Monte Carlo using Langevin Dynamics. The idea of the algorithm is to start from a random point, and slowly move towards the direction of higher probability using the gradients of E_θ. Nevertheless, this is not enough to fully capture the probability distribution. We need to add noise ω at each gradient step to the current sample. Under certain conditions such as that we perform the gradient steps an infinite amount of times, we would be able to create an exact sample from our modeled distribution. However, as this is not practically possible, we usually limit the chain to K steps (K a hyperparameter that needs to be finetuned). Overall, the sampling procedure can be summarized in the following algorithm:

Applications of Energy-based models beyond generation

Modeling the probability distribution for sampling new data is not the only application of energy-based models. Any application which requires us to compare two elements is much simpler to learn because we just need to go for the higher energy. A couple of examples are shown below (figure credit - Stefano Ermon and Aditya Grover). A classification setup like object recognition or sequence labeling can be considered as an energy-based task as we just need to find the Y input that minimizes the output $E(X, Y)$ (hence maximizes probability). Similarly, a popular application of energy-based models is denoising of images. Given an image X with a lot of noise, we try to minimize the energy by finding the true input image Y.

Nonetheless, we will focus on generative modeling here as in the next couple of lectures, we will discuss more generative deep learning approaches.

4.22.2 Image generation

As an example for energy-based models, we will train a model on image generation. Specifically, we will look at how we can generate MNIST digits with a very simple CNN model. However, it should be noted that energy models are not easy to train and often diverge if the hyperparameters are not well tuned. We will rely on training tricks proposed in the paper Implicit Generation and Generalization in Energy-Based Models by Yilun Du and Igor Mordatch (blog). The important part of this notebook is however to see how the theory above can actually be used in a model.

Dataset

First, we can load the MNIST dataset below. Note that we need to normalize the images between -1 and 1 instead of mean 0 and std 1 because during sampling, we have to limit the input space. Scaling between -1 and 1 makes it easier to implement it.

[3]:
```
# Transformations applied on each image => make them a tensor and normalize between -1␣
↪and 1
transform = transforms.Compose([transforms.ToTensor(),
                                transforms.Normalize((0.5,), (0.5,))
                               ])

# Loading the training dataset. We need to split it into a training and validation part
train_set = MNIST(root=DATASET_PATH, train=True, transform=transform, download=True)

# Loading the test set
test_set = MNIST(root=DATASET_PATH, train=False, transform=transform, download=True)

# We define a set of data loaders that we can use for various purposes later.
# Note that for actually training a model, we will use different data loaders
# with a lower batch size.
train_loader = data.DataLoader(train_set, batch_size=128, shuffle=True,  drop_last=True,␣
↪ num_workers=4, pin_memory=True)
test_loader  = data.DataLoader(test_set,  batch_size=256, shuffle=False, drop_last=False,
↪ num_workers=4)
```

CNN Model

First, we implement our CNN model. The MNIST images are of size 28x28, hence we only need a small model. As an example, we will apply several convolutions with stride 2 that downscale the images. If you are interested, you can also use a deeper model such as a small ResNet, but for simplicity, we will stick with the tiny network.

It is a good practice to use a smooth activation function like Swish instead of ReLU in the energy model. This is because we will rely on the gradients we get back with respect to the input image, which should not be sparse.

[4]:
```
class Swish(nn.Module):

    def forward(self, x):
        return x * torch.sigmoid(x)


class CNNModel(nn.Module):

    def __init__(self, hidden_features=32, out_dim=1, **kwargs):
```

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```
        super().__init__()
        # We increase the hidden dimension over layers. Here pre-calculated for␣
↪simplicity.
        c_hid1 = hidden_features//2
        c_hid2 = hidden_features
        c_hid3 = hidden_features*2

        # Series of convolutions and Swish activation functions
        self.cnn_layers = nn.Sequential(
                nn.Conv2d(1, c_hid1, kernel_size=5, stride=2, padding=4), # [16x16] -␣
↪Larger padding to get 32x32 image
                Swish(),
                nn.Conv2d(c_hid1, c_hid2, kernel_size=3, stride=2, padding=1), #  [8x8]
                Swish(),
                nn.Conv2d(c_hid2, c_hid3, kernel_size=3, stride=2, padding=1), # [4x4]
                Swish(),
                nn.Conv2d(c_hid3, c_hid3, kernel_size=3, stride=2, padding=1), # [2x2]
                Swish(),
                nn.Flatten(),
                nn.Linear(c_hid3*4, c_hid3),
                Swish(),
                nn.Linear(c_hid3, out_dim)
        )

    def forward(self, x):
        x = self.cnn_layers(x).squeeze(dim=-1)
        return x
```

In the rest of the notebook, the output of the model will actually not represent $E_\theta(\mathbf{x})$, but $-E_\theta(\mathbf{x})$. This is a standard implementation practice for energy-based models, as some people also write the energy probability density as $q_\theta(\mathbf{x}) = \frac{\exp(f_\theta(\mathbf{x}))}{Z_\theta}$. In that case, the model would actually represent $f_\theta(\mathbf{x})$. In the training loss etc., we need to be careful to not switch up the signs.

Sampling buffer

In the next part, we look at the training with sampled elements. To use the contrastive divergence objective, we need to generate samples during training. Previous work has shown that due to the high dimensionality of images, we need a lot of iterations inside the MCMC sampling to obtain reasonable samples. However, there is a training trick that significantly reduces the sampling cost: using a sampling buffer. The idea is that we store the samples of the last couple of batches in a buffer, and re-use those as the starting point of the MCMC algorithm for the next batches. This reduces the sampling cost because the model requires a significantly lower number of steps to converge to reasonable samples. However, to not solely rely on previous samples and allow novel samples as well, we re-initialize 5% of our samples from scratch (random noise between -1 and 1).

Below, we implement the sampling buffer. The function `sample_new_exmps` returns a new batch of "fake" images. We refer to those as fake images because they have been generated, but are not actually part of the dataset. As mentioned before, we use initialize 5% randomly, and 95% are randomly picked from our buffer. On this initial batch, we perform MCMC for 60 iterations to improve the image quality and come closer to samples from $q_\theta(\mathbf{x})$. In the function `generate_samples`, we implemented the MCMC for images. Note that the hyperparameters of `step_size`, `steps`, the noise standard deviation σ are specifically set for MNIST, and need to be finetuned for a different dataset if you want to use such.

[5]:
```
class Sampler:

    def __init__(self, model, img_shape, sample_size, max_len=8192):
        """
        Inputs:
            model - Neural network to use for modeling E_theta
            img_shape - Shape of the images to model
            sample_size - Batch size of the samples
            max_len - Maximum number of data points to keep in the buffer
        """
        super().__init__()
        self.model = model
        self.img_shape = img_shape
        self.sample_size = sample_size
        self.max_len = max_len
        self.examples = [(torch.rand((1,)+img_shape)*2-1) for _ in range(self.sample_
↪size)]

    def sample_new_exmps(self, steps=60, step_size=10):
        """
        Function for getting a new batch of "fake" images.
        Inputs:
            steps - Number of iterations in the MCMC algorithm
            step_size - Learning rate nu in the algorithm above
        """
        # Choose 95% of the batch from the buffer, 5% generate from scratch
        n_new = np.random.binomial(self.sample_size, 0.05)
        rand_imgs = torch.rand((n_new,) + self.img_shape) * 2 - 1
        old_imgs = torch.cat(random.choices(self.examples, k=self.sample_size-n_new),␣
↪dim=0)
        inp_imgs = torch.cat([rand_imgs, old_imgs], dim=0).detach().to(device)

        # Perform MCMC sampling
        inp_imgs = Sampler.generate_samples(self.model, inp_imgs, steps=steps, step_
↪size=step_size)

        # Add new images to the buffer and remove old ones if needed
        self.examples = list(inp_imgs.to(torch.device("cpu")).chunk(self.sample_size,␣
↪dim=0)) + self.examples
        self.examples = self.examples[:self.max_len]
        return inp_imgs

    @staticmethod
    def generate_samples(model, inp_imgs, steps=60, step_size=10, return_img_per_
↪step=False):
        """
        Function for sampling images for a given model.
        Inputs:
            model - Neural network to use for modeling E_theta
            inp_imgs - Images to start from for sampling. If you want to generate new␣
↪images, enter noise between -1 and 1.
            steps - Number of iterations in the MCMC algorithm.
            step_size - Learning rate nu in the algorithm above
```

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```
            return_img_per_step - If True, we return the sample at every iteration of␣
↪the MCMC
        """
        # Before MCMC: set model parameters to "required_grad=False"
        # because we are only interested in the gradients of the input.
        is_training = model.training
        model.eval()
        for p in model.parameters():
            p.requires_grad = False
        inp_imgs.requires_grad = True

        # Enable gradient calculation if not already the case
        had_gradients_enabled = torch.is_grad_enabled()
        torch.set_grad_enabled(True)

        # We use a buffer tensor in which we generate noise each loop iteration.
        # More efficient than creating a new tensor every iteration.
        noise = torch.randn(inp_imgs.shape, device=inp_imgs.device)

        # List for storing generations at each step (for later analysis)
        imgs_per_step = []

        # Loop over K (steps)
        for _ in range(steps):
            # Part 1: Add noise to the input.
            noise.normal_(0, 0.005)
            inp_imgs.data.add_(noise.data)
            inp_imgs.data.clamp_(min=-1.0, max=1.0)

            # Part 2: calculate gradients for the current input.
            out_imgs = -model(inp_imgs)
            out_imgs.sum().backward()
            inp_imgs.grad.data.clamp_(-0.03, 0.03) # For stabilizing and preventing too␣
↪high gradients

            # Apply gradients to our current samples
            inp_imgs.data.add_(-step_size * inp_imgs.grad.data)
            inp_imgs.grad.detach_()
            inp_imgs.grad.zero_()
            inp_imgs.data.clamp_(min=-1.0, max=1.0)

            if return_img_per_step:
                imgs_per_step.append(inp_imgs.clone().detach())

        # Reactivate gradients for parameters for training
        for p in model.parameters():
            p.requires_grad = True
        model.train(is_training)

        # Reset gradient calculation to setting before this function
        torch.set_grad_enabled(had_gradients_enabled)
```

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```
        if return_img_per_step:
            return torch.stack(imgs_per_step, dim=0)
        else:
            return inp_imgs
```

The idea of the buffer becomes a bit clearer in the following algorithm.

Training algorithm

With the sampling buffer being ready, we can complete our training algorithm. Below is shown a summary of the full training algorithm of an energy model on image modeling:

The first few statements in each training iteration concern the sampling of the real and fake data, as we have seen above with the sample buffer. Next, we calculate the contrastive divergence objective using our energy model E_θ. However, one additional training trick we need is to add a regularization loss on the output of E_θ. As the output of the network is not constrained and adding a large bias or not to the output doesn't change the contrastive divergence loss, we need to ensure somehow else that the output values are in a reasonable range. Without the regularization loss, the output values will fluctuate in a very large range. With this, we ensure that the values for the real data are around 0, and the fake data likely slightly lower (for noise or outliers the score can be still significantly lower). As the regularization loss is less important than the Contrastive Divergence, we have a weight factor α which is usually quite some smaller than 1. Finally, we perform an update step with an optimizer on the combined loss and add the new samples to the buffer.

Below, we put this training dynamic into a PyTorch Lightning module. Remember that, since we model $f_\theta(x) = -E_\theta(x)$, we need to be careful with switching all important signs, e.g. in the loss function.

[6]:
```
class DeepEnergyModel(pl.LightningModule):

    def __init__(self, img_shape, batch_size, alpha=0.1, lr=1e-4, beta1=0.0, **CNN_args):
        super().__init__()
        self.save_hyperparameters()

        self.cnn = CNNModel(**CNN_args)
        self.sampler = Sampler(self.cnn, img_shape=img_shape, sample_size=batch_size)
        self.example_input_array = torch.zeros(1, *img_shape)

    def forward(self, x):
        z = self.cnn(x)
        return z

    def configure_optimizers(self):
        # Energy models can have issues with momentum as the loss surfaces changes with␣
↪its parameters.
        # Hence, we set it to 0 by default.
        optimizer = optim.Adam(self.parameters(), lr=self.hparams.lr, betas=(self.
↪hparams.beta1, 0.999))
        scheduler = optim.lr_scheduler.StepLR(optimizer, 1, gamma=0.97) # Exponential␣
↪decay over epochs
        return [optimizer], [scheduler]

    def training_step(self, batch, batch_idx):
        # We add minimal noise to the original images to prevent the model from focusing␣
↪on purely "clean" inputs
```

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```
        real_imgs, _ = batch
        small_noise = torch.randn_like(real_imgs) * 0.005
        real_imgs.add_(small_noise).clamp_(min=-1.0, max=1.0)

        # Obtain samples
        fake_imgs = self.sampler.sample_new_exmps(steps=60, step_size=10)

        # Predict energy score for all images
        inp_imgs = torch.cat([real_imgs, fake_imgs], dim=0)
        real_out, fake_out = self.cnn(inp_imgs).chunk(2, dim=0)

        # Calculate losses
        reg_loss = self.hparams.alpha * (real_out ** 2 + fake_out ** 2).mean()
        cdiv_loss = fake_out.mean() - real_out.mean()
        loss = reg_loss + cdiv_loss

        # Logging
        self.log('loss', loss)
        self.log('loss_regularization', reg_loss)
        self.log('loss_contrastive_divergence', cdiv_loss)
        self.log('metrics_avg_real', real_out.mean())
        self.log('metrics_avg_fake', fake_out.mean())
        return loss

    def validation_step(self, batch, batch_idx):
        # For validating, we calculate the contrastive divergence between purely random␣
↪images and unseen examples
        # Note that the validation/test step of energy-based models depends on what we␣
↪are interested in the model
        real_imgs, _ = batch
        fake_imgs = torch.rand_like(real_imgs) * 2 - 1

        inp_imgs = torch.cat([real_imgs, fake_imgs], dim=0)
        real_out, fake_out = self.cnn(inp_imgs).chunk(2, dim=0)

        cdiv = fake_out.mean() - real_out.mean()
        self.log('val_contrastive_divergence', cdiv)
        self.log('val_fake_out', fake_out.mean())
        self.log('val_real_out', real_out.mean())
```

We do not implement a test step because energy-based, generative models are usually not evaluated on a test set. The validation step however is used to get an idea of the difference between ennergy/likelihood of random images to unseen examples of the dataset. Alternative test steps would be to generate new images and evaluate how realistic they are based on FID or Inception score, or try to denoise images.

Callbacks

To track the performance of our model during training, we will make extensive use of PyTorch Lightning's callback framework. Remember that callbacks can be used for running small functions at any point of the training, for instance after finishing an epoch. Here, we will use three different callbacks we define ourselves.

The first callback, called `GenerateCallback`, is used for adding image generations to the model during training. After every N epochs (usually $N = 5$ to reduce output to TensorBoard), we take a small batch of random images and perform many MCMC iterations until the model's generation converges. Compared to the training that used 60 iterations, we use 256 here because (1) we only have to do it once compared to the training that has to do it every iteration, and (2) we do not start from a buffer here, but from scratch. It is implemented as follows:

[7]:
```
class GenerateCallback(pl.Callback):

    def __init__(self, batch_size=8, vis_steps=8, num_steps=256, every_n_epochs=5):
        super().__init__()
        self.batch_size = batch_size         # Number of images to generate
        self.vis_steps = vis_steps           # Number of steps within generation to␣
↪visualize
        self.num_steps = num_steps           # Number of steps to take during generation
        self.every_n_epochs = every_n_epochs # Only save those images every N epochs␣
↪(otherwise tensorboard gets quite large)

    def on_epoch_end(self, trainer, pl_module):
        # Skip for all other epochs
        if trainer.current_epoch % self.every_n_epochs == 0:
            # Generate images
            imgs_per_step = self.generate_imgs(pl_module)
            # Plot and add to tensorboard
            for i in range(imgs_per_step.shape[1]):
                step_size = self.num_steps // self.vis_steps
                imgs_to_plot = imgs_per_step[step_size-1::step_size,i]
                grid = torchvision.utils.make_grid(imgs_to_plot, nrow=imgs_to_plot.
↪shape[0], normalize=True, range=(-1,1))
                trainer.logger.experiment.add_image(f"generation_{i}", grid, global_
↪step=trainer.current_epoch)

    def generate_imgs(self, pl_module):
        pl_module.eval()
        start_imgs = torch.rand((self.batch_size,) + pl_module.hparams["img_shape"]).
↪to(pl_module.device)
        start_imgs = start_imgs * 2 - 1
        torch.set_grad_enabled(True)  # Tracking gradients for sampling necessary
        imgs_per_step = Sampler.generate_samples(pl_module.cnn, start_imgs, steps=self.
↪num_steps, step_size=10, return_img_per_step=True)
        torch.set_grad_enabled(False)
        pl_module.train()
        return imgs_per_step
```

The second callback is called `SamplerCallback`, and simply adds a randomly picked subset of images in the sampling buffer to the TensorBoard. This helps to understand what images are currently shown to the model as "fake".

[8]:
```
class SamplerCallback(pl.Callback):
```

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```
    def __init__(self, num_imgs=32, every_n_epochs=5):
        super().__init__()
        self.num_imgs = num_imgs             # Number of images to plot
        self.every_n_epochs = every_n_epochs # Only save those images every N epochs␣
↪(otherwise tensorboard gets quite large)

    def on_epoch_end(self, trainer, pl_module):
        if trainer.current_epoch % self.every_n_epochs == 0:
            exmp_imgs = torch.cat(random.choices(pl_module.sampler.examples, k=self.num_
↪imgs), dim=0)
            grid = torchvision.utils.make_grid(exmp_imgs, nrow=4, normalize=True,␣
↪range=(-1,1))
            trainer.logger.experiment.add_image("sampler", grid, global_step=trainer.
↪current_epoch)
```

Finally, our last callback is `OutlierCallback`. This callback evaluates the model by recording the (negative) energy assigned to random noise. While our training loss is almost constant across iterations, this score is likely showing the progress of the model to detect "outliers".

[9]:
```
class OutlierCallback(pl.Callback):

    def __init__(self, batch_size=1024):
        super().__init__()
        self.batch_size = batch_size

    def on_epoch_end(self, trainer, pl_module):
        with torch.no_grad():
            pl_module.eval()
            rand_imgs = torch.rand((self.batch_size,) + pl_module.hparams["img_shape"]).
↪to(pl_module.device)
            rand_imgs = rand_imgs * 2 - 1.0
            rand_out = pl_module.cnn(rand_imgs).mean()
            pl_module.train()

        trainer.logger.experiment.add_scalar("rand_out", rand_out, global_step=trainer.
↪current_epoch)
```

Running the model

Finally, we can add everything together to create our final training function. The function is very similar to any other PyTorch Lightning training function we have seen so far. However, there is the small difference of that we do not test the model on a test set because we will analyse the model afterward by checking its prediction and ability to perform outlier detection.

[10]:
```
def train_model(**kwargs):
    # Create a PyTorch Lightning trainer with the generation callback
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, "MNIST"),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=60,
                         gradient_clip_val=0.1,
```

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```
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="min",␣
↪monitor='val_contrastive_divergence'),
                                    GenerateCallback(every_n_epochs=5),
                                    SamplerCallback(every_n_epochs=5),
                                    OutlierCallback(),
                                    LearningRateMonitor("epoch")
                                   ])
    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, "MNIST.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = DeepEnergyModel.load_from_checkpoint(pretrained_filename)
    else:
        pl.seed_everything(42)
        model = DeepEnergyModel(**kwargs)
        trainer.fit(model, train_loader, test_loader)
        model = DeepEnergyModel.load_from_checkpoint(trainer.checkpoint_callback.best_
↪model_path)
    # No testing as we are more interested in other properties
    return model
```

[11]:
```
model = train_model(img_shape=(1,28,28),
                    batch_size=train_loader.batch_size,
                    lr=1e-4,
                    beta1=0.0)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

4.22.3 Analysis

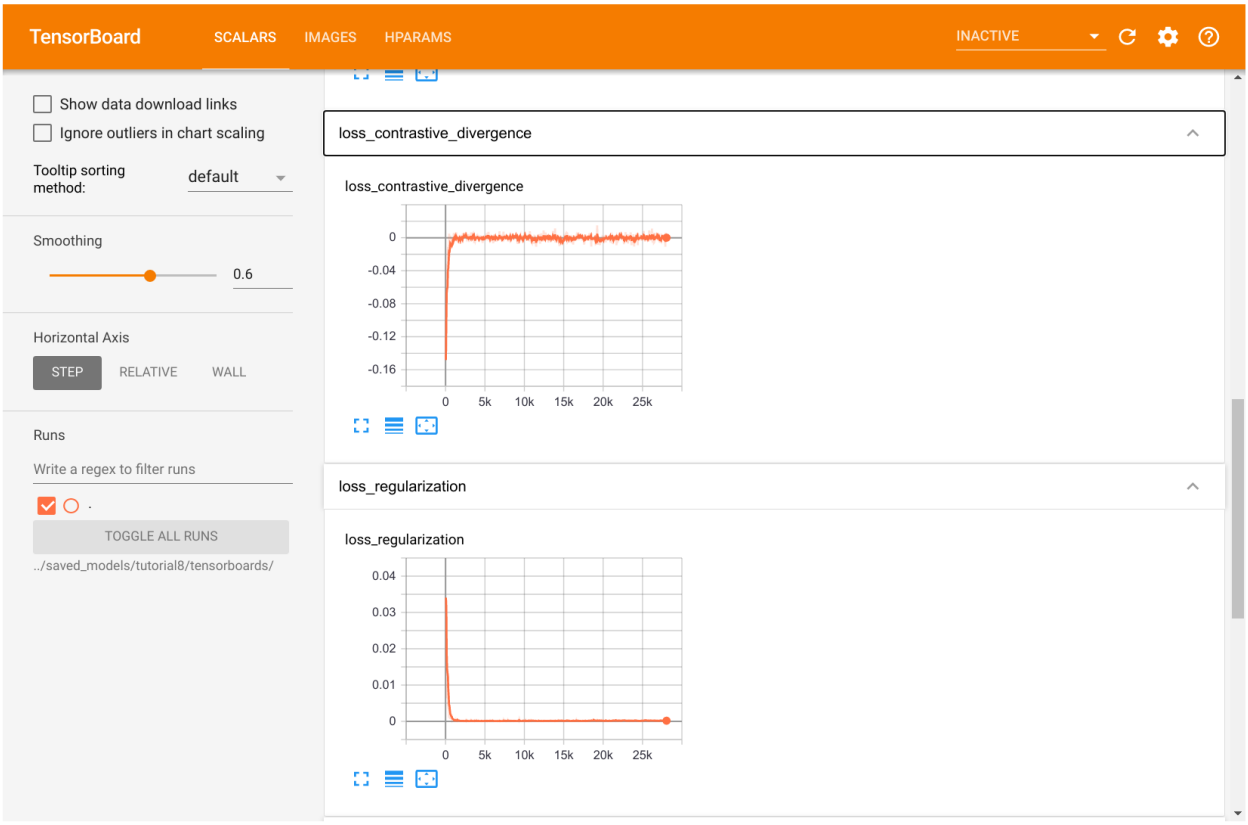
In the last part of the notebook, we will try to take the trained energy-based generative model, and analyse its properties.

TensorBoard

The first thing we can look at is the TensorBoard generate during training. This can help us to understand the training dynamic even better, and shows potential issues. Let's load the TensorBoard below:

[12]:
```
# Import tensorboard
%load_ext tensorboard
```

[13]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH!
%tensorboard --logdir ../saved_models/tutorial8/tensorboards/
```



We see that the contrastive divergence as well as the regularization converge quickly to 0. However, the training continues although the loss is always close to zero. This is because our "training" data changes with the model by sampling. The progress of training can be best measured by looking at the samples across iterations, and the score for random images that decreases constantly over time.

Image Generation

Another way of evaluating generative models is by sampling a few generated images. Generative models need to be good at generating realistic images as this truely shows that they have modeled the true data distribution. Thus, let's sample a few images of the model below:

[14]:
```
model.to(device)
pl.seed_everything(43)
callback = GenerateCallback(batch_size=4, vis_steps=8, num_steps=256)
imgs_per_step = callback.generate_imgs(model)
imgs_per_step = imgs_per_step.cpu()
```

The characteristic of sampling with energy-based models is that they require the iterative MCMC algorithm. To gain an insight in how the images change over iterations, we plot a few intermediate samples in the MCMC as well:

[15]:
```
for i in range(imgs_per_step.shape[1]):
    step_size = callback.num_steps // callback.vis_steps
    imgs_to_plot = imgs_per_step[step_size-1::step_size,i]
    imgs_to_plot = torch.cat([imgs_per_step[0:1,i],imgs_to_plot], dim=0)
    grid = torchvision.utils.make_grid(imgs_to_plot, nrow=imgs_to_plot.shape[0],␣
↪normalize=True, range=(-1,1), pad_value=0.5, padding=2)
```

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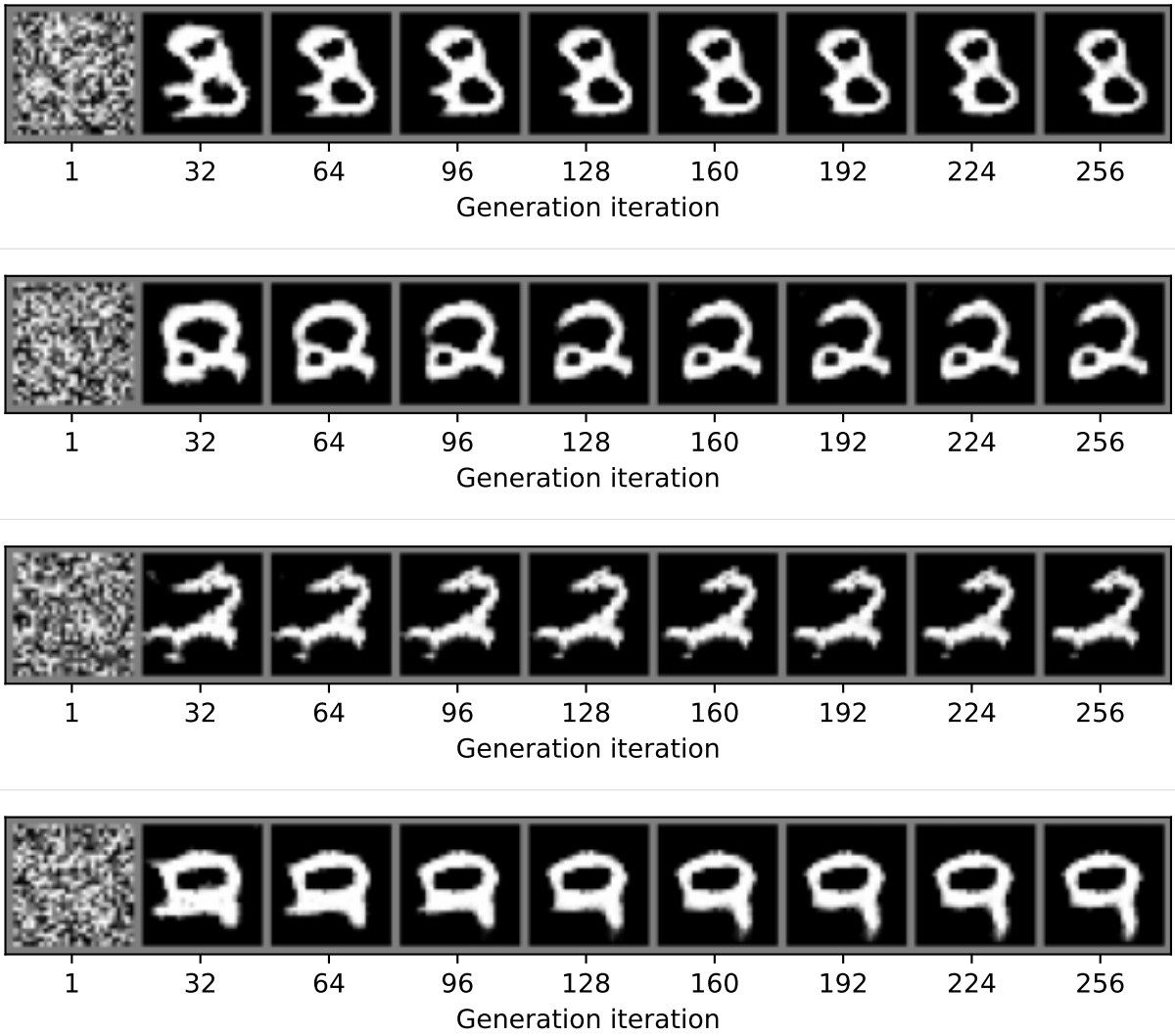
```
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(8,8))
    plt.imshow(grid)
    plt.xlabel("Generation iteration")
    plt.xticks([(imgs_per_step.shape[-1]+2)*(0.5+j) for j in range(callback.vis_
↪steps+1)],
               labels=[1] + list(range(step_size,imgs_per_step.shape[0]+1,step_size)))
    plt.yticks([])
    plt.show()
```



We see that although starting from noise in the very first step, the sampling algorithm obtains reasonable shapes after only 32 steps. Over the next 200 steps, the shapes become clearer and changed towards realistic digits. The specific samples can differ when you run the code on Colab, hence the following description is specific to the plots shown on the website. The first row shows an 8, where we remove unnecessary white parts over iterations. The transformation across iterations can be seen at best for the second sample, which creates a digit of 2. While the first sample after 32 iterations looks a bit like a digit, but not really, the sample is transformed more and more to a typical image of the digit 2.

Out-of-distribution detection

A very common and strong application of energy-based models is out-of-distribution detection (sometimes referred to as "anomaly" detection). As more and more deep learning models are applied in production and applications, a crucial aspect of these models is to know what the models don't know. Deep learning models are usually overconfident, meaning that they classify even random images sometimes with 100% probability. Clearly, this is not something that we want to see in applications. Energy-based models can help with this problem because they are trained to detect images that do not fit the training dataset distribution. Thus, in those applications, you could train an energy-based model along with the classifier, and only output predictions if the energy-based models assign a (unnormalized) probability higher than δ to the image. You can actually combine classifiers and energy-based objectives in a single model, as proposed in this paper.

In this part of the analysis, we want to test the out-of-distribution capability of our energy-based model. Remember that a lower output of the model denotes a low probability. Thus, we hope to see low scores if we enter random noise to the model:

[16]:
```
with torch.no_grad():
    rand_imgs = torch.rand((128,) + model.hparams.img_shape).to(model.device)
    rand_imgs = rand_imgs * 2 - 1.0
    rand_out = model.cnn(rand_imgs).mean()
    print(f"Average score for random images: {rand_out.item():4.2f}")
```

```
Average score for random images: -17.88
```

As we hoped, the model assigns very low probability to those noisy images. As another reference, let's look at predictions for a batch of images from the training set:

[17]:
```
with torch.no_grad():
    train_imgs,_ = next(iter(train_loader))
    train_imgs = train_imgs.to(model.device)
    train_out = model.cnn(train_imgs).mean()
    print(f"Average score for training images: {train_out.item():4.2f}")
```

```
Average score for training images: -0.00
```

The scores are close to 0 because of the regularization objective that was added to the training. So clearly, the model can distinguish between noise and real digits. However, what happens if we change the training images a little, and see which ones gets a very low score?

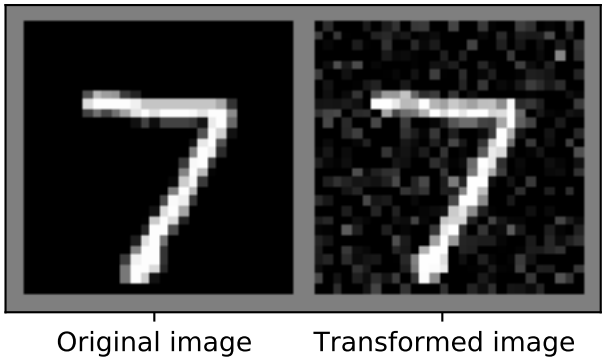
[18]:
```
@torch.no_grad()
def compare_images(img1, img2):
    imgs = torch.stack([img1, img2], dim=0).to(model.device)
    score1, score2 = model.cnn(imgs).cpu().chunk(2, dim=0)
    grid = torchvision.utils.make_grid([img1.cpu(), img2.cpu()], nrow=2, normalize=True,␣
↪range=(-1,1), pad_value=0.5, padding=2)
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(4,4))
    plt.imshow(grid)
    plt.xticks([(img1.shape[2]+2)*(0.5+j) for j in range(2)],
               labels=["Original image", "Transformed image"])
    plt.yticks([])
    plt.show()
    print(f"Score original image: {score1.item():4.2f}")
    print(f"Score transformed image: {score2.item():4.2f}")
```

We use a random test image for this. Feel free to change it to experiment with the model yourself.

[19]:
```
test_imgs, _ = next(iter(test_loader))
exmp_img = test_imgs[0].to(model.device)
```

The first transformation is to add some random noise to the image:

[20]:
```
img_noisy = exmp_img + torch.randn_like(exmp_img) * 0.3
img_noisy.clamp_(min=-1.0, max=1.0)
compare_images(exmp_img, img_noisy)
```

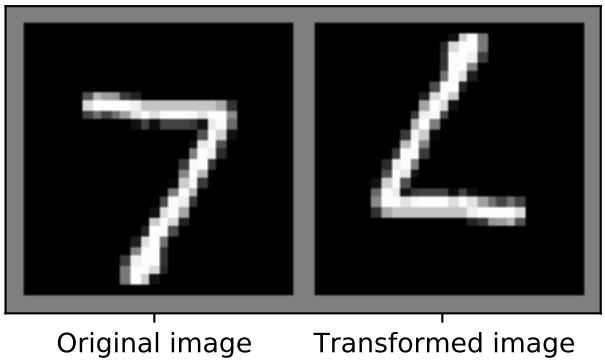



```
Score original image: 0.03
Score transformed image: -0.07
```

We can see that the score considerably drops. Hence, the model can detect random Gaussian noise on the image. This is also to expect as initially, the "fake" samples are pure noise images.

Next, we flip an image and check how this influences the score:

[21]:
```
img_flipped = exmp_img.flip(dims=(1,2))
compare_images(exmp_img, img_flipped)
```

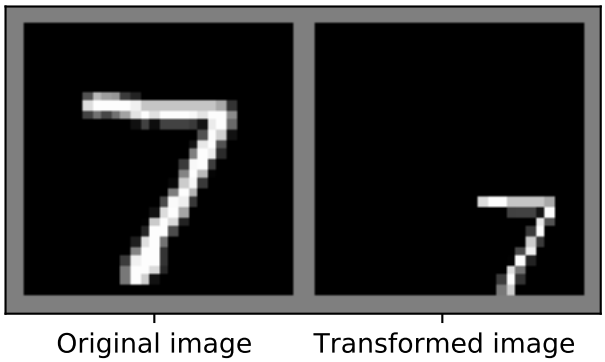



```
Score original image: 0.03
Score transformed image: -0.00
```

If the digit can only be read in this way, for example, the 7, then we can see that the score drops. However, the score only drops slightly. This is likely because of the small size of our model. Keep in mind that generative modeling is a much harder task than classification, as we do not only need to distinguish between classes but learn **all** details/characteristics of the digits. With a deeper model, this could eventually be captured better (but at the cost of greater training instability).

Finally, we check what happens if we reduce the digit significantly in size:

[22]:
```
img_tiny = torch.zeros_like(exmp_img)-1
img_tiny[:,exmp_img.shape[1]//2:,exmp_img.shape[2]//2:] = exmp_img[:,::2,::2]
compare_images(exmp_img, img_tiny)
```




```
Score original image: 0.03
Score transformed image: -0.02
```

The score again drops but not by a large margin, although digits in the MNIST dataset usually are much larger.

Overall, we can conclude that our model is good for detecting Gaussian noise and smaller transformations to existing digits. Nonetheless, to obtain a very good out-of-distribution model, we would need to train deeper models and for more iterations.

Instability

Finally, we should discuss the possible instabilities of energy-based models, in particular for the example of image generation that we have implemented in this notebook. In the process of hyperparameter search for this notebook, there have been several models that diverged. Divergence in energy-based models means that the models assign a high probability to examples of the training set which is a good thing. However, at the same time, the sampling algorithm fails and only generates noise images that obtain minimal probability scores. This happens because the model has created many local maxima in which the generated noise images fall. The energy surface over which we calculate the gradients to reach data points with high probability has "diverged" and is not useful for our MCMC sampling.

Besides finding the optimal hyperparameters, a common trick in energy-based models is to reload stable checkpoints. If we detect that the model is diverging, we stop the training, load the model from one epoch ago where it did not diverge yet. Afterward, we continue training and hope that with a different seed the model is not diverging again. Nevertheless, this should be considered as the "last hope" for stabilizing the models, and careful hyperparameter tuning is the better way to do so. Sensitive hyperparameters include `step_size`, `steps` and the noise standard deviation in the sampler, and the learning rate and feature dimensionality in the CNN model.

4.22.4 Conclusion

In this tutorial, we have discussed energy-based models for generative modeling. The concept relies on the idea that any strictly positive function can be turned into a probability distribution by normalizing over the whole dataset. As this is not reasonable to calculate for high dimensional data like images, we train the model using contrastive divergence and sampling via MCMC. While the idea allows us to turn any neural network into an energy-based model, we have seen that there are multiple training tricks needed to stabilize the training. Furthermore, the training time of these models is relatively long as, during every training iteration, we need to sample new "fake" images, even with a sampling buffer. In the next lectures and assignment, we will see different generative models (e.g. VAE, GAN, NF) that allow us to do generative modeling more stably, but with the cost of more parameters.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.23 Tutorial 9: Deep Autoencoders

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will take a closer look at autoencoders (AE). Autoencoders are trained on encoding input data such as images into a smaller feature vector, and afterward, reconstruct it by a second neural network, called a decoder. The feature vector is called the "bottleneck" of the network as we aim to compress the input data into a smaller amount of features. This property is useful in many applications, in particular in compressing data or comparing images on a metric beyond pixel-level comparisons. Besides learning about the autoencoder framework, we will also see the "deconvolution" (or transposed convolution) operator in action for scaling up feature maps in height and width. Such deconvolution networks are necessary wherever we start from a small feature vector and need to output an image of full size (e.g. in VAE, GANs, or super-resolution applications).

First of all, we again import most of our standard libraries. We will use PyTorch Lightning to reduce the training code overhead.

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
```

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```
import seaborn as sns
sns.reset_orig()
sns.set()

## Progress bar
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import CIFAR10
from torchvision import transforms
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Tensorboard extension (for visualization purposes later)
from torch.utils.tensorboard import SummaryWriter
%load_ext tensorboard

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial9"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)
```

We have 4 pretrained models that we have to download. Remember the adjust the variables `DATASET_PATH` and `CHECKPOINT_PATH` if needed.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial9/"
```

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```
# Files to download
pretrained_files = ["cifar10_64.ckpt", "cifar10_128.ckpt", "cifar10_256.ckpt", "cifar10_
↪384.ckpt"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

In this tutorial, we work with the CIFAR10 dataset. In CIFAR10, each image has 3 color channels and is 32x32 pixels large. As autoencoders do not have the constrain of modeling images probabilistic, we can work on more complex image data (i.e. 3 color channels instead of black-and-white) much easier than for VAEs. In case you have downloaded CIFAR10 already in a different directory, make sure to set DATASET_PATH accordingly to prevent another download.

In contrast to previous tutorials on CIFAR10 like Tutorial 5 (CNN classification), we do not normalize the data explicitly with a mean of 0 and std of 1, but roughly estimate it scaling the data between -1 and 1. This is because limiting the range will make our task of predicting/reconstructing images easier.

[3]:
```
# Transformations applied on each image => only make them a tensor
transform = transforms.Compose([transforms.ToTensor(),
                                transforms.Normalize((0.5,),(0.5,))])

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=transform,␣
↪download=True)
pl.seed_everything(42)
train_set, val_set = torch.utils.data.random_split(train_dataset, [45000, 5000])

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=transform, download=True)

# We define a set of data loaders that we can use for various purposes later.
train_loader = data.DataLoader(train_set, batch_size=256, shuffle=True, drop_last=True,␣
↪pin_memory=True, num_workers=4)
val_loader = data.DataLoader(val_set, batch_size=256, shuffle=False, drop_last=False,␣
↪num_workers=4)
test_loader = data.DataLoader(test_set, batch_size=256, shuffle=False, drop_last=False,␣
↪num_workers=4)

def get_train_images(num):
    return torch.stack([train_dataset[i][0] for i in range(num)], dim=0)
```

```
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```

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4.23.1 Building the autoencoder

In general, an autoencoder consists of an **encoder** that maps the input x to a lower-dimensional feature vector z, and a **decoder** that reconstructs the input $\hat{x}$ from z. We train the model by comparing x to $\hat{x}$ and optimizing the parameters to increase the similarity between x and $\hat{x}$. See below for a small illustration of the autoencoder framework.

We first start by implementing the encoder. The encoder effectively consists of a deep convolutional network, where we scale down the image layer-by-layer using strided convolutions. After downscaling the image three times, we flatten the features and apply linear layers. The latent representation z is therefore a vector of size d which can be flexibly selected.

[4]:
```
class Encoder(nn.Module):

    def __init__(self,
                 num_input_channels : int,
                 base_channel_size : int,
                 latent_dim : int,
                 act_fn : object = nn.GELU):
        """
        Inputs:
            - num_input_channels : Number of input channels of the image. For CIFAR, this parameter is 3
            - base_channel_size : Number of channels we use in the first convolutional layers. Deeper layers might use a duplicate of it.
            - latent_dim : Dimensionality of latent representation z
            - act_fn : Activation function used throughout the encoder network
        """
        super().__init__()
        c_hid = base_channel_size
        self.net = nn.Sequential(
            nn.Conv2d(num_input_channels, c_hid, kernel_size=3, padding=1, stride=2), # 32x32 => 16x16
            act_fn(),
            nn.Conv2d(c_hid, c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.Conv2d(c_hid, 2*c_hid, kernel_size=3, padding=1, stride=2), # 16x16 => 8x8
            act_fn(),
            nn.Conv2d(2*c_hid, 2*c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.Conv2d(2*c_hid, 2*c_hid, kernel_size=3, padding=1, stride=2), # 8x8 => 4x4
            act_fn(),
            nn.Flatten(), # Image grid to single feature vector
            nn.Linear(2*16*c_hid, latent_dim)
        )

    def forward(self, x):
        return self.net(x)
```

Note that we do not apply Batch Normalization here. This is because we want the encoding of each image to be independent of all the other images. Otherwise, we might introduce correlations into the encoding or decoding that we do not want to have. In some implementations, you still can see Batch Normalization being used, because it can also serve as a form of regularization. Nevertheless, the better practice is to go with other normalization techniques if necessary like Instance Normalization or Layer Normalization. Given the small size of the model, we can neglect normalization for now.

The decoder is a mirrored, flipped version of the encoder. The only difference is that we replace strided convolutions by transposed convolutions (i.e. deconvolutions) to upscale the features. Transposed convolutions can be imagined as adding the stride to the input instead of the output, and can thus upscale the input. For an illustration of a `nn.ConvTranspose2d` layer with kernel size 3, stride 2, and padding 1, see below (figure credit - Vincent Dumoulin and Francesco Visin):

You see that for an input of size 3×3, we obtain an output of 5×5. However, to truly have a reverse operation of the convolution, we need to ensure that the layer scales the input shape by a factor of 2 (e.g. $4 \times 4 \rightarrow 8 \times 8$). For this, we can specify the parameter `output_padding` which adds additional values to the output shape. Note that we do not perform zero-padding with this, but rather increase the output shape for calculation.

Overall, the decoder can be implemented as follows:

[5]:
```
class Decoder(nn.Module):

    def __init__(self,
                 num_input_channels : int,
                 base_channel_size : int,
                 latent_dim : int,
                 act_fn : object = nn.GELU):
        """
        Inputs:
            - num_input_channels : Number of channels of the image to reconstruct. For␣
↪CIFAR, this parameter is 3
            - base_channel_size : Number of channels we use in the last convolutional␣
↪layers. Early layers might use a duplicate of it.
            - latent_dim : Dimensionality of latent representation z
            - act_fn : Activation function used throughout the decoder network
        """
        super().__init__()
        c_hid = base_channel_size
        self.linear = nn.Sequential(
            nn.Linear(latent_dim, 2*16*c_hid),
            act_fn()
        )
        self.net = nn.Sequential(
            nn.ConvTranspose2d(2*c_hid, 2*c_hid, kernel_size=3, output_padding=1,␣
↪padding=1, stride=2), # 4x4 => 8x8
            act_fn(),
            nn.Conv2d(2*c_hid, 2*c_hid, kernel_size=3, padding=1),
            act_fn(),
            nn.ConvTranspose2d(2*c_hid, c_hid, kernel_size=3, output_padding=1,␣
↪padding=1, stride=2), # 8x8 => 16x16
            act_fn(),
            nn.Conv2d(c_hid, c_hid, kernel_size=3, padding=1),
            act_fn(),
```

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```
            nn.ConvTranspose2d(c_hid, num_input_channels, kernel_size=3, output_
↪padding=1, padding=1, stride=2), # 16x16 => 32x32
            nn.Tanh() # The input images is scaled between -1 and 1, hence the output␣
↪has to be bounded as well
        )

    def forward(self, x):
        x = self.linear(x)
        x = x.reshape(x.shape[0], -1, 4, 4)
        x = self.net(x)
        return x
```

The encoder and decoder networks we chose here are relatively simple. Usually, more complex networks are applied, especially when using a ResNet-based architecture. For example, see VQ-VAE and NVAE (although the papers discuss architectures for VAEs, they can equally be applied to standard autoencoders).

In a final step, we add the encoder and decoder together into the autoencoder architecture. We define the autoencoder as PyTorch Lightning Module to simplify the needed training code:

[6]:
```
class Autoencoder(pl.LightningModule):

    def __init__(self,
                 base_channel_size: int,
                 latent_dim: int,
                 encoder_class : object = Encoder,
                 decoder_class : object = Decoder,
                 num_input_channels: int = 3,
                 width: int = 32,
                 height: int = 32):
        super().__init__()
        # Saving hyperparameters of autoencoder
        self.save_hyperparameters()
        # Creating encoder and decoder
        self.encoder = encoder_class(num_input_channels, base_channel_size, latent_dim)
        self.decoder = decoder_class(num_input_channels, base_channel_size, latent_dim)
        # Example input array needed for visualizing the graph of the network
        self.example_input_array = torch.zeros(2, num_input_channels, width, height)

    def forward(self, x):
        """
        The forward function takes in an image and returns the reconstructed image
        """
        z = self.encoder(x)
        x_hat = self.decoder(z)
        return x_hat

    def _get_reconstruction_loss(self, batch):
        """
        Given a batch of images, this function returns the reconstruction loss (MSE in␣
↪our case)
        """
        x, _ = batch # We do not need the labels
        x_hat = self.forward(x)
```

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```
        loss = F.mse_loss(x, x_hat, reduction="none")
        loss = loss.sum(dim=[1,2,3]).mean(dim=[0])
        return loss

    def configure_optimizers(self):
        optimizer = optim.Adam(self.parameters(), lr=1e-3)
        # Using a scheduler is optional but can be helpful.
        # The scheduler reduces the LR if the validation performance hasn't improved for␣
↪the last N epochs
        scheduler = optim.lr_scheduler.ReduceLROnPlateau(optimizer,
                                                         mode='min',
                                                         factor=0.2,
                                                         patience=20,
                                                         min_lr=5e-5)
        return {"optimizer": optimizer, "lr_scheduler": scheduler, "monitor": "val_loss"}

    def training_step(self, batch, batch_idx):
        loss = self._get_reconstruction_loss(batch)
        self.log('train_loss', loss)
        return loss

    def validation_step(self, batch, batch_idx):
        loss = self._get_reconstruction_loss(batch)
        self.log('val_loss', loss)

    def test_step(self, batch, batch_idx):
        loss = self._get_reconstruction_loss(batch)
        self.log('test_loss', loss)
```

For the loss function, we use the mean squared error (MSE). The mean squared error pushes the network to pay special attention to those pixel values its estimate is far away. Predicting 127 instead of 128 is not important when reconstructing, but confusing 0 with 128 is much worse. Note that in contrast to VAEs, we do not predict the probability per pixel value, but instead use a distance measure. This saves a lot of parameters and simplifies training. To get a better intuition per pixel, we report the summed squared error averaged over the batch dimension (any other mean/sum leads to the same result/parameters).

However, MSE has also some considerable disadvantages. Usually, MSE leads to blurry images where small noise/high-frequent patterns are removed as those cause a very low error. To ensure realistic images to be reconstructed, one could combine Generative Adversarial Networks (lecture 10) with autoencoders as done in several works (e.g. see here, here or these slides). Additionally, comparing two images using MSE does not necessarily reflect their visual similarity. For instance, suppose the autoencoder reconstructs an image shifted by one pixel to the right and bottom. Although the images are almost identical, we can get a higher loss than predicting a constant pixel value for half of the image (see code below). An example solution for this issue includes using a separate, pre-trained CNN, and use a distance of visual features in lower layers as a distance measure instead of the original pixel-level comparison.

[7]:
```
def compare_imgs(img1, img2, title_prefix=""):
    # Calculate MSE loss between both images
    loss = F.mse_loss(img1, img2, reduction="sum")
    # Plot images for visual comparison
    grid = torchvision.utils.make_grid(torch.stack([img1, img2], dim=0), nrow=2,␣
↪normalize=True, range=(-1,1))
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(4,2))
```

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```
    plt.title(f"{title_prefix} Loss: {loss.item():4.2f}")
    plt.imshow(grid)
    plt.axis('off')
    plt.show()

for i in range(2):
    # Load example image
    img, _ = train_dataset[i]
    img_mean = img.mean(dim=[1,2], keepdims=True)

    # Shift image by one pixel
    SHIFT = 1
    img_shifted = torch.roll(img, shifts=SHIFT, dims=1)
    img_shifted = torch.roll(img_shifted, shifts=SHIFT, dims=2)
    img_shifted[:,:1,:] = img_mean
    img_shifted[:,:,:1] = img_mean
    compare_imgs(img, img_shifted, "Shifted -")

    # Set half of the image to zero
    img_masked = img.clone()
    img_masked[:,:img_masked.shape[1]//2,:] = img_mean
    compare_imgs(img, img_masked, "Masked -")
```

Training the model

During the training, we want to keep track of the learning progress by seeing reconstructions made by our model. For this, we implement a callback object in PyTorch Lightning which will add reconstructions every N epochs to our tensorboard:

[8]:
```
class GenerateCallback(pl.Callback):

    def __init__(self, input_imgs, every_n_epochs=1):
        super().__init__()
        self.input_imgs = input_imgs # Images to reconstruct during training
        self.every_n_epochs = every_n_epochs # Only save those images every N epochs␣
↪(otherwise tensorboard gets quite large)

    def on_train_epoch_end(self, trainer, pl_module):
        if trainer.current_epoch % self.every_n_epochs == 0:
            # Reconstruct images
            input_imgs = self.input_imgs.to(pl_module.device)
            with torch.no_grad():
                pl_module.eval()
                reconst_imgs = pl_module(input_imgs)
                pl_module.train()
            # Plot and add to tensorboard
            imgs = torch.stack([input_imgs, reconst_imgs], dim=1).flatten(0,1)
            grid = torchvision.utils.make_grid(imgs, nrow=2, normalize=True, range=(-1,
↪1))
            trainer.logger.experiment.add_image("Reconstructions", grid, global_
↪step=trainer.global_step)
```

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We will now write a training function that allows us to train the autoencoder with different latent dimensionality and returns both the test and validation score. We provide pre-trained models and recommend you using those, especially when you work on a computer without GPU. Of course, feel free to train your own models on Snellius.

[9]:
```
def train_cifar(latent_dim):
    # Create a PyTorch Lightning trainer with the generation callback
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, f"cifar10_
↪{latent_dim}"),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=500,
                         callbacks=[ModelCheckpoint(save_weights_only=True),
                                    GenerateCallback(get_train_images(8), every_n_
↪epochs=10),
                                    LearningRateMonitor("epoch")])
    trainer.logger._log_graph = True         # If True, we plot the computation graph in␣
↪tensorboard
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, f"cifar10_{latent_dim}.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = Autoencoder.load_from_checkpoint(pretrained_filename)
    else:
        model = Autoencoder(base_channel_size=32, latent_dim=latent_dim)
        trainer.fit(model, train_loader, val_loader)
    # Test best model on validation and test set
    val_result = trainer.test(model, val_loader, verbose=False)
    test_result = trainer.test(model, test_loader, verbose=False)
    result = {"test": test_result, "val": val_result}
    return model, result
```

Comparing latent dimensionality

When training an autoencoder, we need to choose a dimensionality for the latent representation z. The higher the latent dimensionality, the better we expect the reconstruction to be. However, the idea of autoencoders is to *compress* data. Hence, we are also interested in keeping the dimensionality low. To find the best tradeoff, we can train multiple models with different latent dimensionalities. The original input has $32 \times 32 \times 3 = 3072$ pixels. Keeping this in mind, a reasonable choice for the latent dimensionality might be between 64 and 384:

[10]:
```
model_dict = {}
for latent_dim in [64, 128, 256, 384]:
    model_ld, result_ld = train_cifar(latent_dim)
    model_dict[latent_dim] = {"model": model_ld, "result": result_ld}
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```
GPU available: True, used: True
WARNING: Logging before flag parsing goes to stderr.
I1123 10:35:57.297765 140189561788224 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1123 10:35:57.298832 140189561788224 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1123 10:35:57.299675 140189561788224 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```
GPU available: True, used: True
I1123 10:35:58.741801 140189561788224 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1123 10:35:58.742980 140189561788224 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1123 10:35:58.743852 140189561788224 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```
GPU available: True, used: True
I1123 10:36:00.166019 140189561788224 distributed.py:49] GPU available: True, used: True
TPU available: False, using: 0 TPU cores
I1123 10:36:00.167815 140189561788224 distributed.py:49] TPU available: False, using: 0␣
↪TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
I1123 10:36:00.169288 140189561788224 accelerator_connector.py:385] LOCAL_RANK: 0 - CUDA_
↪VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', description='Testing',␣
↪layout=Layout(flex='2'), max=...
```

```

```

After training the models, we can plot the reconstruction loss over the latent dimensionality to get an intuition how these two properties are correlated:

[11]:
```
latent_dims = sorted([k for k in model_dict])
val_scores = [model_dict[k]["result"]["val"][0]["test_loss"] for k in latent_dims]

fig = plt.figure(figsize=(6,4))
plt.plot(latent_dims, val_scores, '--', color="#000", marker="*", markeredgecolor="#000",
↪ markerfacecolor="y", markersize=16)
plt.xscale("log")
plt.xticks(latent_dims, labels=latent_dims)
plt.title("Reconstruction error over latent dimensionality", fontsize=14)
plt.xlabel("Latent dimensionality")
plt.ylabel("Reconstruction error")
plt.minorticks_off()
plt.ylim(0,100)
plt.show()
```

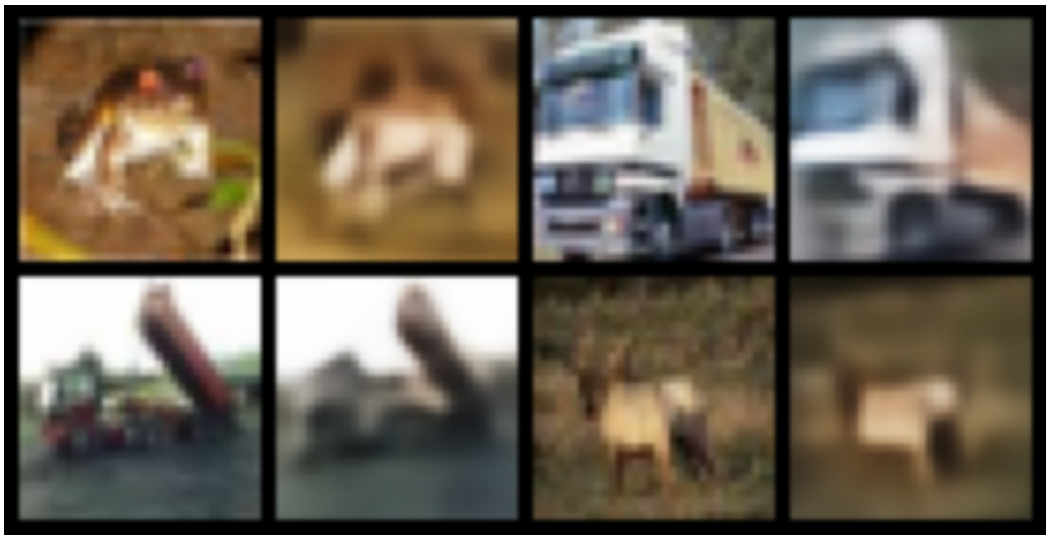
As we initially expected, the reconstruction loss goes down with increasing latent dimensionality. For our model and

setup, the two properties seem to be exponentially (or double exponentially) correlated. To understand what these differences in reconstruction error mean, we can visualize example reconstructions of the four models. For simplicity, we visualize four training images of CIFAR10 we have seen already before. For larger models that may overfit, it is recommended to use images from the validation set.

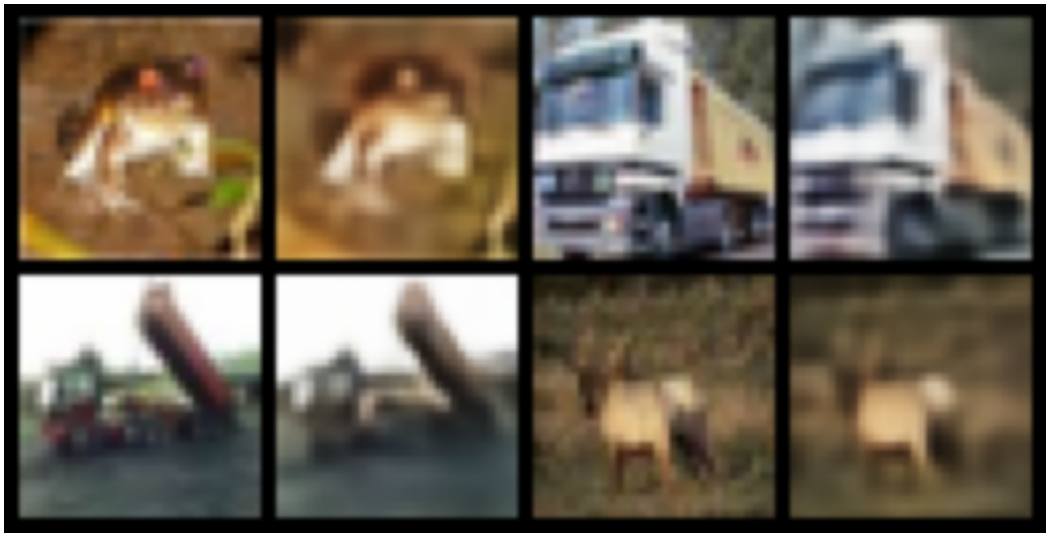
[12]:
```
def visualize_reconstructions(model, input_imgs):
    # Reconstruct images
    model.eval()
    with torch.no_grad():
        reconst_imgs = model(input_imgs.to(model.device))
    reconst_imgs = reconst_imgs.cpu()

    # Plotting
    imgs = torch.stack([input_imgs, reconst_imgs], dim=1).flatten(0,1)
    grid = torchvision.utils.make_grid(imgs, nrow=4, normalize=True, range=(-1,1))
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(7,4.5))
    plt.title(f"Reconstructed from {model.hparams.latent_dim} latents")
    plt.imshow(grid)
    plt.axis('off')
    plt.show()
```

[13]:
```
input_imgs = get_train_images(4)
for latent_dim in model_dict:
    visualize_reconstructions(model_dict[latent_dim]["model"], input_imgs)
```

Reconstructed from 128 latents



Reconstructed from 256 latents



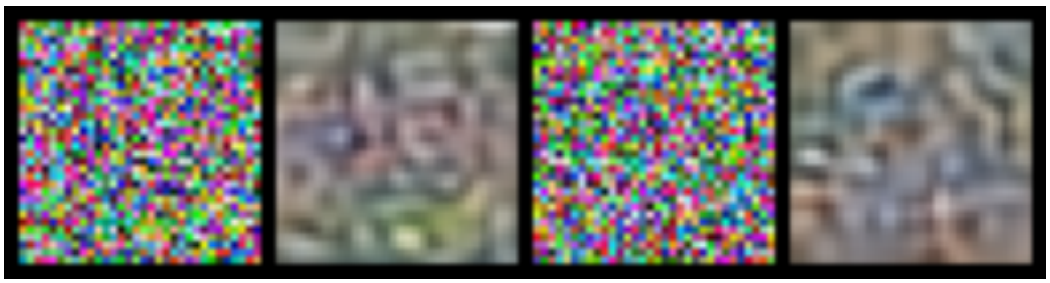
Clearly, the smallest latent dimensionality can only save information about the rough shape and color of the object, but the reconstructed image is extremely blurry and it is hard to recognize the original object in the reconstruction. With 128 features, we can recognize some shapes again although the picture remains blurry. The models with the highest two dimensionalities reconstruct the images quite well. The difference between 256 and 384 is marginal at first sight but can be noticed when comparing, for instance, the backgrounds of the first image (the 384 features model more of the pattern than 256).

Out-of-distribution images

Before continuing with the applications of autoencoder, we can actually explore some limitations of our autoencoder. For example, what happens if we try to reconstruct an image that is clearly out of the distribution of our dataset? We expect the decoder to have learned some common patterns in the dataset, and thus might in particular fail to reconstruct images that do not follow these patterns.

The first experiment we can try is to reconstruct noise. We, therefore, create two images whose pixels are randomly sampled from a uniform distribution over pixel values, and visualize the reconstruction of the model (feel free to test different latent dimensionalities):

[14]:
```
rand_imgs = torch.rand(2, 3, 32, 32) * 2 - 1
visualize_reconstructions(model_dict[256]["model"], rand_imgs)
```

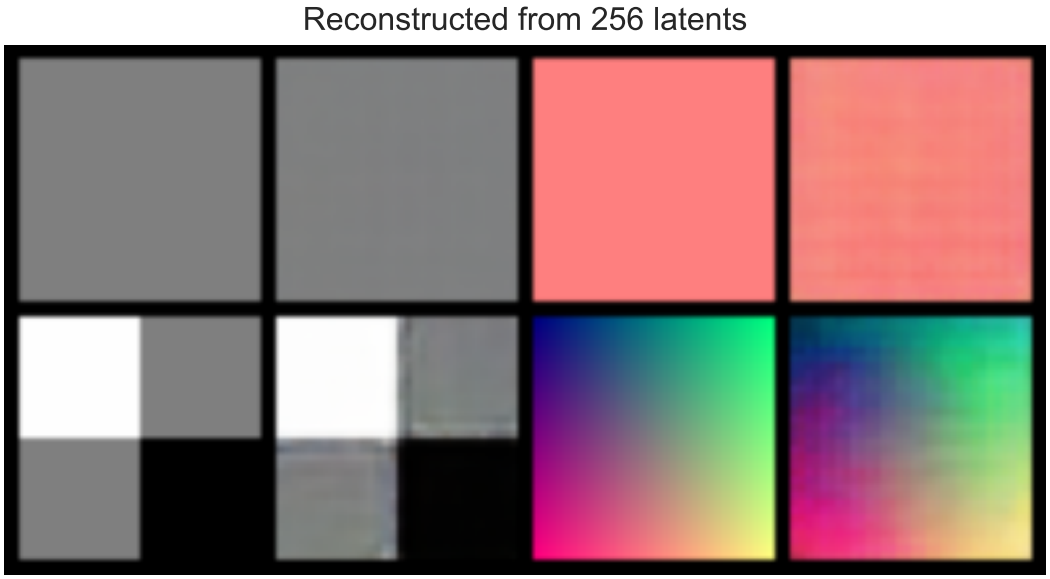


The reconstruction of the noise is quite poor, and seems to introduce some rough patterns. As the input does not follow

the patterns of the CIFAR dataset, the model has issues reconstructing it accurately.

We can also check how well the model can reconstruct other manually-coded patterns:

[15]:
```
plain_imgs = torch.zeros(4, 3, 32, 32)

# Single color channel
plain_imgs[1,0] = 1
# Checkboard pattern
plain_imgs[2,:,:16,:16] = 1
plain_imgs[2,:,16:,16:] = -1
# Color progression
xx, yy = torch.meshgrid(torch.linspace(-1,1,32), torch.linspace(-1,1,32))
plain_imgs[3,0,:,:] = xx
plain_imgs[3,1,:,:] = yy

visualize_reconstructions(model_dict[256]["model"], plain_imgs)
```



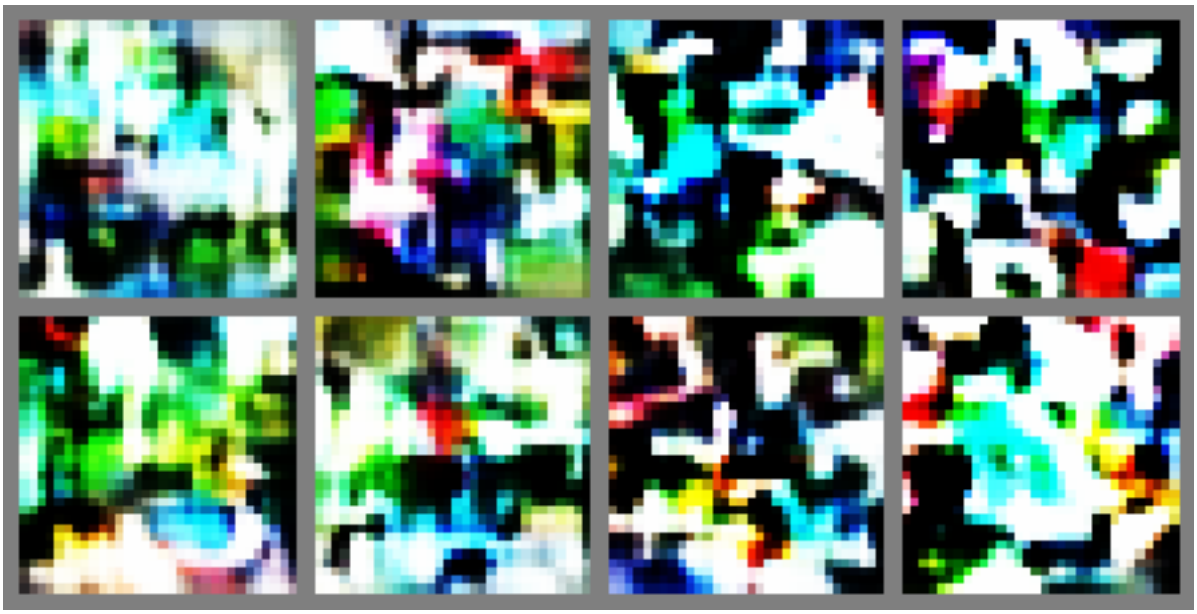
The plain, constant images are reconstructed relatively good although the single color channel contains some noticeable noise. The hard borders of the checkboard pattern are not as sharp as intended, as well as the color progression, both because such patterns never occur in the real-world pictures of CIFAR.

In general, autoencoders tend to fail reconstructing high-frequent noise (i.e. sudden, big changes across few pixels) due to the choice of MSE as loss function (see our previous discussion about loss functions in autoencoders). Small misalignments in the decoder can lead to huge losses so that the model settles for the expected value/mean in these regions. For low-frequent noise, a misalignment of a few pixels does not result in a big difference to the original image. However, the larger the latent dimensionality becomes, the more of this high-frequent noise can be accurately reconstructed.

Generating new images

Variational autoencoders are a generative version of the autoencoders because we regularize the latent space to follow a Gaussian distribution. However, in vanilla autoencoders, we do not have any restrictions on the latent vector. So what happens if we would actually input a randomly sampled latent vector into the decoder? Let's find it out below:

[16]:
```
model = model_dict[256]["model"]
latent_vectors = torch.randn(8, model.hparams.latent_dim, device=model.device)
with torch.no_grad():
    imgs = model.decoder(latent_vectors)
    imgs = imgs.cpu()

grid = torchvision.utils.make_grid(imgs, nrow=4, normalize=True, range=(-1,1), pad_
↪value=0.5)
grid = grid.permute(1, 2, 0)
plt.figure(figsize=(8,5))
plt.imshow(grid)
plt.axis('off')
plt.show()
```



As we can see, the generated images more look like art than realistic images. As the autoencoder was allowed to structure the latent space in whichever way it suits the reconstruction best, there is no incentive to map every possible latent vector to realistic images. Furthermore, the distribution in latent space is unknown to us and doesn't necessarily follow a multivariate normal distribution. Thus, we can conclude that vanilla autoencoders are indeed not generative.

4.23.2 Finding visually similar images

One application of autoencoders is to build an image-based search engine to retrieve visually similar images. This can be done by representing all images as their latent dimensionality, and find the closest K images in this domain. The first step to such a search engine is to encode all images into z. In the following, we will use the training set as a search corpus, and the test set as queries to the system.

(Warning: the following cells can be computationally heavy for a weak CPU-only system. If you do not have a strong computer and are not on Google Colab, you might want to skip the execution of the following cells and rely on the results shown in the filled notebook)

[17]:
```
# We use the following model throughout this section.
# If you want to try a different latent dimensionality, change it here!
model = model_dict[128]["model"]
```

[18]:
```
def embed_imgs(model, data_loader):
    # Encode all images in the data_laoder using model, and return both images and␣
↪encodings
    img_list, embed_list = [], []
    model.eval()
    for imgs, _ in tqdm(data_loader, desc="Encoding images", leave=False):
        with torch.no_grad():
            z = model.encoder(imgs.to(model.device))
        img_list.append(imgs)
        embed_list.append(z)
    return (torch.cat(img_list, dim=0), torch.cat(embed_list, dim=0))

train_img_embeds = embed_imgs(model, train_loader)
test_img_embeds = embed_imgs(model, test_loader)
```

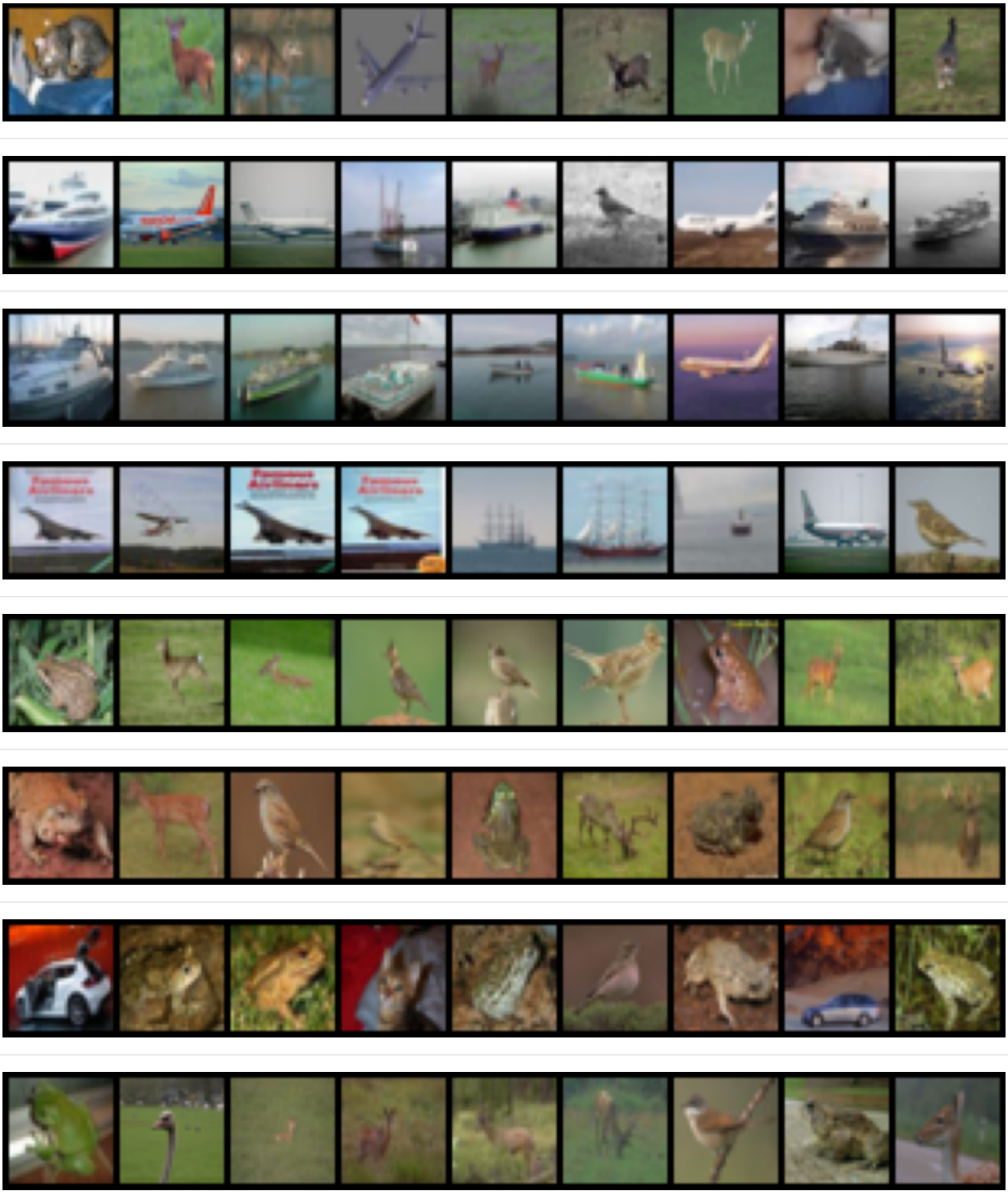
```
HBox(children=(FloatProgress(value=0.0, description='Encoding images', max=175.0,␣
↪style=ProgressStyle(descript...
```

```
HBox(children=(FloatProgress(value=0.0, description='Encoding images', max=40.0,␣
↪style=ProgressStyle(descripti...
```

After encoding all images, we just need to write a function that finds the closest K images and returns (or plots) those:

[19]:
```
def find_similar_images(query_img, query_z, key_embeds, K=8):
    # Find closest K images. We use the euclidean distance here but other like cosine␣
↪distance can also be used.
    dist = torch.cdist(query_z[None,:], key_embeds[1], p=2)
    dist = dist.squeeze(dim=0)
    dist, indices = torch.sort(dist)
    # Plot K closest images
    imgs_to_display = torch.cat([query_img[None], key_embeds[0][indices[:K]]], dim=0)
    grid = torchvision.utils.make_grid(imgs_to_display, nrow=K+1, normalize=True,␣
↪range=(-1,1))
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(12,3))
    plt.imshow(grid)
    plt.axis('off')
    plt.show()
```

[20]:
```
# Plot the closest images for the first N test images as example
for i in range(8):
    find_similar_images(test_img_embeds[0][i], test_img_embeds[1][i], key_embeds=train_
↪img_embeds)
```



Based on our autoencoder, we see that we are able to retrieve many similar images to the test input. In particular, in row 4, we can spot that some test images might not be that different from the training set as we thought (same poster, just

different scaling/color scaling). We also see that although we haven't given the model any labels, it can cluster different classes in different parts of the latent space (airplane + ship, animals, etc.). This is why autoencoders can also be used as a pre-training strategy for deep networks, especially when we have a large set of unlabeled images (often the case). However, it should be noted that the background still plays a big role in autoencoders while it doesn't for classification. Hence, we don't get "perfect" clusters and need to finetune such models for classification.

Tensorboard clustering

Another way of exploring the similarity of images in the latent space is by dimensionality-reduction methods like PCA or T-SNE. Luckily, Tensorboard provides a nice interface for this and we can make use of it in the following:

[21]:
```
# We use the following model throughout this section.
# If you want to try a different latent dimensionality, change it here!
model = model_dict[128]["model"]
```

[22]:
```
# Create a summary writer
writer = SummaryWriter("tensorboard/")
```

The function `add_embedding` allows us to add high-dimensional feature vectors to TensorBoard on which we can perform clustering. What we have to provide in the function are the feature vectors, additional metadata such as the labels, and the original images so that we can identify a specific image in the clustering.

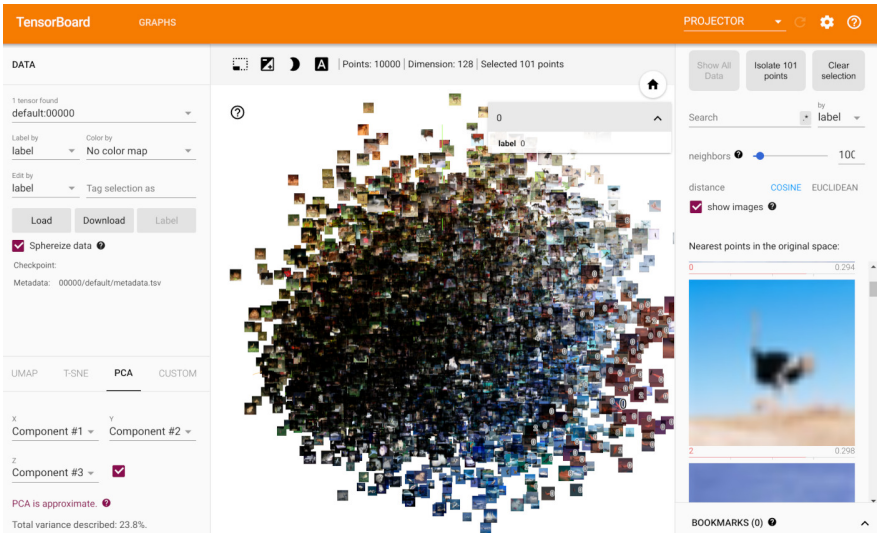
[23]:
```
## In case you obtain the following error in the next cell, execute the import␣
↪statements and last line in this cell
##   AttributeError: module 'tensorflow._api.v2.io.gfile' has no attribute 'get_filesystem'

# import tensorflow as tf
# import tensorboard as tb
# tf.io.gfile = tb.compat.tensorflow_stub.io.gfile
```

[24]:
```
# Note: the embedding projector in tensorboard is computationally heavy.
# Reduce the image amount below if your computer struggles with visualizing all 10k␣
↪points
NUM_IMGS = len(test_set)

writer.add_embedding(test_img_embeds[1][:NUM_IMGS], # Encodings per image
                     metadata=[test_set[i][1] for i in range(NUM_IMGS)], # Adding the␣
↪labels per image to the plot
                     label_img=(test_img_embeds[0][:NUM_IMGS]+1)/2.0) # Adding the␣
↪original images to the plot
```

Finally, we can run tensorboard to explore similarities among images:

[25]:
```
%tensorboard --logdir tensorboard/
```

You should be able to see something similar as in the following image. In case the projector stays empty, try to start the TensorBoard outside of the Jupyter notebook.



Overall, we can see that the model indeed clustered images together that are visually similar. Especially the background color seems to be a crucial factor in the encoding. This correlates to the chosen loss function, here Mean Squared Error on pixel-level because the background is responsible for more than half of the pixels in an average image. Hence, the model learns to focus on it. Nevertheless, we can see that the encodings also separate a couple of classes in the latent space although it hasn't seen any labels. This shows again that autoencoding can also be used as a "pre-training"/transfer learning task before classification.

[26]:
```
# Closing the summary writer
writer.close()
```

4.23.3 Conclusion

In this tutorial, we have implemented our own autoencoder on small RGB images and explored various properties of the model. In contrast to variational autoencoders, vanilla AEs are not generative and can work on MSE loss functions. This makes them often easier to train. Both versions of AE can be used for dimensionality reduction, as we have seen for finding visually similar images beyond pixel distances. Despite autoencoders gaining less interest in the research community due to their more "theoretically" challenging counterpart of VAEs, autoencoders still find usage in a lot of applications like denoising and compression. Hence, AEs are an essential tool that every Deep Learning engineer/researcher should be familiar with.

If you found this tutorial helpful, consider -ing our repository.

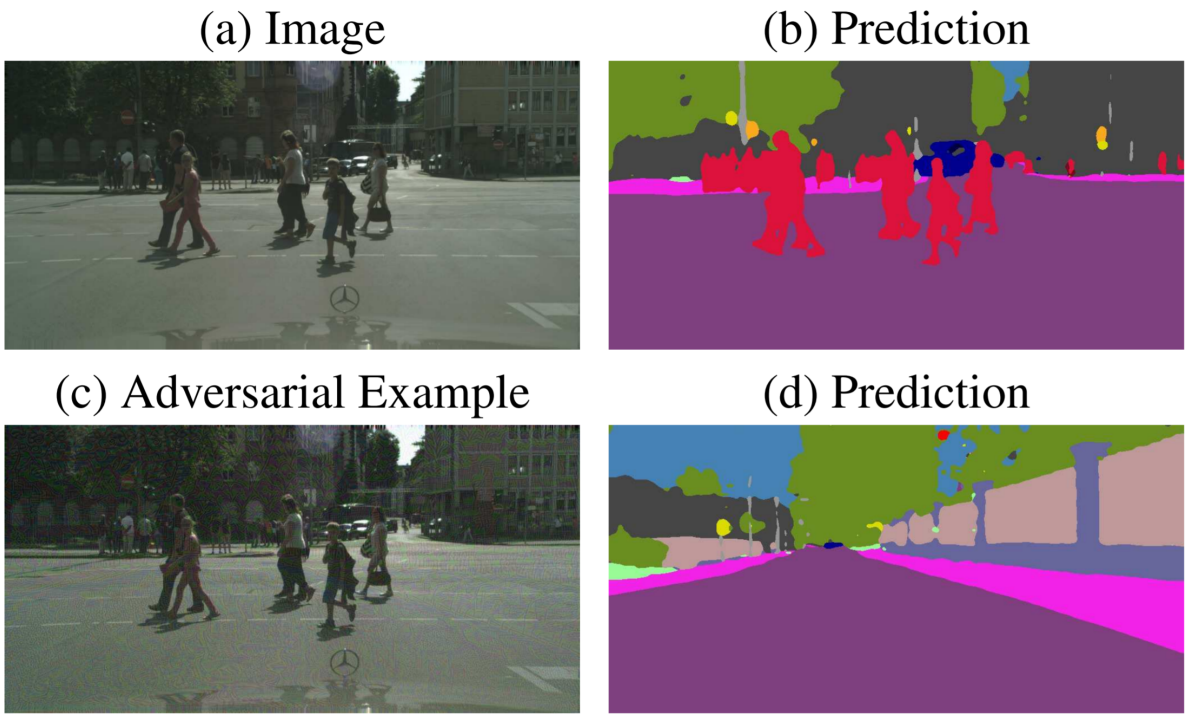
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.24 Tutorial 10: Adversarial attacks

Filled notebook:
Pre-trained models and dataset:
Recordings:
Author: Phillip Lippe

In this tutorial, we will discuss adversarial attacks on deep image classification models. As we have seen in many of the previous tutorials so far, Deep Neural Networks are a very powerful tool to recognize patterns in data, and, for example, perform image classification on a human-level. However, we have not tested yet how robust these models actually are. Can we "trick" the model and find failure modes? Can we design images that the networks naturally classify incorrectly? Due to the high classification accuracy on unseen test data, we would expect that this can be difficult. However, in 2014, a research group at Google and NYU showed that deep CNNs can be easily fooled, just by adding some salient but carefully constructed noise to the images. For instance, take a look at the example below (figure credit - Goodfellow et al.):

The image on the left is the original image from ImageNet, and a deep CNN classifies the image correctly as "panda" with a class likelihood of 57%. Nevertheless, if we add a little noise to every pixel of the image, the prediction of the model changes completely. Instead of a panda, our CNN tells us that the image contains a "gibbon" with the confidence of over 99%. For a human, however, these two images look exactly alike, and you cannot distinguish which one has noise added and which doesn't. While this first seems like a fun game to fool trained networks, it can have a serious impact on the usage of neural networks. More and more deep learning models are used in applications, such as for example autonomous driving. Imagine that someone who gains access to the camera input of the car, could make pedestrians "disappear" for the image understanding network by simply adding some noise to the input as shown below (the figure is taken from J.H. Metzen et al.). The first row shows the original image with the semantic segmentation output on the right (pedestrians red), while the second row shows the image with small noise and the corresponding segmentation prediction. The pedestrian becomes invisible for the network, and the car would think the road is clear ahead.



Some attack types don't even require to add noise, but minor changes on a stop sign can be already sufficient for the network to recognize it as a "50km/h" speed sign (paper, paper). The consequences of such attacks can be devastating. Hence, every deep learning engineer who designs models for an application should be aware of the possibility of adversarial attacks.

To understand what makes CNNs vulnerable to such attacks, we will implement our own adversarial attack strategies in this notebook, and try to fool a deep neural network. Let's being with importing our standard libraries:

[1]:
```
## Standard libraries
import os
import json
import math
import time
import numpy as np
import scipy.linalg

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.set()

## Progress bar
from tqdm.notebook import tqdm
```

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```
## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import CIFAR10
from torchvision import transforms
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial10"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

# Fetching the device that will be used throughout this notebook
device = torch.device("cpu") if not torch.cuda.is_available() else torch.device("cuda:0")
print("Using device", device)
```

```
Using device cuda:0
```

We have again a few download statements. This includes both a dataset, and a few pretrained patches we will use later.

[2]:
```
import urllib.request
from urllib.error import HTTPError
import zipfile
# Github URL where the dataset is stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial10/"
# Files to download
pretrained_files = [(DATASET_PATH, "TinyImageNet.zip"), (CHECKPOINT_PATH, "patches.zip")]
# Create checkpoint path if it doesn't exist yet
os.makedirs(DATASET_PATH, exist_ok=True)
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for dir_name, file_name in pretrained_files:
    file_path = os.path.join(dir_name, file_name)
```

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```
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
        if file_name.endswith(".zip"):
            print("Unzipping file...")
            with zipfile.ZipFile(file_path, 'r') as zip_ref:
                zip_ref.extractall(file_path.rsplit("/",1)[0])
```

4.24.1 Deep CNNs on ImageNet

For our experiments in this notebook, we will use common CNN architectures trained on the ImageNet dataset. Such models are luckily provided by PyTorch's torchvision package, and hence we just need to load the model of our preference. For the results on the website and default on Google Colab, we use a ResNet34. Feel free to experiment with other architectures as well, the code is mainly independent of the specific architecture we choose.

[3]:
```
# Load CNN architecture pretrained on ImageNet
os.environ["TORCH_HOME"] = CHECKPOINT_PATH
pretrained_model = torchvision.models.resnet34(weights='IMAGENET1K_V1')
pretrained_model = pretrained_model.to(device)

# No gradients needed for the network
pretrained_model.eval()
for p in pretrained_model.parameters():
    p.requires_grad = False
```

To perform adversarial attacks, we also need a dataset to work on. Given that the CNN model has been trained on ImageNet, it is only fair to perform the attacks on data from ImageNet. For this, we provide a small set of pre-processed images from the original ImageNet dataset (note that this dataset is shared under the same license as the original ImageNet dataset). Specifically, we have 5 images for each of the 1000 labels of the dataset. We can load the data below, and create a corresponding data loader.

[4]:
```
# Mean and Std from ImageNet
NORM_MEAN = np.array([0.485, 0.456, 0.406])
NORM_STD = np.array([0.229, 0.224, 0.225])
# No resizing and center crop necessary as images are already preprocessed.
plain_transforms = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize(mean=NORM_MEAN,
                         std=NORM_STD)
])

# Load dataset and create data loader
imagenet_path = os.path.join(DATASET_PATH, "TinyImageNet/")
assert os.path.isdir(imagenet_path), f"Could not find the ImageNet dataset at expected␣
↪path \"{imagenet_path}\". " + \
```

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```
                                    f"Please make sure to have downloaded the ImageNet␣
↪dataset here, or change the {DATASET_PATH=} variable."
dataset = torchvision.datasets.ImageFolder(root=imagenet_path, transform=plain_
↪transforms)
data_loader = data.DataLoader(dataset, batch_size=32, shuffle=False, drop_last=False,␣
↪num_workers=8)

# Load label names to interpret the label numbers 0 to 999
with open(os.path.join(imagenet_path, "label_list.json"), "r") as f:
    label_names = json.load(f)

def get_label_index(lab_str):
    assert lab_str in label_names, f"Label \"{lab_str}\" not found. Check the spelling␣
↪of the class."
    return label_names.index(lab_str)
```

Before we start with our attacks, we should verify the performance of our model. As ImageNet has 1000 classes, simply looking at the accuracy is not sufficient to tell the performance of a model. Imagine a model that always predicts the true label as the second-highest class in its softmax output. Although we would say it recognizes the object in the image, it achieves an accuracy of 0. In ImageNet with 1000 classes, there is not always one clear label we can assign an image to. This is why for image classifications over so many classes, a common alternative metric is "Top-5 accuracy", which tells us how many times the true label has been within the 5 most-likely predictions of the model. As models usually perform quite well on those, we report the error (1 - accuracy) instead of the accuracy:

[5]:
```
def eval_model(dataset_loader, img_func=None):
    tp, tp_5, counter = 0., 0., 0.
    for imgs, labels in tqdm(dataset_loader, desc="Validating..."):
        imgs = imgs.to(device)
        labels = labels.to(device)
        if img_func is not None:
            imgs = img_func(imgs, labels)
        with torch.no_grad():
            preds = pretrained_model(imgs)
        tp += (preds.argmax(dim=-1) == labels).sum()
        tp_5 += (preds.topk(5, dim=-1)[1] == labels[...,None]).any(dim=-1).sum()
        counter += preds.shape[0]
    acc = tp.float().item()/counter
    top5 = tp_5.float().item()/counter
    print(f"Top-1 error: {(100.0 * (1 - acc)):4.2f}%")
    print(f"Top-5 error: {(100.0 * (1 - top5)):4.2f}%")
    return acc, top5
```

[6]:
```
_ = eval_model(data_loader)
```

```
HBox(children=(FloatProgress(value=0.0, description='Validating...', max=157.0,␣
↪style=ProgressStyle(descriptio...
```

```
Top-1 error: 19.10%
Top-5 error: 4.30%
```

The ResNet34 achives a decent error rate of 4.3% for the top-5 predictions. Next, we can look at some predictions of the model to get more familiar with the dataset. The function below plots an image along with a bar diagram of its predictions. We also prepare it to show adversarial examples for later applications.

[7]:
```
def show_prediction(img, label, pred, K=5, adv_img=None, noise=None):

    if isinstance(img, torch.Tensor):
        # Tensor image to numpy
        img = img.cpu().permute(1, 2, 0).numpy()
        img = (img * NORM_STD[None,None]) + NORM_MEAN[None,None]
        img = np.clip(img, a_min=0.0, a_max=1.0)
        label = label.item()

    # Plot on the left the image with the true label as title.
    # On the right, have a horizontal bar plot with the top k predictions including␣
↪probabilities
    if noise is None or adv_img is None:
        fig, ax = plt.subplots(1, 2, figsize=(10,2), gridspec_kw={'width_ratios': [1, 1]}
↪)
    else:
        fig, ax = plt.subplots(1, 5, figsize=(12,2), gridspec_kw={'width_ratios': [1, 1,␣
↪1, 1, 2]})

    ax[0].imshow(img)
    ax[0].set_title(label_names[label])
    ax[0].axis('off')

    if adv_img is not None and noise is not None:
        # Visualize adversarial images
        adv_img = adv_img.cpu().permute(1, 2, 0).numpy()
        adv_img = (adv_img * NORM_STD[None,None]) + NORM_MEAN[None,None]
        adv_img = np.clip(adv_img, a_min=0.0, a_max=1.0)
        ax[1].imshow(adv_img)
        ax[1].set_title('Adversarial')
        ax[1].axis('off')
        # Visualize noise
        noise = noise.cpu().permute(1, 2, 0).numpy()
        noise = noise * 0.5 + 0.5 # Scale between 0 to 1
        ax[2].imshow(noise)
        ax[2].set_title('Noise')
        ax[2].axis('off')
        # buffer
        ax[3].axis('off')

    if abs(pred.sum().item() - 1.0) > 1e-4:
        pred = torch.softmax(pred, dim=-1)
    topk_vals, topk_idx = pred.topk(K, dim=-1)
    topk_vals, topk_idx = topk_vals.cpu().numpy(), topk_idx.cpu().numpy()
    ax[-1].barh(np.arange(K), topk_vals*100.0, align='center', color=["C0" if topk_
↪idx[i]!=label else "C2" for i in range(K)])
    ax[-1].set_yticks(np.arange(K))
    ax[-1].set_yticklabels([label_names[c] for c in topk_idx])
    ax[-1].invert_yaxis()
    ax[-1].set_xlabel('Confidence')
    ax[-1].set_title('Predictions')

    plt.show()
```

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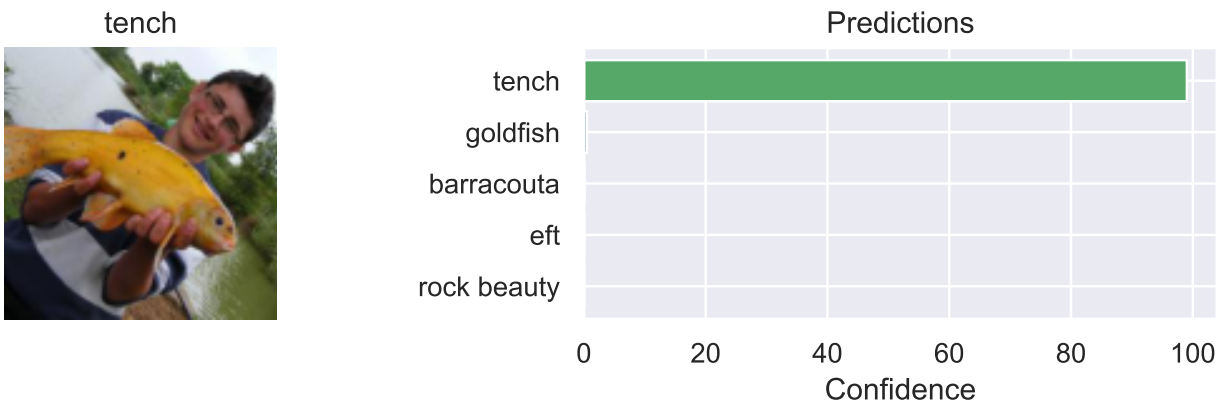
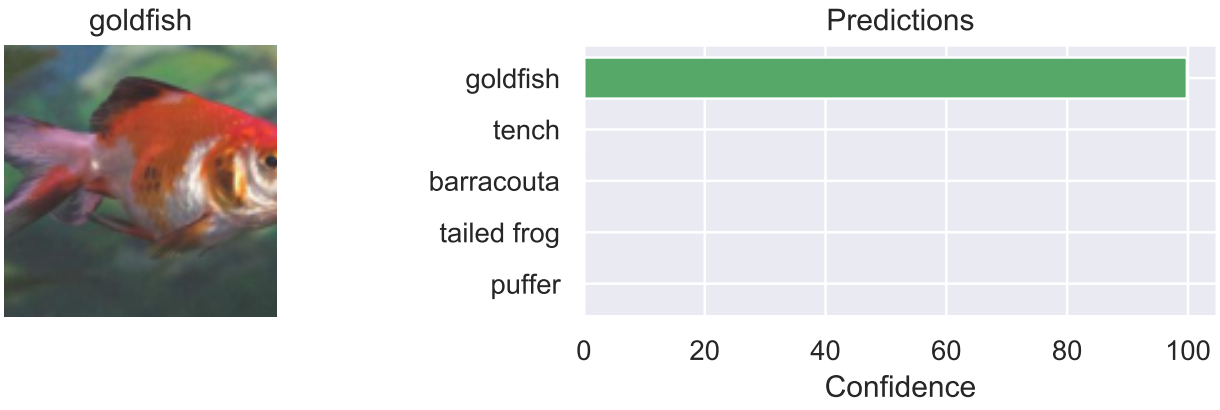
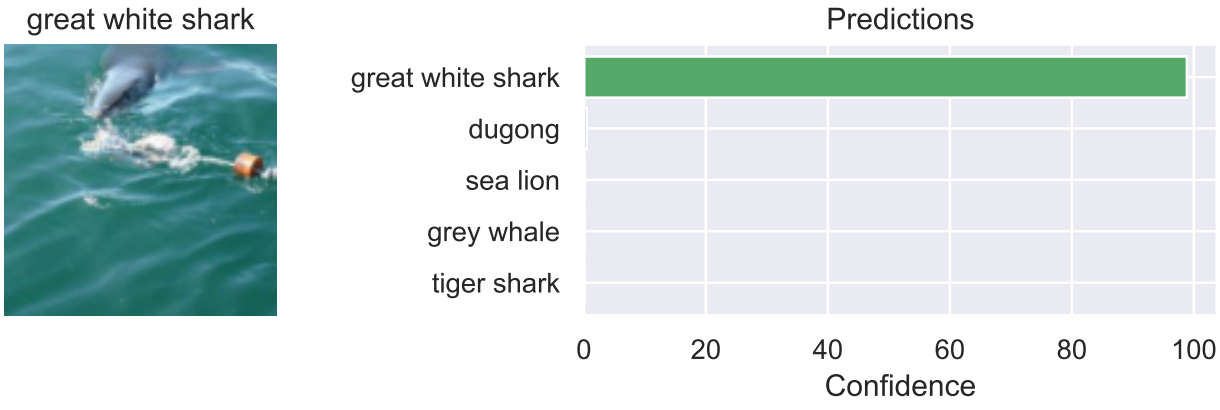
```
    plt.close()
```

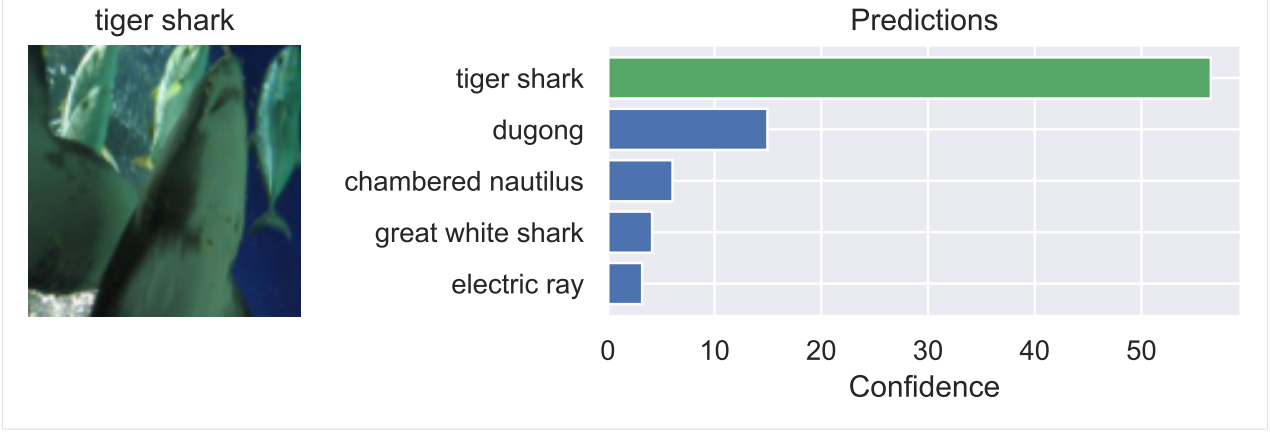
Let's visualize a few images below:

[8]:
```
exmp_batch, label_batch = next(iter(data_loader))
with torch.no_grad():
    preds = pretrained_model(exmp_batch.to(device))
for i in range(1,17,5):
    show_prediction(exmp_batch[i], label_batch[i], preds[i])
```









The bar plot on the right shows the top-5 predictions of the model with their class probabilities. We denote the class probabilities with "confidence" as it somewhat resembles how confident the network is that the image is of one specific class. Some of the images have a highly peaked probability distribution, and we would expect the model to be rather robust against noise for those. However, we will see below that this is not always the case. Note that all of the images are of fish because the data loader doesn't shuffle the dataset. Otherwise, we would get different images every time we run the notebook, which would make it hard to discuss the results on the static version.

4.24.2 White-box adversarial attacks

There have been proposed many possible adversarial attack strategies, which all share the same goal: alternate the data/image input only a little bit to have a great impact on the model's prediction. Specifically, if we look at the ImageNet predictions above, how can we have to change the image of the goldfish so that the model does not recognize the goldfish anymore? At the same time, the label of the image should not change, in the sense that a human would still clearly classify it as a goldfish. This is the same objective that the generator network has in the Generative Adversarial Network framework: try to fool another network (discriminator) by changing its input.

Adversarial attacks are usually grouped into "white-box" and "black-box" attacks. White-box attacks assume that we have access to the model parameter and can, for example, calculate the gradients with respect to the input (similar as in GANs). Black-box attacks on the other hand have the harder task of not having any knowledge about the network, and can only obtain predictions for an image, but no gradients or the like. In this notebook, we will focus on white-box attacks as they are usually easier to implement and follow the intuition of Generative Adversarial Networks (GAN) as studied in lecture 10.

Fast Gradient Sign Method (FGSM)

One of the first attack strategies proposed is Fast Gradient Sign Method (FGSM), developed by Ian Goodfellow et al. in 2014. Given an image, we create an adversarial example by the following expression:

$$\tilde{x} = x + \epsilon \cdot \text{sign}(\nabla_x J(\theta, x, y))$$

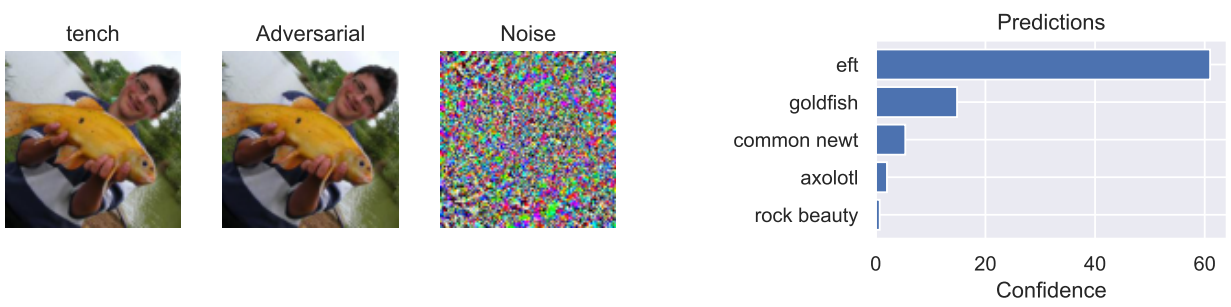
The term $J(\theta, x, y)$ represents the loss of the network for classifying input image x as label y; ϵ is the intensity of the noise, and $\tilde{x}$ the final adversarial example. The equation resembles SGD and is actually nothing else than that. We change the input image x in the direction of *maximizing* the loss $J(\theta, x, y)$. This is exactly the other way round as during training, where we try to minimize the loss. The sign function and ϵ can be seen as gradient clipping and learning rate specifically. We only allow our attack to change each pixel value by ϵ. You can also see that the attack can be performed very fast, as it only requires a single forward and backward pass. Let's implement it below:

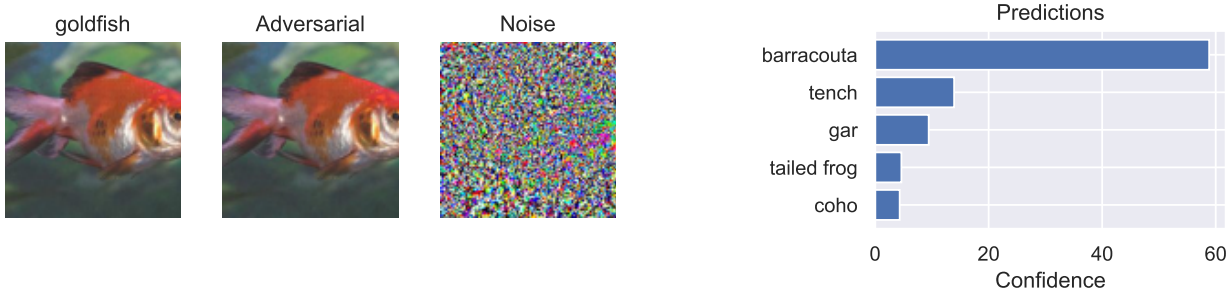
[9]:
```
def fast_gradient_sign_method(model, imgs, labels, epsilon=0.02):
    # Determine prediction of the model
    inp_imgs = imgs.clone().requires_grad_()
    preds = model(inp_imgs.to(device))
    preds = F.log_softmax(preds, dim=-1)
    # Calculate loss by NLL
    loss = -torch.gather(preds, 1, labels.to(device).unsqueeze(dim=-1))
    loss.sum().backward()
    # Update image to adversarial example as written above
    noise_grad = torch.sign(inp_imgs.grad.to(imgs.device))
    fake_imgs = imgs + epsilon * noise_grad
    fake_imgs.detach_()
    return fake_imgs, noise_grad
```

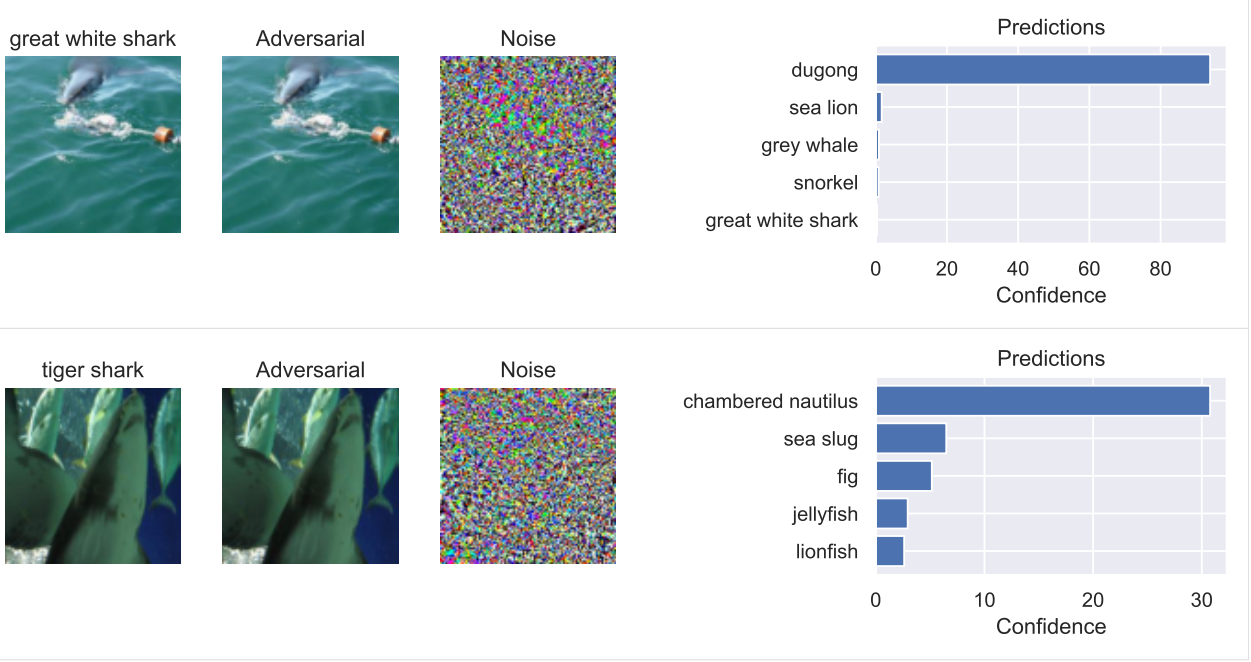
The default value of $\epsilon = 0.02$ corresponds to changing a pixel value by about 1 in the range of 0 to 255, e.g. changing 127 to 128. This difference is marginal and can often not be recognized by humans. Let's try it below on our example images:

[10]:
```
adv_imgs, noise_grad = fast_gradient_sign_method(pretrained_model, exmp_batch, label_
↪batch, epsilon=0.02)
with torch.no_grad():
    adv_preds = pretrained_model(adv_imgs.to(device))

for i in range(1,17,5):
    show_prediction(exmp_batch[i], label_batch[i], adv_preds[i], adv_img=adv_imgs[i],␣
↪noise=noise_grad[i])
```







Despite the minor amount of noise, we are able to fool the network on all of our examples. None of the labels have made it into the top-5 for the four images, showing that we indeed fooled the model. We can also check the accuracy of the model on the adversarial images:

[11]:
```
_ = eval_model(data_loader, img_func=lambda x, y: fast_gradient_sign_method(pretrained_
↪model, x, y, epsilon=0.02)[0])
```

```
HBox(children=(FloatProgress(value=0.0, description='Validating...', max=157.0,␣
↪style=ProgressStyle(descriptio...
```

```
Top-1 error: 93.56%
Top-5 error: 60.52%
```

As expected, the model is fooled on almost every image at least for the top-1 error, and more than half don't have the true label in their top-5. This is a quite significant difference compared to the error rate of 4.3% on the clean images. However, note that the predictions remain semantically similar. For instance, in the images we visualized above, the tench is still recognized as another fish, as well as the great white shark being a dugong. FGSM could be adapted to increase the probability of a specific class instead of minimizing the probability of a label, but for those, there are usually better attacks such as the adversarial patch.

Adversarial Patches

Instead of changing every pixel by a little bit, we can also try to change a small part of the image into whatever values we would like. In other words, we will create a small image patch that covers a minor part of the original image but causes the model to confidentially predict a specific class we choose. This form of attack is an even bigger threat in real-world applications than FSGM. Imagine a network in an autonomous car that receives a live image from a camera. Another driver could print out a specific pattern and put it on the back of his/her vehicle to make the autonomous car believe that the car is actually a pedestrian. Meanwhile, humans would not notice it. Tom Brown et al. proposed a way of learning such adversarial image patches robustly in 2017 and provided a short demonstration on YouTube. Interestingly, if you add a small picture of the target class (here *toaster*) to the original image, the model does not pick it up at all. A specifically designed patch, however, which only roughly looks like a toaster, can change the network's prediction instantaneously.

Let's take a closer look at how we can actually train such patches. The general idea is very similar to FSGM in the sense that we calculate gradients for the input, and update our adversarial input correspondingly. However, there are also some differences in the setup. Firstly, we do not calculate a gradient for every pixel. Instead, we replace parts of the input image with our patch and then calculate the gradients just for our patch. Secondly, we don't just do it for one image, but we want the patch to work with any possible image. Hence, we have a whole training loop where we train the patch using SGD. Lastly, image patches are usually designed to make the model predict a specific class, not just any other arbitrary class except the true label. For instance, we can try to create a patch for the class "toaster" and train the patch so that our pretrained model predicts the class "toaster" for any image with the patch in it.

Additionally, to the setup described above, there are a couple of design choices we can take. For instance, Brown et al. randomly rotated and scaled the patch during training before placing it at a random position in an input image. This makes the patch more robust to small changes and is necessary if we want to fool a neural network in a real-world application. For simplicity, we will only focus on making the patch robust to the location in the image. Given a batch of input images and a patch, we can add the patch as follows:

[12]:
```
def place_patch(img, patch):
    for i in range(img.shape[0]):
        h_offset = np.random.randint(0,img.shape[2]-patch.shape[1]-1)
        w_offset = np.random.randint(0,img.shape[3]-patch.shape[2]-1)
        img[i,:,h_offset:h_offset+patch.shape[1],w_offset:w_offset+patch.shape[2]] =␣
↪patch_forward(patch)
    return img
```

The patch itself will be an `nn.Parameter` whose values are in the range between $-\infty$ and ∞. Images are, however, naturally limited in their range, and thus we write a small function that maps the parameter into the image value range of ImageNet:

[13]:
```
TENSOR_MEANS, TENSOR_STD = torch.FloatTensor(NORM_MEAN)[:,None,None], torch.
↪FloatTensor(NORM_STD)[:,None,None]
def patch_forward(patch):
    # Map patch values from [-infty,infty] to ImageNet min and max
```

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```
    patch = (torch.tanh(patch) + 1 - 2 * TENSOR_MEANS) / (2 * TENSOR_STD)
    return patch
```

Before looking at the actual training code, we can write a small evaluation function. We evaluate the success of a patch by how many times we were able to fool the network into predicting our target class. A simple function for this is implemented below.

[14]:
```
def eval_patch(model, patch, val_loader, target_class):
    model.eval()
    tp, tp_5, counter = 0., 0., 0.
    with torch.no_grad():
        for img, img_labels in tqdm(val_loader, desc="Validating...", leave=False):
            # For stability, place the patch at 4 random locations per image, and␣
↪average the performance
            for _ in range(4):
                patch_img = place_patch(img, patch)
                patch_img = patch_img.to(device)
                img_labels = img_labels.to(device)
                pred = model(patch_img)
                # In the accuracy calculation, we need to exclude the images that are of␣
↪our target class
                # as we would not "fool" the model into predicting those
                tp += torch.logical_and(pred.argmax(dim=-1) == target_class, img_labels !
↪= target_class).sum()
                tp_5 += torch.logical_and((pred.topk(5, dim=-1)[1] == target_class).
↪any(dim=-1), img_labels != target_class).sum()
                counter += (img_labels != target_class).sum()
    acc = tp/counter
    top5 = tp_5/counter
    return acc, top5
```

Finally, we can look at the training loop. Given a model to fool, a target class to design the patch for, and a size k of the patch in the number of pixels, we first start by creating a parameter of size $3 \times k \times k$. These are the only parameters we will train, and the network itself remains untouched. We use a simple SGD optimizer with momentum to minimize the classification loss of the model given the patch in the image. While we first start with a very high loss due to the good initial performance of the network, the loss quickly decreases once we start changing the patch. In the end, the patch will represent patterns that are characteristic of the class. For instance, if we would want the model to predict a "goldfish" in every image, we would expect the pattern to look somewhat like a goldfish. Over the iterations, the model finetunes the pattern and, hopefully, achieves a high fooling accuracy.

[15]:
```
def patch_attack(model, target_class, patch_size=64, num_epochs=5):
    # Leave a small set of images out to check generalization
    # In most of our experiments, the performance on the hold-out data points
    # was as good as on the training set. Overfitting was little possible due
    # to the small size of the patches.
    train_set, val_set = torch.utils.data.random_split(dataset, [4500, 500])
    train_loader = data.DataLoader(train_set, batch_size=32, shuffle=True, drop_
↪last=True, num_workers=8)
    val_loader = data.DataLoader(val_set, batch_size=32, shuffle=False, drop_last=False,␣
↪num_workers=4)

    # Create parameter and optimizer
```

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```
    if not isinstance(patch_size, tuple):
        patch_size = (patch_size, patch_size)
    patch = nn.Parameter(torch.zeros(3, patch_size[0], patch_size[1]), requires_
↪grad=True)
    optimizer = torch.optim.SGD([patch], lr=1e-1, momentum=0.8)
    loss_module = nn.CrossEntropyLoss()

    # Training loop
    for epoch in range(num_epochs):
        t = tqdm(train_loader, leave=False)
        for img, _ in t:
            img = place_patch(img, patch)
            img = img.to(device)
            pred = model(img)
            labels = torch.zeros(img.shape[0], device=pred.device, dtype=torch.long).
↪fill_(target_class)
            loss = loss_module(pred, labels)
            optimizer.zero_grad()
            loss.mean().backward()
            optimizer.step()
            t.set_description(f"Epoch {epoch}, Loss: {loss.item():4.2f}")

    # Final validation
    acc, top5 = eval_patch(model, patch, val_loader, target_class)

    return patch.data, {"acc": acc.item(), "top5": top5.item()}
```

To get some experience with what to expect from an adversarial patch attack, we want to train multiple patches for different classes. As the training of a patch can take one or two minutes on a GPU, we have provided a couple of pre-trained patches including their results on the full dataset. The results are saved in a JSON file, which is loaded below.

[16]:
```
# Load evaluation results of the pretrained patches
json_results_file = os.path.join(CHECKPOINT_PATH, "patch_results.json")
json_results = {}
if os.path.isfile(json_results_file):
    with open(json_results_file, "r") as f:
        json_results = json.load(f)

# If you train new patches, you can save the results via calling this function
def save_results(patch_dict):
    result_dict = {cname: {psize: [t.item() if isinstance(t, torch.Tensor) else t
                                   for t in patch_dict[cname][psize]["results"]]
                           for psize in patch_dict[cname]}
                   for cname in patch_dict}
    with open(os.path.join(CHECKPOINT_PATH, "patch_results.json"), "w") as f:
        json.dump(result_dict, f, indent=4)
```

Additionally, we implement a function to train and evaluate patches for a list of classes and patch sizes. The pretrained patches include the classes *toaster*, *goldfish*, *school bus*, *lipstick*, and *pineapple*. We chose the classes arbitrarily to cover multiple domains (animals, vehicles, fruits, devices, etc.). We trained each class for three different patch sizes: 32×32 pixels, 48×48 pixels, and 64×64 pixels. We can load them in the two cells below.

[17]:
```
def get_patches(class_names, patch_sizes):
    result_dict = dict()

    # Loop over all classes and patch sizes
    for name in class_names:
        result_dict[name] = dict()
        for patch_size in patch_sizes:
            c = label_names.index(name)
            file_name = os.path.join(CHECKPOINT_PATH, f"{name}_{patch_size}_patch.pt")
            # Load patch if pretrained file exists, otherwise start training
            if not os.path.isfile(file_name):
                patch, val_results = patch_attack(pretrained_model, target_class=c,␣
↪patch_size=patch_size, num_epochs=5)
                print(f"Validation results for {name} and {patch_size}:", val_results)
                torch.save(patch, file_name)
            else:
                patch = torch.load(file_name)
            # Load evaluation results if exist, otherwise manually evaluate the patch
            if name in json_results:
                results = json_results[name][str(patch_size)]
            else:
                results = eval_patch(pretrained_model, patch, data_loader, target_
↪class=c)

            # Store results and the patches in a dict for better access
            result_dict[name][patch_size] = {
                "results": results,
                "patch": patch
            }

    return result_dict
```

Feel free to add any additional classes and/or patch sizes.

[18]:
```
class_names = ['toaster', 'goldfish', 'school bus', 'lipstick', 'pineapple']
patch_sizes = [32, 48, 64]

patch_dict = get_patches(class_names, patch_sizes)
# save_results(patch_dict) # Uncomment if you add new class names and want to save the␣
↪new results
```

Before looking at the quantitative results, we can actually visualize the patches.

[19]:
```
def show_patches():
    fig, ax = plt.subplots(len(patch_sizes), len(class_names), figsize=(len(class_
↪names)*2.2, len(patch_sizes)*2.2))
    for c_idx, cname in enumerate(class_names):
        for p_idx, psize in enumerate(patch_sizes):
            patch = patch_dict[cname][psize]["patch"]
            patch = (torch.tanh(patch) + 1) / 2 # Parameter to pixel values
            patch = patch.cpu().permute(1, 2, 0).numpy()
            patch = np.clip(patch, a_min=0.0, a_max=1.0)
            ax[p_idx][c_idx].imshow(patch)
```

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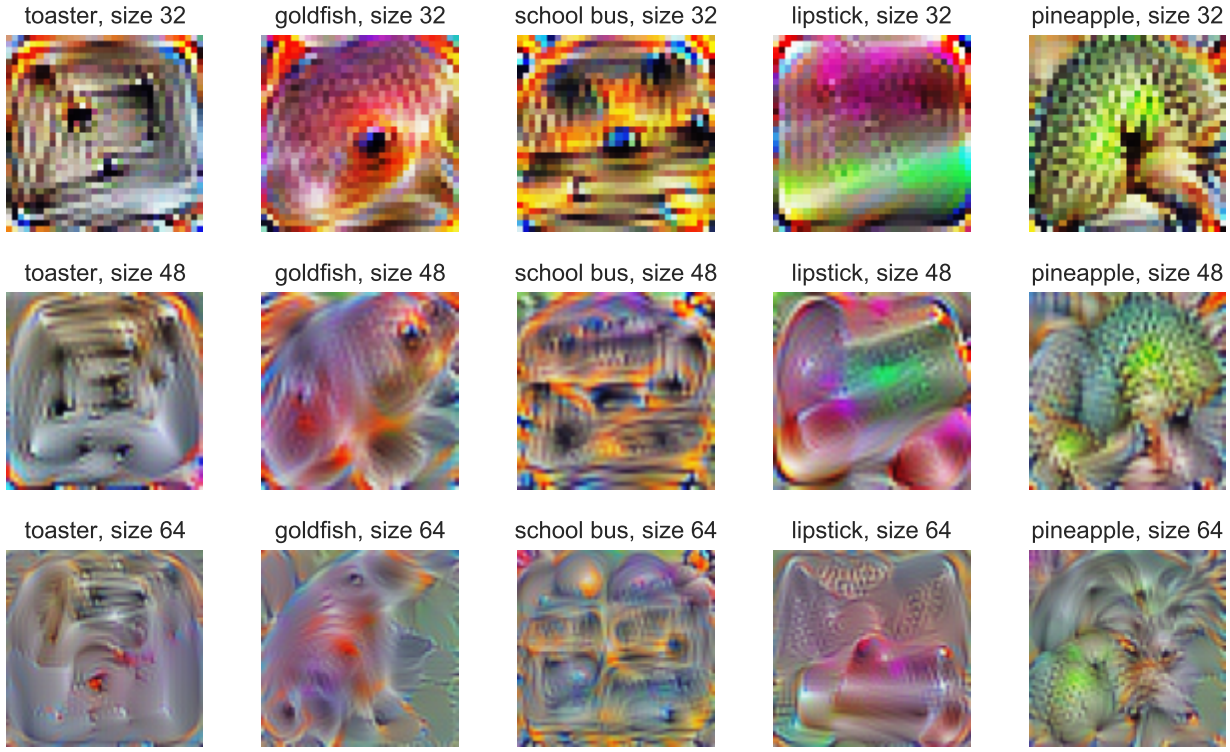
```
            ax[p_idx][c_idx].set_title(f"{cname}, size {psize}")
            ax[p_idx][c_idx].axis('off')
    fig.subplots_adjust(hspace=0.3, wspace=0.3)
    plt.show()
show_patches()
```



We can see a clear difference between patches of different classes and sizes. In the smallest size, 32×32 pixels, some of the patches clearly resemble their class. For instance, the goldfish patch clearly shows a goldfish. The eye and the color are very characteristic of the class. Overall, the patches with 32 pixels have very strong colors that are typical for their class (yellow school bus, pink lipstick, greenish pineapple). The larger the patch becomes, the more stretched the pattern becomes. For the goldfish, we can still spot regions that might represent eyes and the characteristic orange color, but it is not clearly a single fish anymore. For the pineapple, we might interpret the top part of the image as the leaves of pineapple fruit, but it is more abstract than our small patches. Nevertheless, we can easily spot the alignment of the patch to class, even on the largest scale.

Let's now look at the quantitative results.

[20]:
```
%%html
<!-- Some HTML code to increase font size in the following table -->
<style>
th {font-size: 120%;}
td {font-size: 120%;}
</style>
```

```
<IPython.core.display.HTML object>
```

[21]:
```
import tabulate
from IPython.display import display, HTML
```

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```
def show_table(top_1=True):
    i = 0 if top_1 else 1
    table = [[name] + [f"{(100.0 * patch_dict[name][psize]['results'][i]):4.2f}%" for psize in patch_sizes]
             for name in class_names]
    display(HTML(tabulate.tabulate(table, tablefmt='html', headers=["Class name"] + [f"Patch size {psize}x{psize}" for psize in patch_sizes])))
```

First, we will create a table of top-1 accuracy, meaning that how many images have been classified with the target class as highest prediction?

[22]:
```
show_table(top_1=True)
```

```
<IPython.core.display.HTML object>
```

The clear trend, that we would also have expected, is that the larger the patch, the easier it is to fool the model. For the largest patch size of 64×64, we are able to fool the model on almost all images, despite the patch covering only 8% of the image. The smallest patch actually covers 2% of the image, which is almost neglectable. Still, the fooling accuracy is quite remarkable. A large variation can be however seen across classes. While *school bus* and *pineapple* seem to be classes that were easily predicted, *toaster* and *lipstick* seem to be much harder for creating a patch. It is hard to intuitively explain why our patches underperform on those classes. Nonetheless, a fooling accuracy of >40% is still very good for such a tiny patch.

Let's also take a look at the top-5 accuracy:

[23]:
```
show_table(top_1=False)
```

```
<IPython.core.display.HTML object>
```

We see a very similar pattern across classes and patch sizes. The patch size 64 obtains >99.7% top-5 accuracy for any class, showing that we can almost fool the network on any image. A top-5 accuracy of >70% for the hard classes and small patches is still impressive and shows how vulnerable deep CNNs are to such attacks.

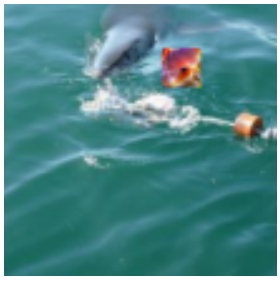
Finally, let's create some example visualizations of the patch attack in action.

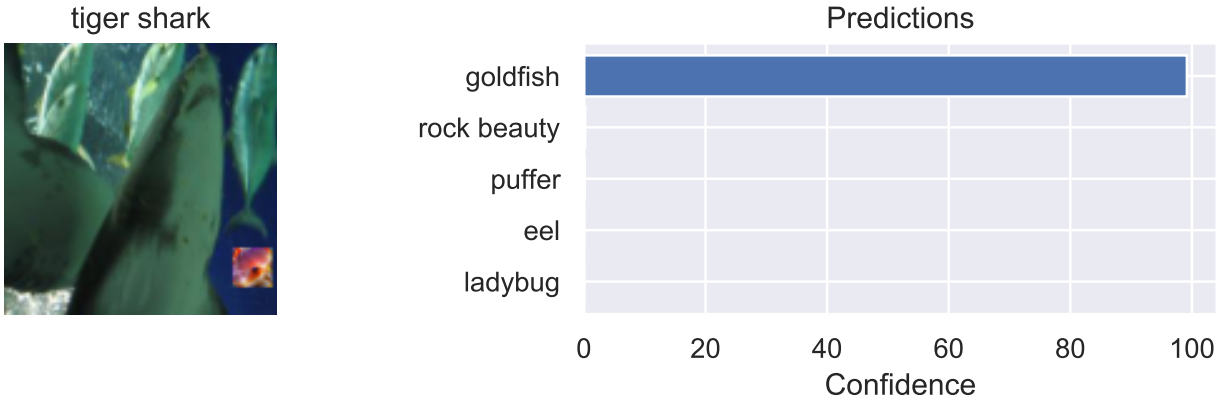
[24]:
```
def perform_patch_attack(patch):
    patch_batch = exmp_batch.clone()
    patch_batch = place_patch(patch_batch, patch)
    with torch.no_grad():
        patch_preds = pretrained_model(patch_batch.to(device))
    for i in range(1,17,5):
        show_prediction(patch_batch[i], label_batch[i], patch_preds[i])
```

[25]:
```
perform_patch_attack(patch_dict['goldfish'][32]['patch'])
```


tench
Predictions
goldfish
tench
rock beauty
barracouta
eft
0
20
40
60
Confidence

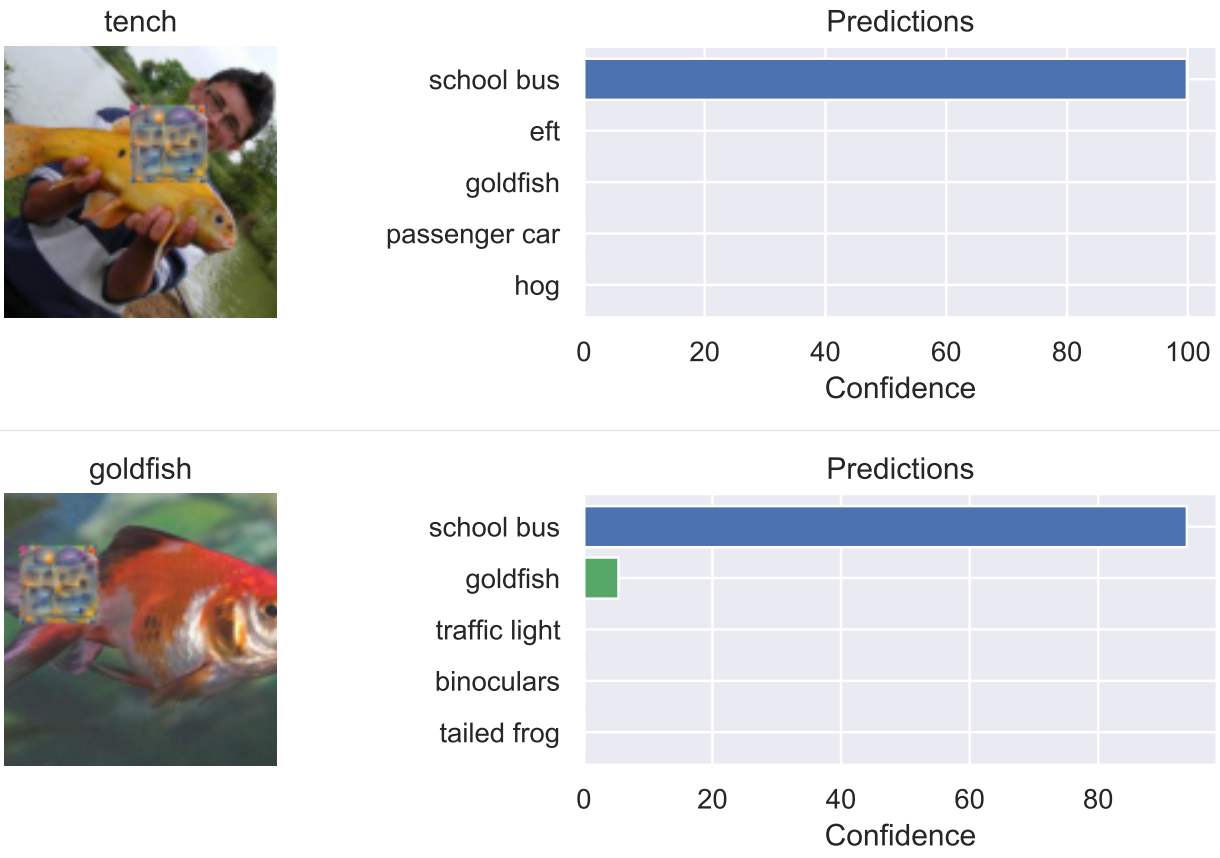

goldfish
Predictions
goldfish
tench
rock beauty
tailed frog
barracouta
0
20
40
60
80
100
Confidence

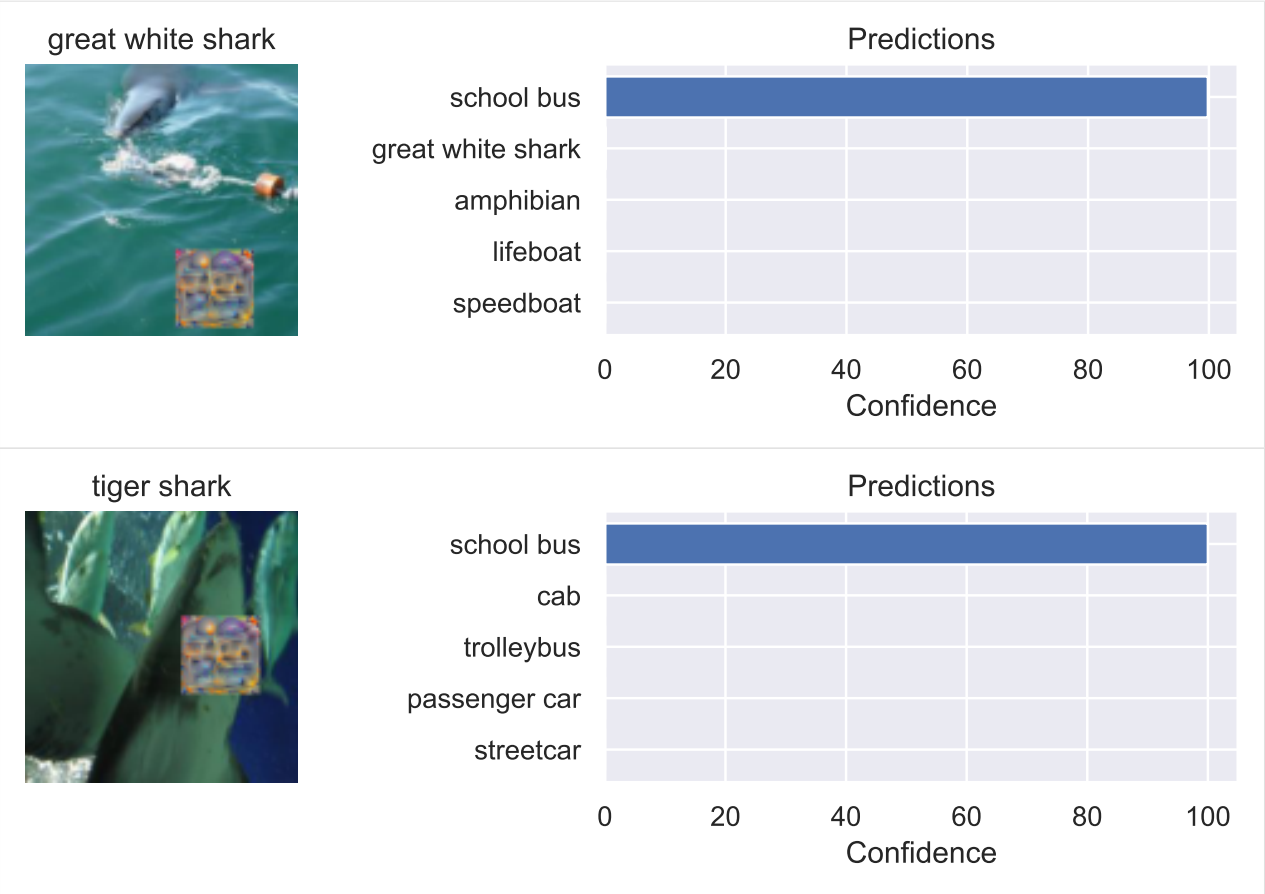

great white shark
Predictions
goldfish
great white shark
ladybug
snorkel
ice bear
0
10
20
30
40
50
Confidence



The tiny goldfish patch can change all of the predictions to "goldfish" as top class. Note that the patch attacks work especially well if the input image is semantically similar to the target class (e.g. a fish and the target class "goldfish" works better than an airplane image with that patch). Nevertheless, we can also let the network predict semantically dis-similar classes by using a larger patch:

[26]:
```
perform_patch_attack(patch_dict['school bus'][64]['patch'])
```





Although none of the images have anything to do with an American school bus, the high confidence of often 100% shows how powerful such attacks can be. With a few lines of code and access to the model, we were able to generate patches that we add to any image to make the model predict any class we want.

Transferability of white-box attacks

FGSM and the adversarial patch attack were both focused on one specific image. However, can we transfer those attacks to other models? The adversarial patch attack as proposed in Brown et al., was originally trained on multiple models, and hence was also able to work on many different network architecture. But how different are the patches for different models anyway? For instance, let's evaluate some of our patches trained above on a different network, e.g. DenseNet121.

[27]:
```
transfer_model = torchvision.models.densenet121(weights='IMAGENET1K_V1')
transfer_model = transfer_model.to(device)

# No gradients needed for the network
transfer_model.eval()
for p in transfer_model.parameters():
    p.requires_grad = False
```

Feel free to change the class name and/or patch size below to test out different patches.

[28]:
```
class_name = 'pineapple'
patch_size = 64
```

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```
print(f"Testing patch \"{class_name}\" of size {patch_size}x{patch_size}")

results = eval_patch(transfer_model,
                     patch_dict[class_name][patch_size]["patch"],
                     data_loader,
                     target_class=label_names.index(class_name))

print(f"Top-1 fool accuracy: {(results[0] * 100.0):4.2f}%")
print(f"Top-5 fool accuracy: {(results[1] * 100.0):4.2f}%")
```

```
Testing patch "pineapple" of size 64x64
```

```
HBox(children=(FloatProgress(value=0.0, description='Validating...', max=157.0,␣
↪style=ProgressStyle(descriptio...
```

```
Top-1 fool accuracy: 65.28%
Top-5 fool accuracy: 82.58%
```

Although the fool accuracy is significantly lower than on the original ResNet34, it still has a considerable impact on DenseNet although the networks have completely different architectures and weights. If you would compare more patches and models, some would work better than others. However, one aspect which allows patch attacks to generalize well is if all the networks have been trained on the same data. In this case, all networks have been trained on ImageNet. Dataset biases make the networks recognize specific patterns in the underlying image data that humans would not have seen, and/or only work for the given dataset. This is why the knowledge of what data has been used to train a specific model is already worth a lot in the context of adversarial attacks.

4.24.3 Protecting against adversarial attacks

There are many more attack strategies than just FGSM and adversarial patches that we haven't discussed and implemented ourselves here. However, what about the other perspective? What can we do to *protect* a network against adversarial attacks? The sad truth to this is: not much.

White-box attacks require access to the model and its gradient calculation. The easiest way of preventing this is by ensuring safe, private storage of the model and its weights. However, some attacks, called black-box attacks, also work without access to the model's parameters, or white-box attacks can also generalize as we have seen above on our short test on transferability.

So, how could we eventually protect a model? An intuitive approach would to train/finetune a model on such adversarial images, leading to an adversarial training similar to a GAN. During training, we would pretend to be the attacker, and use for example FGSM as an augmentation strategy. However, this usually just ends up in an oscillation of the defending network between weak spots. Another common trick to increase robustness against adversarial attacks is defensive distillation (Papernot et al.). Instead of training the model on the dataset labels, we train a secondary model on the softmax predictions of the first one. This way, the loss surface is "smoothed" in the directions an attacker might try to exploit, and it becomes more difficult for the attacker to find adversarial examples. Nevertheless, there hasn't been found the one, true strategy that works against all possible adversarial attacks.

Why are CNNs, or neural networks in general, so vulnerable to adversarial attacks? While there are many possible explanations, the most intuitive is that neural networks don't know what they don't know. Even a large dataset represents just a few sparse points in the extremely large space of possible images. A lot of the input space has not been seen by the network during training, and hence, we cannot guarantee that the prediction for those images is any useful. The network instead learns a very good classification on a smaller region, often referred to as manifold, while ignoring the points outside of it. NNs with uncertainty prediction could potentially help to discover what the network does not know. Another possible explanation lies in the activation function. As we know, most CNNs use ReLU-based activation functions. While those have enabled great success in training deep neural networks due to their stable gradient for positive values, they also constitute a possible flaw. The output range of a ReLU neuron can be arbitrarily high. Thus,

if we design a patch or the noise in the image to cause a very high value for a single neuron, it can overpower many other features in the network. Thus, although ReLU stabilizes training, it also offers a potential point of attack for adversaries.

4.24.4 Conclusion

In this tutorial, we have looked at different forms of adversarial attacks. Deep CNNs can be fooled by only slight modifications to the input. Whether it is a carefully designed noise pattern, unnoticeable for a human, or a small patch, we are able to manipulate the networks' predictions significantly. The fact that even white-box attacks can be transferable across networks, and that there exist no suitable protections against all possible adversarial attacks, make this concept a massive problem for real-world applications. While adversarial attacks can also be used for improving/training a robust model or a GAN, it is not close to being solved yet. This is also because neural networks are currently complex, unknown non-linear functions in high-dimensional looking for correlations instead of causation. In the next years, we might hopefully see an improvement in the stability of such models by using causal approaches and/or introducing uncertainty.

4.24.5 References

[1] Goodfellow, Ian J., Jonathon Shlens, and Christian Szegedy. "Explaining and harnessing adversarial examples." ICLR 2015.

[2] Hendrik Metzen, Jan, et al. "Universal adversarial perturbations against semantic image segmentation." Proceedings of the IEEE International Conference on Computer Vision. 2017.

[3] Anant Jain. "Breaking neural networks with adversarial attacks." Blog post 2019.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.25 Tutorial 11: Normalizing Flows for image modeling

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will take a closer look at complex, deep normalizing flows. The most popular, current application of deep normalizing flows is to model datasets of images. As for other generative models, images are a good domain to start working on because (1) CNNs are widely studied and strong models exist, (2) images are high-dimensional and complex, and (3) images are discrete integers. In this tutorial, we will review current advances in normalizing flows for image modeling, and get hands-on experience on coding normalizing flows. Note that normalizing flows are commonly parameter heavy and therefore computationally expensive. We will use relatively simple and shallow flows to save computational cost and allow you to run the notebook on CPU, but keep in mind that a simple way to improve the scores of the flows we study here is to make them deeper.

Throughout this notebook, we make use of PyTorch Lightning. The first cell imports our usual libraries.

[1]:
```
## Standard libraries
import os
import math
import time
import numpy as np

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## Progress bar
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import MNIST
from torchvision import transforms
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial11"
```

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```
# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

# Fetching the device that will be used throughout this notebook
device = torch.device("cpu") if not torch.cuda.is_available() else torch.device("cuda:0")
print("Using device", device)
```

```
Global seed set to 42
```

```
Using device cuda:0
```

Again, we have a few pretrained models. We download them below to the specified path above.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial11/"
# Files to download
pretrained_files = ["MNISTFlow_simple.ckpt", "MNISTFlow_vardeq.ckpt", "MNISTFlow_
↪multiscale.ckpt"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

We will use the MNIST dataset in this notebook. MNIST constitutes, despite its simplicity, a challenge for small generative models as it requires the global understanding of an image. At the same time, we can easily judge whether generated images come from the same distribution as the dataset (i.e. represent real digits), or not.

To deal better with the discrete nature of the images, we transform them from a range of 0-1 to a range of 0-255 as integers.

[3]:
```
# Convert images from 0-1 to 0-255 (integers)
def discretize(sample):
    return (sample * 255).to(torch.int32)

# Transformations applied on each image => make them a tensor and discretize
transform = transforms.Compose([transforms.ToTensor(),
```

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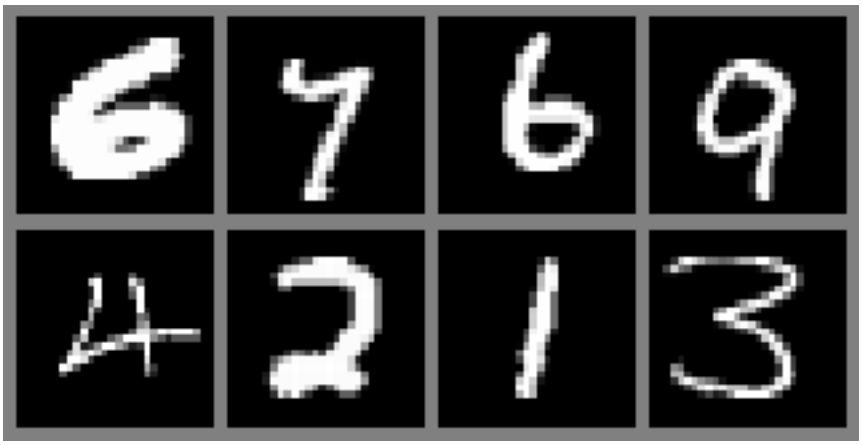
```
                                discretize])

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = MNIST(root=DATASET_PATH, train=True, transform=transform, download=True)
pl.seed_everything(42)
train_set, val_set = torch.utils.data.random_split(train_dataset, [50000, 10000])

# Loading the test set
test_set = MNIST(root=DATASET_PATH, train=False, transform=transform, download=True)

# We define a set of data loaders that we can use for various purposes later.
# Note that for actually training a model, we will use different data loaders
# with a lower batch size.
train_loader = data.DataLoader(train_set, batch_size=256, shuffle=False, drop_last=False)
val_loader = data.DataLoader(val_set, batch_size=64, shuffle=False, drop_last=False, num_
↪workers=4)
test_loader = data.DataLoader(test_set, batch_size=64, shuffle=False, drop_last=False,␣
↪num_workers=4)
```

```
Global seed set to 42
```

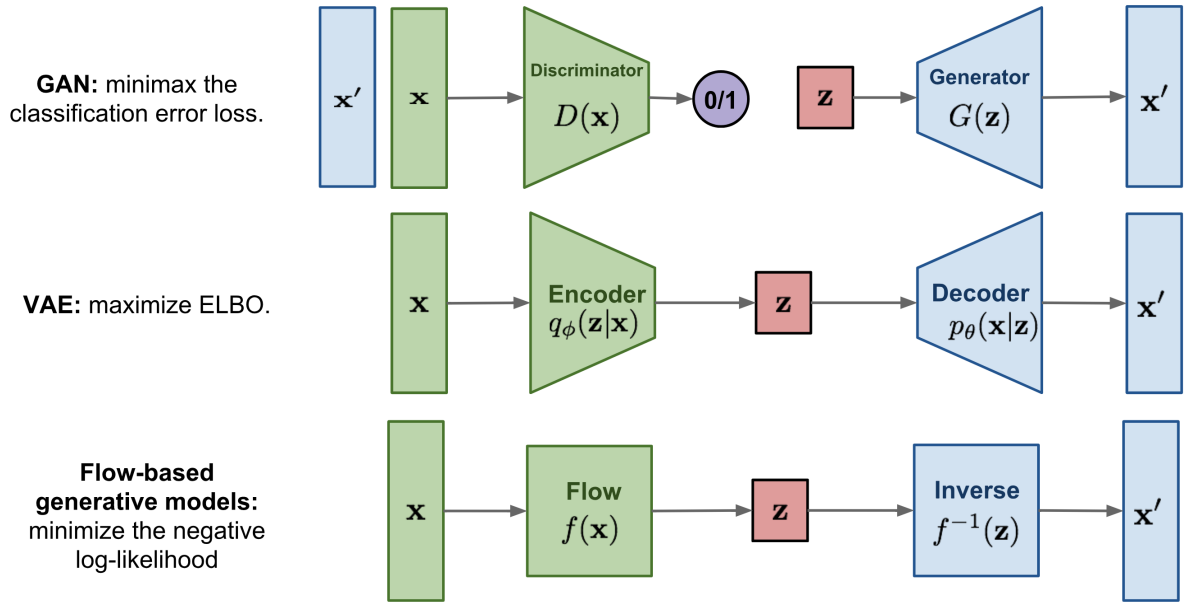
In addition, we will define below a function to simplify the visualization of images/samples. Some training examples of the MNIST dataset is shown below.

[4]:
```
def show_imgs(imgs, title=None, row_size=4):
    # Form a grid of pictures (we use max. 8 columns)
    num_imgs = imgs.shape[0] if isinstance(imgs, torch.Tensor) else len(imgs)
    is_int = imgs.dtype==torch.int32 if isinstance(imgs, torch.Tensor) else imgs[0].
↪dtype==torch.int32
    nrow = min(num_imgs, row_size)
    ncol = int(math.ceil(num_imgs/nrow))
    imgs = torchvision.utils.make_grid(imgs, nrow=nrow, pad_value=128 if is_int else 0.5)
    np_imgs = imgs.cpu().numpy()
    # Plot the grid
    plt.figure(figsize=(1.5*nrow, 1.5*ncol))
    plt.imshow(np.transpose(np_imgs, (1,2,0)), interpolation='nearest')
    plt.axis('off')
    if title is not None:
        plt.title(title)
    plt.show()
    plt.close()

show_imgs([train_set[i][0] for i in range(8)])
```



4.25.1 Normalizing Flows as generative model

In the previous lectures, we have seen Energy-based models, Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) as example of generative models. However, none of them explicitly learn the probability density function $p(x)$ of the real input data. While VAEs model a lower bound, energy-based models only implicitly learn the probability density. GANs on the other hand provide us a sampling mechanism for generating new data, without offering a likelihood estimate. The generative model we will look at here, called Normalizing Flows, actually models the true data distribution $p(x)$ and provides us with an exact likelihood estimate. Below, we can visually compare VAEs, GANs and Flows (figure credit - Lilian Weng):



The major difference compared to VAEs is that flows use *invertible* functions f to map the input data x to a latent representation z. To realize this, z must be of the same shape as x. This is in contrast to VAEs where z is usually much lower dimensional than the original input data. However, an invertible mapping also means that for every data point x, we have a corresponding latent representation z which allows us to perform lossless reconstruction (z to x). In the visualization above, this means that $x = x'$ for flows, no matter what invertible function f and input x we choose.

Nonetheless, how are normalizing flows modeling a probability density with an invertible function? The answer to this question is the rule for change of variables. Specifically, given a prior density $p_z(z)$ (e.g. Gaussian) and an invertible function f, we can determine $p_x(x)$ as follows:

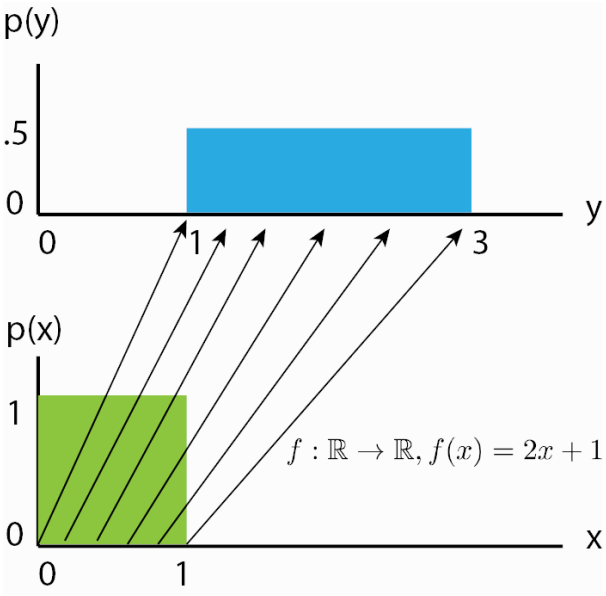
$$\int p_x(x)dx = \int p_z(z)dz = 1 \qquad \text{(by definition of a probability distribution)}$$

$$\Leftrightarrow p_x(x) = p_z(z)\left|\frac{dz}{dx}\right| = p_z(f(x))\left|\frac{df(x)}{dx}\right|$$

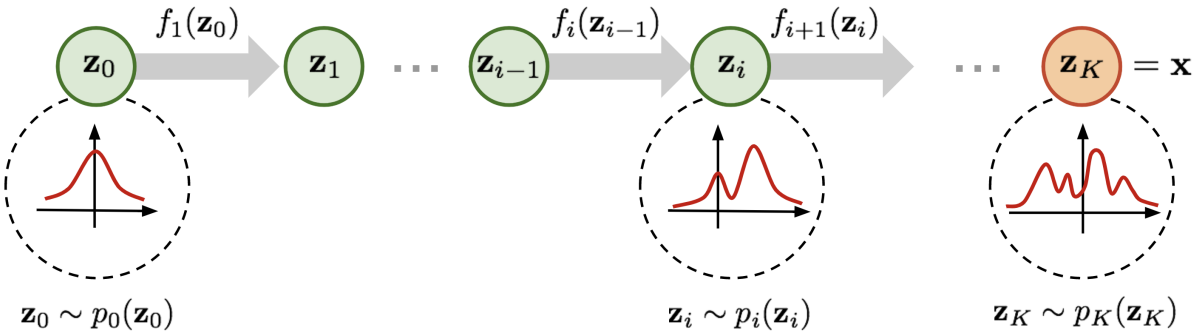
Hence, in order to determine the probability of x, we only need to determine its probability in latent space, and get the derivate of f. Note that this is for a univariate distribution, and f is required to be invertible and smooth. For a multivariate case, the derivative becomes a Jacobian of which we need to take the determinant. As we usually use the log-likelihood as objective, we write the multivariate term with logarithms below:

$$\log p_x(\mathbf{x}) = \log p_z(f(\mathbf{x})) + \log\left|\det\frac{df(\mathbf{x})}{d\mathbf{x}}\right|$$

Although we now know how a normalizing flow obtains its likelihood, it might not be clear what a normalizing flow does intuitively. For this, we should look from the inverse perspective of the flow starting with the prior probability density $p_z(z)$. If we apply an invertible function on it, we effectively "transform" its probability density. For instance, if $f^{-1}(z) = z + 1$, we shift the density by one while still remaining a valid probability distribution, and being invertible. We can also apply more complex transformations, like scaling: $f^{-1}(z) = 2z + 1$, but there you might see a difference. When you scale, you also change the volume of the probability density, as for example on uniform distributions (figure credit - Eric Jang):



You can see that the height of $p(y)$ should be lower than $p(x)$ after scaling. This change in volume represents $\left|\frac{df(x)}{dx}\right|$ in our equation above, and ensures that even after scaling, we still have a valid probability distribution. We can go on with making our function f more complex. However, the more complex f becomes, the harder it will be to find the inverse f^{-1} of it, and to calculate the log-determinant of the Jacobian $\log\left|\det\frac{df(\mathbf{x})}{d\mathbf{x}}\right|$. An easier trick to stack multiple invertible functions $f_{1,\dots,K}$ after each other, as all together, they still represent a single, invertible function. Using multiple, learnable invertible functions, a normalizing flow attempts to transform $p_z(z)$ slowly into a more complex distribution which should finally be $p_x(x)$. We visualize the idea below (figure credit - Lilian Weng):



Starting from z_0, which follows the prior Gaussian distribution, we sequentially apply the invertible functions $f_1, f_2, ..., f_K$, until z_K represents x. Note that in the figure above, the functions f represent the inverted function from f we had above (here: $f : Z \to X$, above: $f : X \to Z$). This is just a different notation and has no impact on the actual flow design because all f need to be invertible anyways. When we estimate the log likelihood of a data point x as in the equations above, we run the flows in the opposite direction than visualized above. Multiple flow layers have been proposed that use a neural network as learnable parameters, such as the planar and radial flow. However, we will focus here on flows that are commonly used in image modeling, and will discuss them in the rest of the notebook along with the details of how to train a normalizing flow.

4.25.2 Normalizing Flows on images

To become familiar with normalizing flows, especially for the application of image modeling, it is best to discuss the different elements in a flow along with the implementation. As a general concept, we want to build a normalizing flow that maps an input image (here MNIST) to an equally sized latent space:

As a first step, we will implement a template of a normalizing flow in PyTorch Lightning. During training and validation, a normalizing flow performs density estimation in the forward direction. For this, we apply a series of flow transformations on the input x and estimate the probability of the input by determining the probability of the transformed point z given a prior, and the change of volume caused by the transformations. During inference, we can do both density estimation and sampling new points by inverting the flow transformations. Therefore, we define a function `_get_likelihood` which performs density estimation, and `sample` to generate new examples. The functions `training_step`, `validation_step` and `test_step` all make use of `_get_likelihood`.

The standard metric used in generative models, and in particular normalizing flows, is bits per dimensions (bpd). Bpd is motivated from an information theory perspective and describes how many bits we would need to encode a particular example in our modeled distribution. The less bits we need, the more likely the example in our distribution. When we test for the bits per dimension of our test dataset, we can judge whether our model generalizes to new samples of the dataset and didn't memorize the training dataset. In order to calculate the bits per dimension score, we can rely on the negative log-likelihood and change the log base (as bits are binary while NLL is usually exponential):

$$\text{bpd} = \text{nll} \cdot \log_2\left(\exp(1)\right) \cdot \left(\prod d_i\right)^{-1}$$

where $d_1, ..., d_K$ are the dimensions of the input. For images, this would be the height, width and channel number. We divide the log likelihood by these extra dimensions to have a metric which we can compare for different image resolutions. In the original image space, MNIST examples have a bits per dimension score of 8 (we need 8 bits to encode each pixel as there are 256 possible values).

[5]:
```
class ImageFlow(pl.LightningModule):
```

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```
    def __init__(self, flows, import_samples=8):
        """
        Inputs:
            flows - A list of flows (each a nn.Module) that should be applied on the␣
↪images.
            import_samples - Number of importance samples to use during testing (see␣
↪explanation below). Can be changed at any time
        """
        super().__init__()
        self.flows = nn.ModuleList(flows)
        self.import_samples = import_samples
        # Create prior distribution for final latent space
        self.prior = torch.distributions.normal.Normal(loc=0.0, scale=1.0)
        # Example input for visualizing the graph
        self.example_input_array = train_set[0][0].unsqueeze(dim=0)

    def forward(self, imgs):
        # The forward function is only used for visualizing the graph
        return self._get_likelihood(imgs)

    def encode(self, imgs):
        # Given a batch of images, return the latent representation z and ldj of the␣
↪transformations
        z, ldj = imgs, torch.zeros(imgs.shape[0], device=self.device)
        for flow in self.flows:
            z, ldj = flow(z, ldj, reverse=False)
        return z, ldj

    def _get_likelihood(self, imgs, return_ll=False):
        """
        Given a batch of images, return the likelihood of those.
        If return_ll is True, this function returns the log likelihood of the input.
        Otherwise, the ouptut metric is bits per dimension (scaled negative log␣
↪likelihood)
        """
        z, ldj = self.encode(imgs)
        log_pz = self.prior.log_prob(z).sum(dim=[1,2,3])
        log_px = ldj + log_pz
        nll = -log_px
        # Calculating bits per dimension
        bpd = nll * np.log2(np.exp(1)) / np.prod(imgs.shape[1:])
        return bpd.mean() if not return_ll else log_px

    @torch.no_grad()
    def sample(self, img_shape, z_init=None):
        """
        Sample a batch of images from the flow.
        """
        # Sample latent representation from prior
        if z_init is None:
            z = self.prior.sample(sample_shape=img_shape).to(device)
        else:
```

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```
            z = z_init.to(device)

        # Transform z to x by inverting the flows
        ldj = torch.zeros(img_shape[0], device=device)
        for flow in reversed(self.flows):
            z, ldj = flow(z, ldj, reverse=True)
        return z

    def configure_optimizers(self):
        optimizer = optim.Adam(self.parameters(), lr=1e-3)
        # An scheduler is optional, but can help in flows to get the last bpd improvement
        scheduler = optim.lr_scheduler.StepLR(optimizer, 1, gamma=0.99)
        return [optimizer], [scheduler]

    def training_step(self, batch, batch_idx):
        # Normalizing flows are trained by maximum likelihood => return bpd
        loss = self._get_likelihood(batch[0])
        self.log('train_bpd', loss)
        return loss

    def validation_step(self, batch, batch_idx):
        loss = self._get_likelihood(batch[0])
        self.log('val_bpd', loss)

    def test_step(self, batch, batch_idx):
        # Perform importance sampling during testing => estimate likelihood M times for␣
↪each image
        samples = []
        for _ in range(self.import_samples):
            img_ll = self._get_likelihood(batch[0], return_ll=True)
            samples.append(img_ll)
        img_ll = torch.stack(samples, dim=-1)

        # To average the probabilities, we need to go from log-space to exp, and back to␣
↪log.
        # Logsumexp provides us a stable implementation for this
        img_ll = torch.logsumexp(img_ll, dim=-1) - np.log(self.import_samples)

        # Calculate final bpd
        bpd = -img_ll * np.log2(np.exp(1)) / np.prod(batch[0].shape[1:])
        bpd = bpd.mean()

        self.log('test_bpd', bpd)
```

The `test_step` function differs from the training and validation step in that it makes use of importance sampling. We will discuss the motiviation and details behind this after understanding how flows model discrete images in continuous space.

Dequantization

Normalizing flows rely on the rule of change of variables, which is naturally defined in continuous space. Applying flows directly on discrete data leads to undesired density models where arbitrarily high likelihood are placed on a few, particular values. See the illustration below:

The black points represent the discrete points, and the green volume the density modeled by a normalizing flow in continuous space. The flow would continue to increase the likelihood for $x = 0, 1, 2, 3$ while having no volume on any other point. Remember that in continuous space, we have the constraint that the overall volume of the probability density must be 1 ($\int p(x)dx = 1$). Otherwise, we don't model a probability distribution anymore. However, the discrete points $x = 0, 1, 2, 3$ represent delta peaks with no width in continuous space. This is why the flow can place an infinite high likelihood on these few points while still representing a distribution in continuous space. Nonetheless, the learned density does not tell us anything about the distribution among the discrete points, as in discrete space, the likelihoods of those four points would have to sum to 1, not to infinity.

To prevent such degenerated solutions, a common solution is to add a small amount of noise to each discrete value, which is also referred to as dequantization. Considering x as an integer (as it is the case for images), the dequantized representation v can be formulated as $v = x + u$ where $u \in [0, 1)^D$. Thus, the discrete value 1 is modeled by a distribution over the interval $[1.0, 2.0)$, the value 2 by an volume over $[2.0, 3.0)$, etc. Our objective of modeling $p(x)$ becomes:

$$p(x) = \int p(x+u)du = \int \frac{q(u|x)}{q(u|x)} p(x+u)du = \mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right]$$

with $q(u|x)$ being the noise distribution. For now, we assume it to be uniform, which can also be written as $p(x) = \mathbb{E}_{u \sim U(0,1)^D} [p(x+u)]$.

In the following, we will implement Dequantization as a flow transformation itself. After adding noise to the discrete values, we additionally transform the volume into a Gaussian-like shape. This is done by scaling $x + u$ between 0 and 1, and applying the invert of the sigmoid function $\sigma(z)^{-1} = \log z - \log 1 - z$. If we would not do this, we would face two problems:

1. The input is scaled between 0 and 256 while the prior distribution is a Gaussian with mean 0 and standard deviation 1. In the first iterations after initializing the parameters of the flow, we would have extremely low likelihoods for large values like 256. This would cause the training to diverge instantaneously.
2. As the output distribution is a Gaussian, it is beneficial for the flow to have a similarly shaped input distribution. This will reduce the modeling complexity that is required by the flow.

Overall, we can implement dequantization as follows:

[6]:
```
class Dequantization(nn.Module):

    def __init__(self, alpha=1e-5, quants=256):
        """
        Inputs:
            alpha - small constant that is used to scale the original input.
                    Prevents dealing with values very close to 0 and 1 when inverting␣
↪the sigmoid
            quants - Number of possible discrete values (usually 256 for 8-bit image)
        """
        super().__init__()
        self.alpha = alpha
        self.quants = quants

    def forward(self, z, ldj, reverse=False):
```

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```
        if not reverse:
            z, ldj = self.dequant(z, ldj)
            z, ldj = self.sigmoid(z, ldj, reverse=True)
        else:
            z, ldj = self.sigmoid(z, ldj, reverse=False)
            z = z * self.quants
            ldj += np.log(self.quants) * np.prod(z.shape[1:])
            z = torch.floor(z).clamp(min=0, max=self.quants-1).to(torch.int32)
        return z, ldj

    def sigmoid(self, z, ldj, reverse=False):
        # Applies an invertible sigmoid transformation
        if not reverse:
            ldj += (-z-2*F.softplus(-z)).sum(dim=[1,2,3])
            z = torch.sigmoid(z)
            # Reversing scaling for numerical stability
            ldj -= np.log(1 - self.alpha) * np.prod(z.shape[1:])
            z = (z - 0.5 * self.alpha) / (1 - self.alpha)
        else:
            z = z * (1 - self.alpha) + 0.5 * self.alpha  # Scale to prevent boundaries 0␣
↪and 1
            ldj += np.log(1 - self.alpha) * np.prod(z.shape[1:])
            ldj += (-torch.log(z) - torch.log(1-z)).sum(dim=[1,2,3])
            z = torch.log(z) - torch.log(1-z)
        return z, ldj

    def dequant(self, z, ldj):
        # Transform discrete values to continuous volumes
        z = z.to(torch.float32)
        z = z + torch.rand_like(z).detach()
        z = z / self.quants
        ldj -= np.log(self.quants) * np.prod(z.shape[1:])
        return z, ldj
```

A good check whether a flow is correctly implemented or not, is to verify that it is invertible. Hence, we will dequantize a randomly chosen training image, and then quantize it again. We would expect that we would get the exact same image out:

[7]:
```
## Testing invertibility of dequantization layer
pl.seed_everything(42)
orig_img = train_set[0][0].unsqueeze(dim=0)
ldj = torch.zeros(1,)
dequant_module = Dequantization()
deq_img, ldj = dequant_module(orig_img, ldj, reverse=False)
reconst_img, ldj = dequant_module(deq_img, ldj, reverse=True)

d1, d2 = torch.where(orig_img.squeeze() != reconst_img.squeeze())
if len(d1) != 0:
    print("Dequantization was not invertible.")
    for i in range(d1.shape[0]):
        print("Original value:", orig_img[0,0,d1[i], d2[i]].item())
        print("Reconstructed value:", reconst_img[0,0,d1[i], d2[i]].item())
```

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```
else:
    print("Successfully inverted dequantization")

# Layer is not strictly invertible due to float precision constraints
# assert (orig_img == reconst_img).all().item()
```

```
Global seed set to 42
```

```
Successfully inverted dequantization
```

The test succeeds as we would expect. However, there is a chance that the test fails due to numerical inaccuracies in the sigmoid invert. While the input space to the inverted sigmoid is scaled between 0 and 1, the output space is between $-\infty$ and ∞. And as we use 32 bits to represent the numbers (in addition to applying logs over and over again), such inaccuries can occur and should not be worrisome. Nevertheless, it is good to be aware of them, and can be improved by using a double tensor (float64).

Finally, we can take our dequantization and actually visualize the distribution it transforms the discrete values into:

[8]:
```
def visualize_dequantization(quants, prior=None):
    """
    Function for visualizing the dequantization values of discrete values in continuous␣
↪space
    """
    # Prior over discrete values. If not given, a uniform is assumed
    if prior is None:
        prior = np.ones(quants, dtype=np.float32) / quants
    prior = prior / prior.sum()  # Ensure proper categorical distribution

    inp = torch.arange(-4, 4, 0.01).view(-1, 1, 1, 1) # Possible continuous values we␣
↪want to consider
    ldj = torch.zeros(inp.shape[0])
    dequant_module = Dequantization(quants=quants)
    # Invert dequantization on continuous values to find corresponding discrete value
    out, ldj = dequant_module.forward(inp, ldj, reverse=True)
    inp, out, prob = inp.squeeze().numpy(), out.squeeze().numpy(), ldj.exp().numpy()
    prob = prob * prior[out] # Probability scaled by categorical prior

    # Plot volumes and continuous distribution
    sns.set_style("white")
    fig = plt.figure(figsize=(6,3))
    x_ticks = []
    for v in np.unique(out):
        indices = np.where(out==v)
        color = to_rgb(f"C{v}")
        plt.fill_between(inp[indices], prob[indices], np.zeros(indices[0].shape[0]),␣
↪color=color+(0.5,), label=str(v))
        plt.plot([inp[indices[0][0]]]*2,  [0, prob[indices[0][0]]],  color=color)
        plt.plot([inp[indices[0][-1]]]*2, [0, prob[indices[0][-1]]], color=color)
        x_ticks.append(inp[indices[0][0]])
    x_ticks.append(inp.max())
    plt.xticks(x_ticks, [f"{x:.1f}" for x in x_ticks])
    plt.plot(inp,prob, color=(0.0,0.0,0.0))
    # Set final plot properties
    plt.ylim(0, prob.max()*1.1)
```

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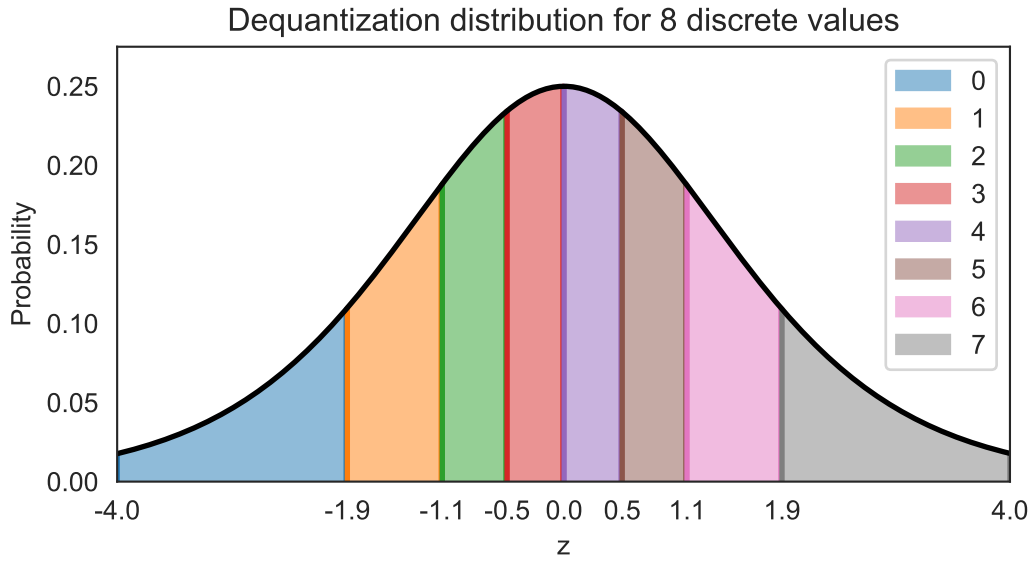
```
    plt.xlim(inp.min(), inp.max())
    plt.xlabel("z")
    plt.ylabel("Probability")
    plt.title(f"Dequantization distribution for {quants} discrete values")
    plt.legend()
    plt.show()
    plt.close()

visualize_dequantization(quants=8)
```



The visualized distribution show the sub-volumes that are assigned to the different discrete values. The value 0 has its volume between $[-\infty, -1.9)$, the value 1 is represented by the interval $[-1.9, -1.1)$, etc. The volume for each discrete value has the same probability mass. That's why the volumes close to the center (e.g. 3 and 4) have a smaller area on the z-axis as others (z is being used to denote the output of the whole dequantization flow).

Effectively, the consecutive normalizing flow models discrete images by the following objective:

$$\log p(x) = \log \mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right] \geq \mathbb{E}_u \left[\log \frac{p(x+u)}{q(u|x)} \right]$$

Although normalizing flows are exact in likelihood, we have a lower bound. Specifically, this is an example of the Jensen inequality because we need to move the log into the expectation so we can use Monte-carlo estimates. In general, this bound is considerably smaller than the ELBO in variational autoencoders. Actually, we can reduce the bound ourselves by estimating the expectation not by one, but by M samples. In other words, we can apply importance sampling which leads to the following inequality:

$$\log p(x) = \log \mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right] \geq \mathbb{E}_u \left[\log \frac{1}{M} \sum_{m=1}^{M} \frac{p(x+u_m)}{q(u_m|x)} \right] \geq \mathbb{E}_u \left[\log \frac{p(x+u)}{q(u|x)} \right]$$

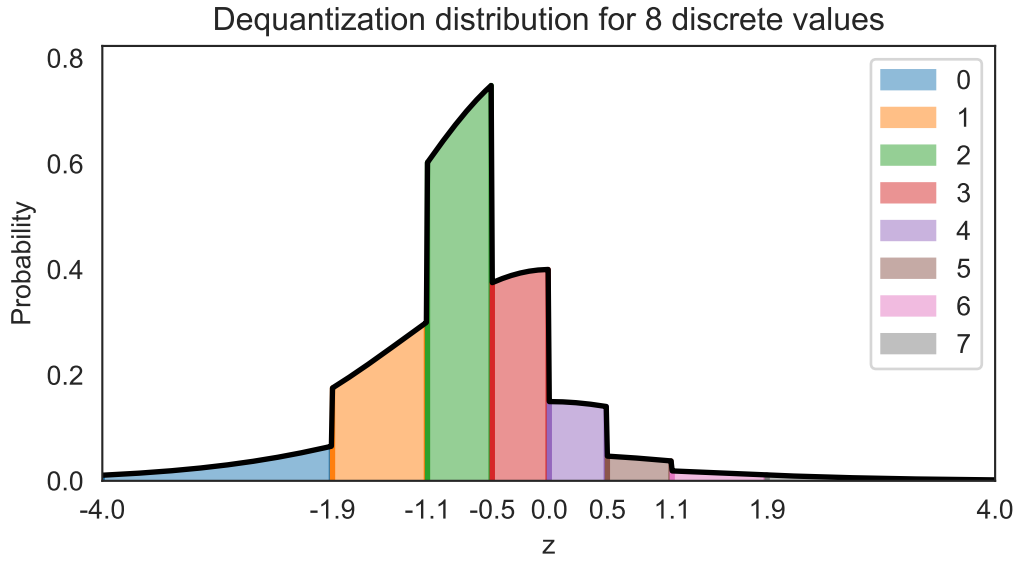
The importance sampling $\frac{1}{M} \sum_{m=1}^{M} \frac{p(x+u_m)}{q(u_m|x)}$ becomes $\mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right]$ if $M \to \infty$, so that the more samples we use, the tighter the bound is. During testing, we can make use of this property and have it implemented in `test_step` in `ImageFlow`. In theory, we could also use this tighter bound during training. However, related work has shown that this does not necessarily lead to an improvement given the additional computational cost, and it is more efficient to stick with a single estimate [5].

Variational Dequantization

Dequantization uses a uniform distribution for the noise u which effectively leads to images being represented as hypercubes (cube in high dimensions) with sharp borders. However, modeling such sharp borders is not easy for a flow as it uses smooth transformations to convert it into a Gaussian distribution.

Another way of looking at it is if we change the prior distribution in the previous visualization. Imagine we have independent Gaussian noise on pixels which is commonly the case for any real-world taken picture. Therefore, the flow would have to model a distribution as above, but with the individual volumes scaled as follows:

[9]:
```
visualize_dequantization(quants=8, prior=np.array([0.075, 0.2, 0.4, 0.2, 0.075, 0.025, 0.
↪0125, 0.0125]))
```



Transforming such a probability into a Gaussian is a difficult task, especially with such hard borders. Dequantization has therefore been extended to more sophisticated, learnable distributions beyond uniform in a variational framework. In particular, if we remember the learning objective $\log p(x) = \log \mathbb{E}_u \left[\frac{p(x+u)}{q(u|x)} \right]$, the uniform distribution can be replaced by a learned distribution $q_\theta(u|x)$ with support over $u \in [0,1)^D$. This approach is called Variational Dequantization and has been proposed by Ho et al. [3]. How can we learn such a distribution? We can use a second normalizing flow that takes x as external input and learns a flexible distribution over u. To ensure a support over $[0,1)^D$, we can apply a sigmoid activation function as final flow transformation.

Inheriting the original dequantization class, we can implement variational dequantization as follows:

[10]:
```
class VariationalDequantization(Dequantization):

    def __init__(self, var_flows, alpha=1e-5):
        """
        Inputs:
            var_flows - A list of flow transformations to use for modeling q(u|x)
            alpha - Small constant, see Dequantization for details
        """
        super().__init__(alpha=alpha)
        self.flows = nn.ModuleList(var_flows)

    def dequant(self, z, ldj):
```

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```
        z = z.to(torch.float32)
        img = (z / 255.0) * 2 - 1 # We condition the flows on x, i.e. the original image

        # Prior of u is a uniform distribution as before
        # As most flow transformations are defined on [-infinity,+infinity], we apply an␣
↪inverse sigmoid first.
        deq_noise = torch.rand_like(z).detach()
        deq_noise, ldj = self.sigmoid(deq_noise, ldj, reverse=True)
        for flow in self.flows:
            deq_noise, ldj = flow(deq_noise, ldj, reverse=False, orig_img=img)
        deq_noise, ldj = self.sigmoid(deq_noise, ldj, reverse=False)

        # After the flows, apply u as in standard dequantization
        z = (z + deq_noise) / 256.0
        ldj -= np.log(256.0) * np.prod(z.shape[1:])
        return z, ldj
```

Variational dequantization can be used as a substitute for dequantization. We will compare dequantization and variational dequantization in later experiments.

Coupling layers

Next, we look at possible transformations to apply inside the flow. A recent popular flow layer, which works well in combination with deep neural networks, is the coupling layer introduced by Dinh et al. [1]. The input z is arbitrarily split into two parts, $z_{1:j}$ and $z_{j+1:d}$, of which the first remains unchanged by the flow. Yet, $z_{1:j}$ is used to parameterize the transformation for the second part, $z_{j+1:d}$. Various transformations have been proposed in recent time [3,4], but here we will settle for the simplest and most efficient one: affine coupling. In this coupling layer, we apply an affine transformation by shifting the input by a bias μ and scale it by σ. In other words, our transformation looks as follows:

$$z'_{j+1:d} = \mu_\theta(z_{1:j}) + \sigma_\theta(z_{1:j}) \odot z_{j+1:d}$$

The functions μ and σ are implemented as a shared neural network, and the sum and multiplication are performed element-wise. The LDJ is thereby the sum of the logs of the scaling factors: $\sum_i [\log \sigma_\theta(z_{1:j})]_i$. Inverting the layer can as simply be done as subtracting the bias and dividing by the scale:

$$z_{j+1:d} = \left(z'_{j+1:d} - \mu_\theta(z_{1:j})\right) / \sigma_\theta(z_{1:j})$$

We can also visualize the coupling layer in form of a computation graph, where z_1 represents $z_{1:j}$, and z_2 represents $z_{j+1:d}$:

In our implementation, we will realize the splitting of variables as masking. The variables to be transformed, $z_{j+1:d}$, are masked when passing z to the shared network to predict the transformation parameters. When applying the transformation, we mask the parameters for $z_{1:j}$ so that we have an identity operation for those variables:

[11]:
```
class CouplingLayer(nn.Module):

    def __init__(self, network, mask, c_in):
        """
        Coupling layer inside a normalizing flow.
        Inputs:
            network - A PyTorch nn.Module constituting the deep neural network for mu␣
↪and sigma.
```

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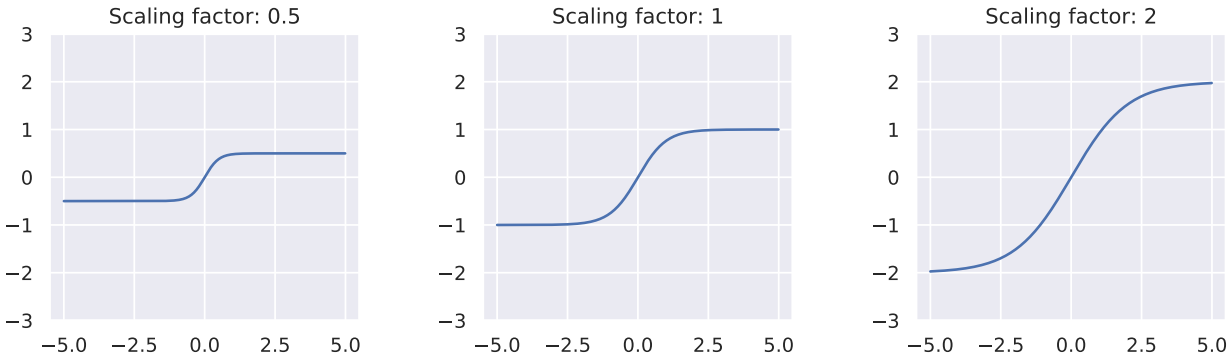
```
                    Output shape should be twice the channel size as the input.
            mask - Binary mask (0 or 1) where 0 denotes that the element should be␣
↪transformed,
                   while 1 means the latent will be used as input to the NN.
            c_in - Number of input channels
        """
        super().__init__()
        self.network = network
        self.scaling_factor = nn.Parameter(torch.zeros(c_in))
        # Register mask as buffer as it is a tensor which is not a parameter,
        # but should be part of the modules state.
        self.register_buffer('mask', mask)

    def forward(self, z, ldj, reverse=False, orig_img=None):
        """
        Inputs:
            z - Latent input to the flow
            ldj - The current ldj of the previous flows.
                  The ldj of this layer will be added to this tensor.
            reverse - If True, we apply the inverse of the layer.
            orig_img (optional) - Only needed in VarDeq. Allows external
                                  input to condition the flow on (e.g. original image)
        """
        # Apply network to masked input
        z_in = z * self.mask
        if orig_img is None:
            nn_out = self.network(z_in)
        else:
            nn_out = self.network(torch.cat([z_in, orig_img], dim=1))
        s, t = nn_out.chunk(2, dim=1)

        # Stabilize scaling output
        s_fac = self.scaling_factor.exp().view(1, -1, 1, 1)
        s = torch.tanh(s / s_fac) * s_fac

        # Mask outputs (only transform the second part)
        s = s * (1 - self.mask)
        t = t * (1 - self.mask)

        # Affine transformation
        if not reverse:
            # Whether we first shift and then scale, or the other way round,
            # is a design choice, and usually does not have a big impact
            z = (z + t) * torch.exp(s)
            ldj += s.sum(dim=[1,2,3])
        else:
            z = (z * torch.exp(-s)) - t
            ldj -= s.sum(dim=[1,2,3])

        return z, ldj
```

For stabilization purposes, we apply a $\tanh$ activation function on the scaling output. This prevents sudden large output values for the scaling that can destabilize training. To still allow scaling factors smaller or larger than -1 and 1

respectively, we have a learnable parameter per dimension, called `scaling_factor`. This scales the tanh to different limits. Below, we visualize the effect of the scaling factor on the output activation of the scaling terms:

[12]:
```
with torch.no_grad():
    x = torch.arange(-5,5,0.01)
    scaling_factors = [0.5, 1, 2]
    sns.set()
    fig, ax = plt.subplots(1, 3, figsize=(12,3))
    for i, scale in enumerate(scaling_factors):
        y = torch.tanh(x / scale) * scale
        ax[i].plot(x.numpy(), y.numpy())
        ax[i].set_title("Scaling factor: " + str(scale))
        ax[i].set_ylim(-3, 3)
    plt.subplots_adjust(wspace=0.4)
    sns.reset_orig()
    plt.show()
```



Coupling layers generalize to any masking technique we could think of. However, the most common approach for images is to split the input z in half, using a checkerboard mask or channel mask. A checkerboard mask splits the variables across the height and width dimensions and assigns each other pixel to $z_{j+1:d}$. Thereby, the mask is shared across channels. In contrast, the channel mask assigns half of the channels to $z_{j+1:d}$, and the other half to $z_{1:j+1}$. Note that when we apply multiple coupling layers, we invert the masking for each other layer so that each variable is transformed a similar amount of times.

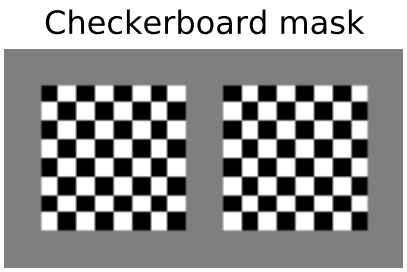
Let's implement a function that creates a checkerboard mask and a channel mask for us:

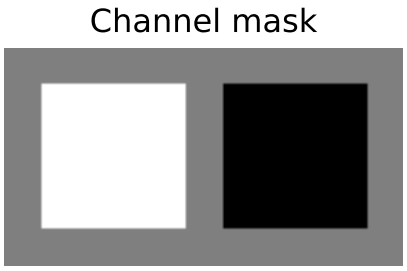
[13]:
```
def create_checkerboard_mask(h, w, invert=False):
    x, y = torch.arange(h, dtype=torch.int32), torch.arange(w, dtype=torch.int32)
    xx, yy = torch.meshgrid(x, y, indexing='ij')
    mask = torch.fmod(xx + yy, 2)
    mask = mask.to(torch.float32).view(1, 1, h, w)
    if invert:
        mask = 1 - mask
    return mask

def create_channel_mask(c_in, invert=False):
    mask = torch.cat([torch.ones(c_in//2, dtype=torch.float32),
                      torch.zeros(c_in-c_in//2, dtype=torch.float32)])
    mask = mask.view(1, c_in, 1, 1)
    if invert:
        mask = 1 - mask
    return mask
```

We can also visualize the corresponding masks for an image of size $8 \times 8 \times 2$ (2 channels):

[14]:
```
checkerboard_mask = create_checkerboard_mask(h=8, w=8).expand(-1,2,-1,-1)
channel_mask = create_channel_mask(c_in=2).expand(-1,-1,8,8)

show_imgs(checkerboard_mask.transpose(0,1), "Checkerboard mask")
show_imgs(channel_mask.transpose(0,1), "Channel mask")
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/torch/functional.py:568:␣
↪UserWarning: torch.meshgrid: in an upcoming release, it will be required to pass the␣
↪indexing argument. (Triggered internally at  /opt/conda/conda-bld/pytorch_
↪1646755953518/work/aten/src/ATen/native/TensorShape.cpp:2228.)
  return _VF.meshgrid(tensors, **kwargs)  # type: ignore[attr-defined]
```





As a last aspect of coupling layers, we need to decide for the deep neural network we want to apply in the coupling layers. The input to the layers is an image, and hence we stick with a CNN. Because the input to a transformation depends on all transformations before, it is crucial to ensure a good gradient flow through the CNN back to the input, which can be optimally achieved by a ResNet-like architecture. Specifically, we use a Gated ResNet that adds a σ-gate to the skip connection, similarly to the input gate in LSTMs. The details are not necessarily important here, and the network is strongly inspired from Flow++ [3] in case you are interested in building even stronger models.

[15]:
```
class ConcatELU(nn.Module):
    """
    Activation function that applies ELU in both direction (inverted and plain).
    Allows non-linearity while providing strong gradients for any input (important for␣
↪final convolution)
    """

    def forward(self, x):
        return torch.cat([F.elu(x), F.elu(-x)], dim=1)


class LayerNormChannels(nn.Module):
```

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```
    def __init__(self, c_in, eps=1e-5):
        """
        This module applies layer norm across channels in an image.
        Inputs:
            c_in - Number of channels of the input
            eps - Small constant to stabilize std
        """
        super().__init__()
        self.gamma = nn.Parameter(torch.ones(1, c_in, 1, 1))
        self.beta = nn.Parameter(torch.zeros(1, c_in, 1, 1))
        self.eps = eps

    def forward(self, x):
        mean = x.mean(dim=1, keepdim=True)
        var = x.var(dim=1, unbiased=False, keepdim=True)
        y = (x - mean) / torch.sqrt(var + self.eps)
        y = y * self.gamma + self.beta
        return y


class GatedConv(nn.Module):

    def __init__(self, c_in, c_hidden):
        """
        This module applies a two-layer convolutional ResNet block with input gate
        Inputs:
            c_in - Number of channels of the input
            c_hidden - Number of hidden dimensions we want to model (usually similar to␣
↪c_in)
        """
        super().__init__()
        self.net = nn.Sequential(
            ConcatELU(),
            nn.Conv2d(2*c_in, c_hidden, kernel_size=3, padding=1),
            ConcatELU(),
            nn.Conv2d(2*c_hidden, 2*c_in, kernel_size=1)
        )

    def forward(self, x):
        out = self.net(x)
        val, gate = out.chunk(2, dim=1)
        return x + val * torch.sigmoid(gate)


class GatedConvNet(nn.Module):

    def __init__(self, c_in, c_hidden=32, c_out=-1, num_layers=3):
        """
        Module that summarizes the previous blocks to a full convolutional neural␣
↪network.
        Inputs:
            c_in - Number of input channels
```

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```
            c_hidden - Number of hidden dimensions to use within the network
            c_out - Number of output channels. If -1, 2 times the input channels are␣
↪used (affine coupling)
            num_layers - Number of gated ResNet blocks to apply
        """
        super().__init__()
        c_out = c_out if c_out > 0 else 2 * c_in
        layers = []
        layers += [nn.Conv2d(c_in, c_hidden, kernel_size=3, padding=1)]
        for layer_index in range(num_layers):
            layers += [GatedConv(c_hidden, c_hidden),
                       LayerNormChannels(c_hidden)]
        layers += [ConcatELU(),
                   nn.Conv2d(2*c_hidden, c_out, kernel_size=3, padding=1)]
        self.nn = nn.Sequential(*layers)

        self.nn[-1].weight.data.zero_()
        self.nn[-1].bias.data.zero_()

    def forward(self, x):
        return self.nn(x)
```

Training loop

Finally, we can add Dequantization, Variational Dequantization and Coupling Layers together to build our full normalizing flow on MNIST images. We apply 8 coupling layers in the main flow, and 4 for variational dequantization if applied. We apply a checkerboard mask throughout the network as with a single channel (black-white images), we cannot apply channel mask. The overall architecture is visualized below.

[16]:
```
def create_simple_flow(use_vardeq=True):
    flow_layers = []
    if use_vardeq:
        vardeq_layers = [CouplingLayer(network=GatedConvNet(c_in=2, c_out=2, c_
↪hidden=16),
                                       mask=create_checkerboard_mask(h=28, w=28,␣
↪invert=(i%2==1)),
                                       c_in=1) for i in range(4)]
        flow_layers += [VariationalDequantization(var_flows=vardeq_layers)]
    else:
        flow_layers += [Dequantization()]

    for i in range(8):
        flow_layers += [CouplingLayer(network=GatedConvNet(c_in=1, c_hidden=32),
                                      mask=create_checkerboard_mask(h=28, w=28, invert=(i
↪%2==1)),
                                      c_in=1)]

    flow_model = ImageFlow(flow_layers).to(device)
    return flow_model
```

For implementing the training loop, we use the framework of PyTorch Lightning and reduce the code overhead. If interested, you can take a look at the generated tensorboard file, in particularly the graph to see an overview of flow transformations that are applied. Note that we again provide pre-trained models (see later on in the notebook) as normalizing flows are particularly expensive to train. We have also run validation and testing as this can take some time as well with the added importance sampling.

[17]:
```
def train_flow(flow, model_name="MNISTFlow"):
    # Create a PyTorch Lightning trainer
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, model_name),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=200,
                         gradient_clip_val=1.0,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="min",␣
↪monitor="val_bpd"),
                                    LearningRateMonitor("epoch")],
                         check_val_every_n_epoch=5)
    trainer.logger._log_graph = True
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    train_data_loader = data.DataLoader(train_set, batch_size=128, shuffle=True, drop_
↪last=True, pin_memory=True, num_workers=8)
    result = None

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, model_name + ".ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        ckpt = torch.load(pretrained_filename, map_location=device)
        flow.load_state_dict(ckpt['state_dict'])
        result = ckpt.get("result", None)
    else:
        print("Start training", model_name)
        trainer.fit(flow, train_data_loader, val_loader)

    # Test best model on validation and test set if no result has been found
    # Testing can be expensive due to the importance sampling.
    if result is None:
        val_result = trainer.test(flow, val_loader, verbose=False)
        start_time = time.time()
        test_result = trainer.test(flow, test_loader, verbose=False)
        duration = time.time() - start_time
        result = {"test": test_result, "val": val_result, "time": duration / len(test_
↪loader) / flow.import_samples}

    return flow, result
```

4.25.3 Multi-scale architecture

One disadvantage of normalizing flows is that they operate on the exact same dimensions as the input. If the input is high-dimensional, so is the latent space, which requires larger computational cost to learn suitable transformations. However, particularly in the image domain, many pixels contain less information in the sense that we could remove them without loosing the semantical information of the image.

Based on this intuition, deep normalizing flows on images commonly apply a multi-scale architecture [1]. After the first N flow transformations, we split off half of the latent dimensions and directly evaluate them on the prior. The other half is run through N more flow transformations, and depending on the size of the input, we split it again in half or stop overall at this position. The two operations involved in this setup is `Squeeze` and `Split` which we will review more closely and implement below.

Squeeze and Split

When we want to remove half of the pixels in an image, we have the problem of deciding which variables to cut, and how to rearrange the image. Thus, the squeezing operation is commonly used before split, which divides the image into subsquares of shape $2 \times 2 \times C$, and reshapes them into $1 \times 1 \times 4C$ blocks. Effectively, we reduce the height and width of the image by a factor of 2 while scaling the number of channels by 4. Afterwards, we can perform the split operation over channels without the need of rearranging the pixels. The smaller scale also makes the overall architecture more efficient. Visually, the squeeze operation should transform the input as follows:

The input of $4 \times 4 \times 1$ is scaled to $2 \times 2 \times 4$ following the idea of grouping the pixels in $2 \times 2 \times 1$ subsquares. Next, let's try to implement this layer:

[18]:
```
class SqueezeFlow(nn.Module):

    def forward(self, z, ldj, reverse=False):
        B, C, H, W = z.shape
        if not reverse:
            # Forward direction: H x W x C => H/2 x W/2 x 4C
            z = z.reshape(B, C, H//2, 2, W//2, 2)
            z = z.permute(0, 1, 3, 5, 2, 4)
            z = z.reshape(B, 4*C, H//2, W//2)
        else:
            # Reverse direction: H/2 x W/2 x 4C => H x W x C
            z = z.reshape(B, C//4, 2, 2, H, W)
            z = z.permute(0, 1, 4, 2, 5, 3)
            z = z.reshape(B, C//4, H*2, W*2)
        return z, ldj
```

Before moving on, we can verify our implementation by comparing our output with the example figure above:

[19]:
```
sq_flow = SqueezeFlow()
rand_img = torch.arange(1,17).view(1, 1, 4, 4)
print("Image (before)\n", rand_img)
forward_img, _ = sq_flow(rand_img, ldj=None, reverse=False)
print("\nImage (forward)\n", forward_img.permute(0,2,3,1)) # Permute for readability
reconst_img, _ = sq_flow(forward_img, ldj=None, reverse=True)
print("\nImage (reverse)\n", reconst_img)
```

```
Image (before)
 tensor([[[[ 1,  2,  3,  4],
```

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```
          [ 5,  6,  7,  8],
          [ 9, 10, 11, 12],
          [13, 14, 15, 16]]]])

Image (forward)
 tensor([[[[ 1,  2,  5,  6],
          [ 3,  4,  7,  8]],

         [[ 9, 10, 13, 14],
          [11, 12, 15, 16]]]])

Image (reverse)
 tensor([[[[ 1,  2,  3,  4],
          [ 5,  6,  7,  8],
          [ 9, 10, 11, 12],
          [13, 14, 15, 16]]]])
```

The split operation divides the input into two parts, and evaluates one part directly on the prior. So that our flow operation fits to the implementation of the previous layers, we will return the prior probability of the first part as the log determinant jacobian of the layer. It has the same effect as if we would combine all variable splits at the end of the flow, and evaluate them together on the prior.

[20]:
```
class SplitFlow(nn.Module):

    def __init__(self):
        super().__init__()
        self.prior = torch.distributions.normal.Normal(loc=0.0, scale=1.0)

    def forward(self, z, ldj, reverse=False):
        if not reverse:
            z, z_split = z.chunk(2, dim=1)
            ldj += self.prior.log_prob(z_split).sum(dim=[1,2,3])
        else:
            z_split = self.prior.sample(sample_shape=z.shape).to(device)
            z = torch.cat([z, z_split], dim=1)
            ldj -= self.prior.log_prob(z_split).sum(dim=[1,2,3])
        return z, ldj
```

Building a multi-scale flow

After defining the squeeze and split operation, we are finally able to build our own multi-scale flow. Deep normalizing flows such as Glow and Flow++ [2,3] often apply a split operation directly after squeezing. However, with shallow flows, we need to be more thoughtful about where to place the split operation as we need at least a minimum amount of transformations on each variable. Our setup is inspired by the original RealNVP architecture [1] which is shallower than other, more recent state-of-the-art architectures.

Hence, for the MNIST dataset, we will apply the first squeeze operation after two coupling layers, but don't apply a split operation yet. Because we have only used two coupling layers and each the variable has been only transformed once, a split operation would be too early. We apply two more coupling layers before finally applying a split flow and squeeze again. The last four coupling layers operate on a scale of $7 \times 7 \times 8$. The full flow architecture is shown below.

Note that while the feature maps inside the coupling layers reduce with the height and width of the input, the increased number of channels is not directly considered. To counteract this, we increase the hidden dimensions for the coupling layers on the squeezed input. The dimensions are often scaled by 2 as this approximately increases the computation cost by 4 canceling with the squeezing operation. However, we will choose the hidden dimensionalities $32, 48, 64$ for the three scales respectively to keep the number of parameters reasonable and show the efficiency of multi-scale architectures.

[21]:
```
def create_multiscale_flow():
    flow_layers = []

    vardeq_layers = [CouplingLayer(network=GatedConvNet(c_in=2, c_out=2, c_hidden=16),
                                   mask=create_checkerboard_mask(h=28, w=28, invert=(i
↪%2==1)),
                                   c_in=1) for i in range(4)]
    flow_layers += [VariationalDequantization(vardeq_layers)]

    flow_layers += [CouplingLayer(network=GatedConvNet(c_in=1, c_hidden=32),
                                  mask=create_checkerboard_mask(h=28, w=28, invert=(i
↪%2==1)),
                                  c_in=1) for i in range(2)]
    flow_layers += [SqueezeFlow()]
    for i in range(2):
        flow_layers += [CouplingLayer(network=GatedConvNet(c_in=4, c_hidden=48),
                                      mask=create_channel_mask(c_in=4, invert=(i%2==1)),
                                      c_in=4)]
    flow_layers += [SplitFlow(),
                    SqueezeFlow()]
    for i in range(4):
        flow_layers += [CouplingLayer(network=GatedConvNet(c_in=8, c_hidden=64),
                                      mask=create_channel_mask(c_in=8, invert=(i%2==1)),
                                      c_in=8)]

    flow_model = ImageFlow(flow_layers).to(device)
    return flow_model
```

We can show the difference in number of parameters below:

[22]:
```
def print_num_params(model):
    num_params = sum([np.prod(p.shape) for p in model.parameters()])
    print("Number of parameters: {:,}".format(num_params))

print_num_params(create_simple_flow(use_vardeq=False))
print_num_params(create_simple_flow(use_vardeq=True))
print_num_params(create_multiscale_flow())
```

```
Number of parameters: 556,312
Number of parameters: 628,388
Number of parameters: 1,711,818
```

Although the multi-scale flow has almost 3 times the parameters of the single scale flow, it is not necessarily more computationally expensive than its counterpart. We will compare the runtime in the following experiments as well.

4.25.4 Analysing the flows

In the last part of the notebook, we will train all the models we have implemented above, and try to analyze the effect of the multi-scale architecture and variational dequantization.

Training flow variants

Before we can analyse the flow models, we need to train them first. We provide pre-trained models that contain the validation and test performance, and run-time information. As flow models are computationally expensive, we advice you to rely on those pretrained models for a first run through the notebook.

[23]:
```
flow_dict = {"simple": {}, "vardeq": {}, "multiscale": {}}
flow_dict["simple"]["model"], flow_dict["simple"]["result"] = train_flow(create_simple_
↪flow(use_vardeq=False), model_name="MNISTFlow_simple")
flow_dict["vardeq"]["model"], flow_dict["vardeq"]["result"] = train_flow(create_simple_
↪flow(use_vardeq=True), model_name="MNISTFlow_vardeq")
flow_dict["multiscale"]["model"], flow_dict["multiscale"]["result"] = train_flow(create_
↪multiscale_flow(), model_name="MNISTFlow_multiscale")
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
```

```
Found pretrained model, loading...
Found pretrained model, loading...
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
```

```
Found pretrained model, loading...
```

[24]:
```
flow_dict["simple"]["result"]
```

[24]:
```
{'test': [{'test_bpd': 1.07839834690094}],
 'val': [{'test_bpd': 1.0798484086990356}],
 'time': 0.019570968523147,
 'samp_time': 0.017716965675354003}
```

Density modeling and sampling

Firstly, we can compare the models on their quantitative results. The following table shows all important statistics. The inference time specifies the time needed to determine the probability for a batch of 64 images for each model, and the sampling time the duration it took to sample a batch of 64 images.

[25]:
```
%%html
<!-- Some HTML code to increase font size in the following table -->
<style>
```

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```
th {font-size: 120%;}
td {font-size: 120%;}
</style>
```

```
<IPython.core.display.HTML object>
```

[26]:
```
import tabulate
from IPython.display import display, HTML

table = [[key,
          "%4.3f bpd" % flow_dict[key]["result"]["val"][0]["test_bpd"],
          "%4.3f bpd" % flow_dict[key]["result"]["test"][0]["test_bpd"],
          "%2.0f ms" % (1000 * flow_dict[key]["result"]["time"]),
          "%2.0f ms" % (1000 * flow_dict[key]["result"].get("samp_time", 0)),
          "{:,}".format(sum([np.prod(p.shape) for p in flow_dict[key]["model"].
↪parameters()]))]
         for key in flow_dict]
display(HTML(tabulate.tabulate(table, tablefmt='html', headers=["Model", "Validation Bpd
↪", "Test Bpd", "Inference time", "Sampling time", "Num Parameters"])))
```

```
<IPython.core.display.HTML object>
```

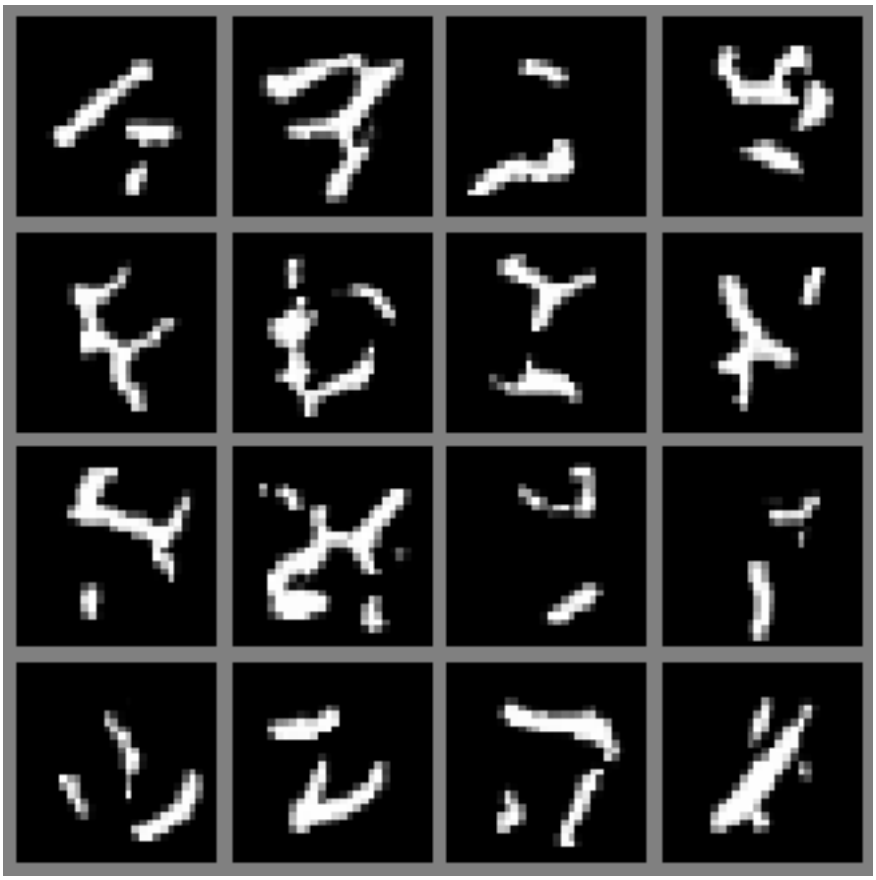
As we have intially expected, using variational dequantization improves upon standard dequantization in terms of bits per dimension. Although the difference with 0.04bpd doesn't seem impressive first, it is a considerably step for generative models (most state-of-the-art models improve upon previous models in a range of 0.02-0.1bpd on CIFAR with three times as high bpd). While it takes longer to evaluate the probability of an image due to the variational dequantization, which also leads to a longer training time, it does not have an effect on the sampling time. This is because inverting variational dequantization is the same as dequantization: finding the next lower integer.

When we compare the two models to multi-scale architecture, we can see that the bits per dimension score again dropped by about 0.02bpd. Additionally, the sampling time improved notably despite having more parameters. Thus, we see that the multi-scale flow is not only stronger for density modeling, but also more efficient.

Next, we can test the sampling quality of the models. We should note that the samples for variational dequantization and standard dequantization are very similar, and hence we visualize here only the ones for variational dequantization and the multi-scale model. However, feel free to also test out the `"simple"` model. The seeds are set to obtain reproducable generations and are not cherry picked.

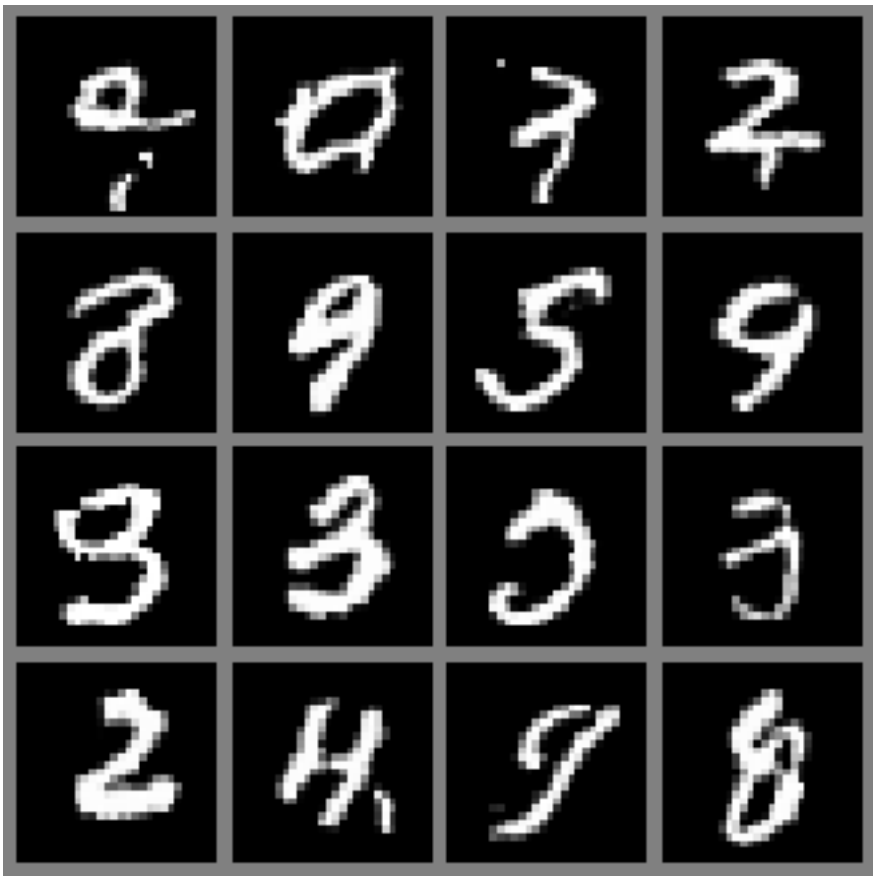
[27]:
```
pl.seed_everything(44)
samples = flow_dict["vardeq"]["model"].sample(img_shape=[16,1,28,28])
show_imgs(samples.cpu())
```

```
Global seed set to 44
```



[28]:
```
pl.seed_everything(42)
samples = flow_dict["multiscale"]["model"].sample(img_shape=[16,8,7,7])
show_imgs(samples.cpu())
```

```
Global seed set to 42
```



From the few samples, we can see a clear difference between the simple and the multi-scale model. The single-scale model has only learned local, small correlations while the multi-scale model was able to learn full, global relations that form digits. This show-cases another benefit of the multi-scale model. In contrast to VAEs, the outputs are sharp as normalizing flows can naturally model complex, multi-modal distributions while VAEs have the independent decoder output noise. Nevertheless, the samples from this flow are far from perfect as not all samples show true digits.

Interpolation in latent space

Another popular test for the smoothness of the latent space of generative models is to interpolate between two training examples. As normalizing flows are strictly invertible, we can guarantee that any image is represented in the latent space. We again compare the variational dequantization model with the multi-scale model below.

[29]:
```
@torch.no_grad()
def interpolate(model, img1, img2, num_steps=8):
    """
    Inputs:
        model - object of ImageFlow class that represents the (trained) flow model
        img1, img2 - Image tensors of shape [1, 28, 28]. Images between which should be␣
↪interpolated.
        num_steps - Number of interpolation steps. 8 interpolation steps mean 6␣
↪intermediate pictures besides img1 and img2
    """
    imgs = torch.stack([img1, img2], dim=0).to(model.device)
```

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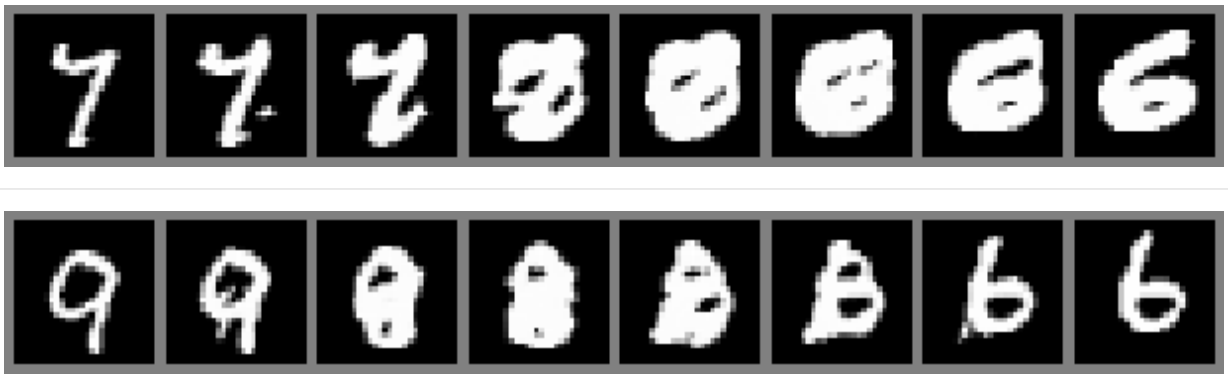
```
    z, _ = model.encode(imgs)
    alpha = torch.linspace(0, 1, steps=num_steps, device=z.device).view(-1, 1, 1, 1)
    interpolations = z[0:1] * alpha + z[1:2] * (1 - alpha)
    interp_imgs = model.sample(interpolations.shape[:1] + imgs.shape[1:], z_
↪init=interpolations)
    show_imgs(interp_imgs, row_size=8)

exmp_imgs, _ = next(iter(train_loader))
```

[30]:
```
pl.seed_everything(42)
for i in range(2):
    interpolate(flow_dict["vardeq"]["model"], exmp_imgs[2*i], exmp_imgs[2*i+1])
```

```
Global seed set to 42
```



[31]:
```
pl.seed_everything(42)
for i in range(2):
    interpolate(flow_dict["multiscale"]["model"], exmp_imgs[2*i], exmp_imgs[2*i+1])
```

```
Global seed set to 42
```

The interpolations of the multi-scale model result in more realistic digits (first row $7 \leftrightarrow 8 \leftrightarrow 6$, second row $9 \leftrightarrow 6$), while the variational dequantization model focuses on local patterns that globally do not form a digit. For the multi-scale model, we actually did not do the "true" interpolation between the two images as we did not consider the variables that were split along the flow (they have been sampled randomly for all samples). However, as we will see in the next experiment, the early variables do not effect the overall image much.

Visualization of latents in different levels of multi-scale

In the following we will focus more on the multi-scale flow. We want to analyse what information is being stored in the variables split at early layers, and what information for the final variables. For this, we sample 8 images where each of them share the same final latent variables, but differ in the other part of the latent variables. Below we visualize three examples of this:

[32]:
```
pl.seed_everything(44)
for _ in range(3):
    z_init = flow_dict["multiscale"]["model"].prior.sample(sample_shape=[1,8,7,7])
    z_init = z_init.expand(8, -1, -1, -1)
    samples = flow_dict["multiscale"]["model"].sample(img_shape=z_init.shape, z_init=z_
↪init)
    show_imgs(samples.cpu())
```

```
Global seed set to 44
```

We see that the early split variables indeed have a smaller effect on the image. Still, small differences can be spot when we look carefully at the borders of the digits. For instance, in the middle, the top part of the 3 has different thicknesses for different samples although all of them represent the same coarse structure. This shows that the flow indeed learns to separate the higher-level information in the final variables, while the early split ones contain local noise patterns.

Visualizing Dequantization

As a final part of this notebook, we will look at the effect of variational dequantization. We have motivated variational dequantization by the issue of sharp edges/boarders being difficult to model, and a flow would rather prefer smooth, prior-like distributions. To check how what noise distribution $q(u|x)$ the flows in the variational dequantization module have learned, we can plot a histogram of output values from the dequantization and variational dequantization module.

[33]:
```
def visualize_dequant_distribution(model : ImageFlow, imgs : torch.Tensor, title:
↪str=None):
    """
    Inputs:
        model - The flow of which we want to visualize the dequantization distribution
        imgs - Example training images of which we want to visualize the dequantization␣
↪distribution
    """
    imgs = imgs.to(device)
    ldj = torch.zeros(imgs.shape[0], dtype=torch.float32).to(device)
    with torch.no_grad():
        dequant_vals = []
        for _ in tqdm(range(8), leave=False):
            d, _ = model.flows[0](imgs, ldj, reverse=False)
            dequant_vals.append(d)
        dequant_vals = torch.cat(dequant_vals, dim=0)
    dequant_vals = dequant_vals.view(-1).cpu().numpy()
    sns.set()
    plt.figure(figsize=(10,3))
    plt.hist(dequant_vals, bins=256, color=to_rgb("C0")+(0.5,), edgecolor="C0",␣
↪density=True)
    if title is not None:
        plt.title(title)
    plt.show()
```

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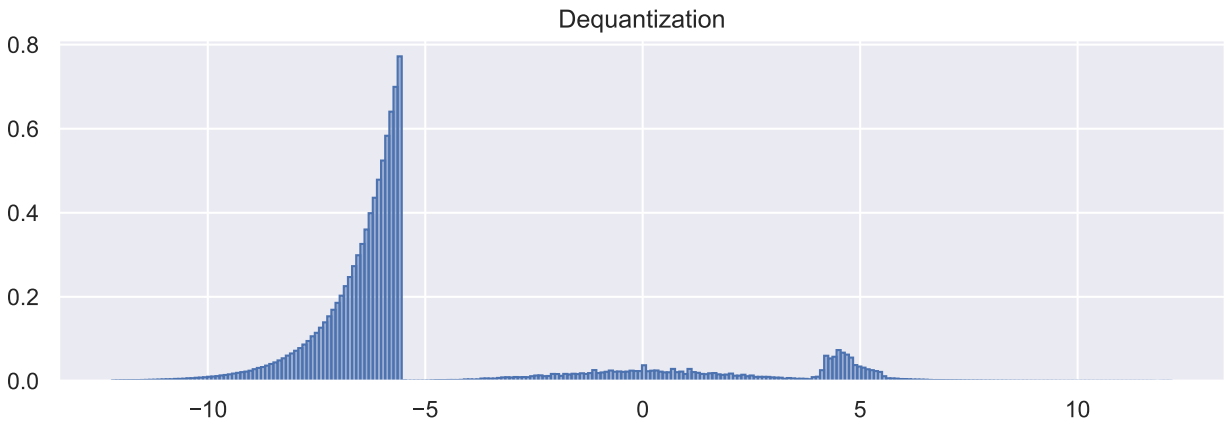
```
    plt.close()

sample_imgs, _ = next(iter(train_loader))
```

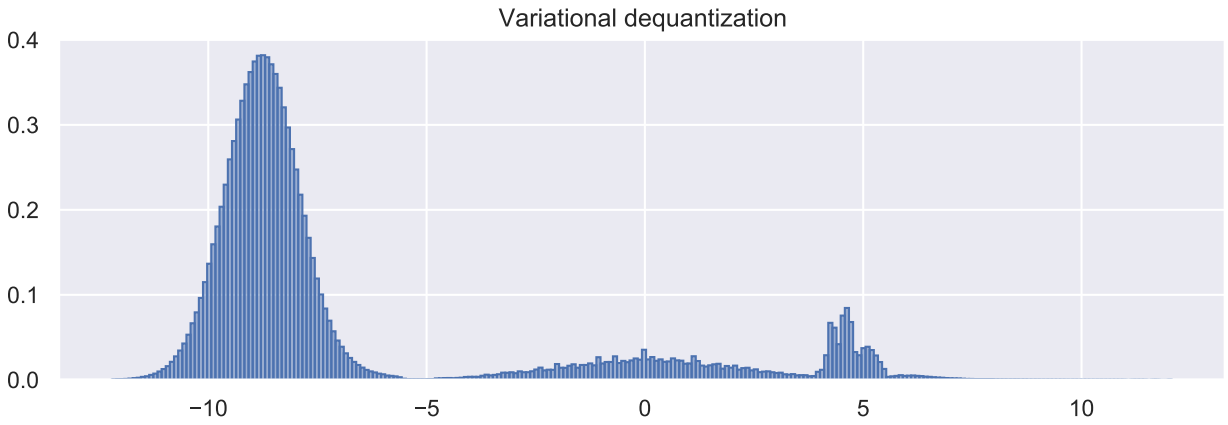
[34]:
```
visualize_dequant_distribution(flow_dict["simple"]["model"], sample_imgs, title=
↪"Dequantization")
```

```
  0%|          | 0/8 [00:00<?, ?it/s]
```



[35]:
```
visualize_dequant_distribution(flow_dict["vardeq"]["model"], sample_imgs, title=
↪"Variational dequantization")
```

```
  0%|          | 0/8 [00:00<?, ?it/s]
```



The dequantization distribution in the first plot shows that the MNIST images have a strong bias towards 0 (black), and the distribution of them have a sharp border as mentioned before. The variational dequantization module has indeed learned a much smoother distribution with a Gaussian-like curve which can be modeled much better. For the other values, we would need to visualize the distribution $q(u|x)$ on a deeper level, depending on x. However, as all u's interact and depend on each other, we would need to visualize a distribution in 784 dimensions, which is not that intuitive anymore.

4.25.5 Conclusion

In conclusion, we have seen how to implement our own normalizing flow, and what difficulties arise if we want to apply them on images. Dequantization is a crucial step in mapping the discrete images into continuous space to prevent underisable delta-peak solutions. While dequantization creates hypercubes with hard border, variational dequantization allows us to fit a flow much better on the data. This allows us to obtain a lower bits per dimension score, while not affecting the sampling speed. The most common flow element, the coupling layer, is simple to implement, and yet effective. Furthermore, multi-scale architectures help to capture the global image context while allowing us to efficiently scale up the flow. Normalizing flows are an interesting alternative to VAEs as they allow an exact likelihood estimate in continuous space, and we have the guarantee that every possible input x has a corresponding latent vector z. However, even beyond continuous inputs and images, flows can be applied and allow us to exploit the data structure in latent space, as e.g. on graphs for the task of molecule generation [6]. Recent advances in Neural ODEs allow a flow with infinite number of layers, called Continuous Normalizing Flows, whose potential is yet to fully explore. Overall, normalizing flows are an exciting research area which will continue over the next couple of years.

4.25.6 References

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[3] Ho, J., Chen, X., Srinivas, A., Duan, Y., and Abbeel, P. (2019). "Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design," in Proceedings of the 36th International Conference on Machine Learning, vol. 97, pp. 2722–2730. Link

[4] Durkan, C., Bekasov, A., Murray, I., and Papamakarios, G. (2019). "Neural Spline Flows," In: Advances in Neural Information Processing Systems, pp. 7509–7520. Link

[5] Hoogeboom, E., Cohen, T. S., and Tomczak, J. M. (2020). "Learning Discrete Distributions by Dequantization," arXiv preprint arXiv2001.11235v1. Link

[6] Lippe, P., and Gavves, E. (2021). "Categorical Normalizing Flows via Continuous Transformations," In: International Conference on Learning Representations, ICLR 2021. Link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.26 Tutorial 12: Autoregressive Image Modeling

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:

Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we implement an autoregressive likelihood model for the task of image modeling. Autoregressive models are naturally strong generative models that constitute one of the current state-of-the-art architectures on likelihood-based image modeling, and are also the basis for large language generation models such as GPT3. Similar to the language generation you have seen in assignment 2, autoregressive models work on images by modeling the likelihood of a pixel given all previous ones. For instance, in the picture below, we model the pixel x_i as a conditional probability distribution based on all previous (here blue) pixels (figure credit - Aaron van den Oord et al.):

Generally, autoregressive model over high-dimensional data $\mathbf{x}$ factor the joint distribution as the following product of conditionals:

$$p(\mathbf{x}) = p(x_1, ..., x_n) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

Learning these conditionals is often much simpler than learning the joint distribution $p(\mathbf{x})$ all together. However, disadvantages of autoregressive models include slow sampling, especially for large images, as we need height-times-width forward passes through the model. In addition, for some applications, we require a latent space as modeled in VAEs and Normalizing Flows. For instance, in autoregressive models, we cannot interpolate between two images because of the lack of a latent representation. We will explore and discuss these benefits and drawbacks alongside with our implementation.

Our implementation will focus on the PixelCNN [2] model which has been discussed in detail in the lecture. Most current SOTA models use PixelCNN as their fundamental architecture, and various additions have been proposed to improve the performance (e.g. PixelCNN++ and PixelSNAIL). Hence, implementing PixelCNN is a good starting point for our short tutorial.

First of all, we need to import our standard libraries. Similarly as in the last couple of tutorials, we will use PyTorch Lightning here as well.

[1]:
```
## Standard libraries
import os
import math
import numpy as np

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import seaborn as sns

## Progress bar
from tqdm.notebook import tqdm

## PyTorch
import torch
```

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```
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim
# Torchvision
import torchvision
from torchvision.datasets import MNIST
from torchvision import transforms
# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial12"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

# Fetching the device that will be used throughout this notebook
device = torch.device("cpu") if not torch.cuda.is_available() else torch.device("cuda:0")
print("Using device", device)
```

```
Using device cuda:0
```

We again provide a pretrained model, which is downloaded below:

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial12/"
# Files to download
pretrained_files = ["PixelCNN.ckpt"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
```

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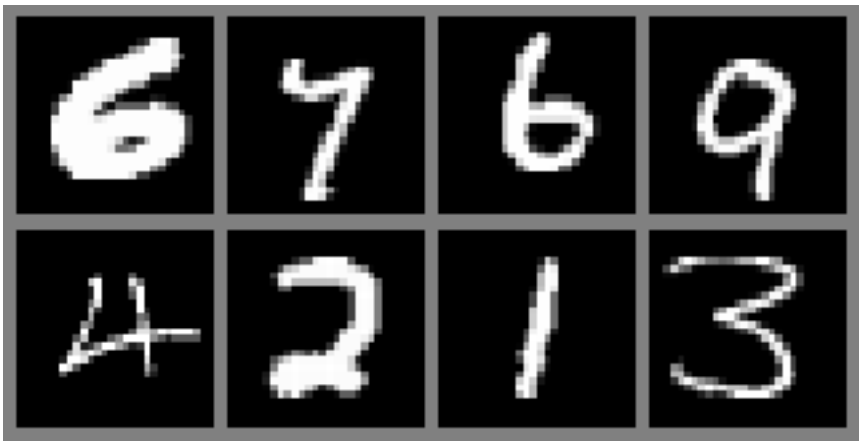
```
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

Similar to the Normalizing Flows in Tutorial 11, we will work on the MNIST dataset and use 8-bits per pixel (values between 0 and 255). The dataset is loaded below:

[3]:
```
# Convert images from 0-1 to 0-255 (integers). We use the long datatype as we will use␣
↪the images as labels as well
def discretize(sample):
    return (sample * 255).to(torch.long)

# Transformations applied on each image => only make them a tensor
transform = transforms.Compose([transforms.ToTensor(),
                                discretize])

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = MNIST(root=DATASET_PATH, train=True, transform=transform, download=True)
pl.seed_everything(42)
train_set, val_set = torch.utils.data.random_split(train_dataset, [50000, 10000])

# Loading the test set
test_set = MNIST(root=DATASET_PATH, train=False, transform=transform, download=True)

# We define a set of data loaders that we can use for various purposes later.
train_loader = data.DataLoader(train_set, batch_size=128, shuffle=True, drop_last=True,␣
↪pin_memory=True, num_workers=4)
val_loader = data.DataLoader(val_set, batch_size=128, shuffle=False, drop_last=False,␣
↪num_workers=4)
test_loader = data.DataLoader(test_set, batch_size=128, shuffle=False, drop_last=False,␣
↪num_workers=4)
```

A good practice is to always visualize some data examples to get an intuition of the data:

[4]:
```
def show_imgs(imgs):
    num_imgs = imgs.shape[0] if isinstance(imgs, torch.Tensor) else len(imgs)
    nrow = min(num_imgs, 4)
    ncol = int(math.ceil(num_imgs/nrow))
    imgs = torchvision.utils.make_grid(imgs, nrow=nrow, pad_value=128)
    imgs = imgs.clamp(min=0, max=255)
    np_imgs = imgs.cpu().numpy()
    plt.figure(figsize=(1.5*nrow, 1.5*ncol))
    plt.imshow(np.transpose(np_imgs, (1,2,0)), interpolation='nearest')
    plt.axis('off')
    plt.show()
    plt.close()

show_imgs([train_set[i][0] for i in range(8)])
```



4.26.1 Masked autoregressive convolutions

The core module of PixelCNN is its masked convolutions. In contrast to language models, we don't apply an LSTM on each pixel one-by-one. This would be inefficient because images are grids instead of sequences. Thus, it is better to rely on convolutions that have shown great success in deep CNN classification models.

Nevertheless, we cannot just apply standard convolutions without any changes. Remember that during training of autoregressive models, we want to use teacher forcing which both helps the model training, and significantly reduces the time needed for training. For image modeling, teacher forcing is implemented by using a training image as input to the model, and we want to obtain as output the prediction for each pixel based on *only* its predecessors. Thus, we need to ensure that the prediction for a specific pixel can only be influenced by its predecessors and not by its own value or any "future" pixels. For this, we apply convolutions with a mask.

Which mask we use depends on the ordering of pixels we decide on, i.e. which is the first pixel we predict, which is the second one, etc. The most commonly used ordering is to denote the upper left pixel as the start pixel, and sort the pixels row by row, as shown in the visualization at the top of the tutorial. Thus, the second pixel is on the right of the first one (first row, second column), and once we reach the end of the row, we start in the second row, first column. If we now want to apply this to our convolutions, we need to ensure that the prediction of pixel 1 is not influenced by its own "true" input, and all pixels on its right and in any lower row. In convolutions, this means that we want to set those entries of the weight matrix to zero that take pixels on the right and below into account. As an example for a 5x5 kernel, see a mask below (figure credit - Aaron van den Oord):

Before looking into the application of masked convolutions in PixelCNN in detail, let's first implement a module that allows us to apply an arbitrary mask to a convolution:

[5]:
```
class MaskedConvolution(nn.Module):

    def __init__(self, c_in, c_out, mask, **kwargs):
        """
        Implements a convolution with mask applied on its weights.
        Inputs:
            c_in - Number of input channels
            c_out - Number of output channels
            mask - Tensor of shape [kernel_size_H, kernel_size_W] with 0s where
                   the convolution should be masked, and 1s otherwise.
            kwargs - Additional arguments for the convolution
```

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```
        """
        super().__init__()
        # For simplicity: calculate padding automatically
        kernel_size = (mask.shape[0], mask.shape[1])
        dilation = 1 if "dilation" not in kwargs else kwargs["dilation"]
        padding = tuple([dilation*(kernel_size[i]-1)//2 for i in range(2)])
        # Actual convolution
        self.conv = nn.Conv2d(c_in, c_out, kernel_size, padding=padding, **kwargs)

        # Mask as buffer => it is no parameter but still a tensor of the module
        # (must be moved with the devices)
        self.register_buffer('mask', mask[None,None])

    def forward(self, x):
        self.conv.weight.data *= self.mask # Ensures zero's at masked positions
        return self.conv(x)
```

Vertical and horizontal convolution stacks

To build our own autoregressive image model, we could simply stack a few masked convolutions on top of each other. This was actually the case for the original PixelCNN model, discussed in the paper Pixel Recurrent Neural Networks, but this leads to a considerable issue. When sequentially applying a couple of masked convolutions, the receptive field of a pixel show to have a "blind spot" on the right upper side, as shown in the figure below (figure credit - Aaron van den Oord et al.):

Although a pixel should be able to take into account all other pixels above and left of it, a stack of masked convolutions does not allow us to look to the upper pixels on the right. This is because the features of the pixels above, which we use for convolution, do not contain any information of the pixels on the right of the same row. If they would, we would be "cheating" and actually looking into the future. To overcome this issue, van den Oord et. al [2] proposed to split the convolutions into a vertical and a horizontal stack. The vertical stack looks at all pixels above the current one, while the horizontal takes into account all on the left. While keeping both of them separate, we can actually look at the pixels on the right with the vertical stack without breaking any of our assumptions. The two convolutions are also shown in the figure above.

Let us implement them here as follows:

[6]:
```
class VerticalStackConvolution(MaskedConvolution):

    def __init__(self, c_in, c_out, kernel_size=3, mask_center=False, **kwargs):
        # Mask out all pixels below. For efficiency, we could also reduce the kernel
        # size in height, but for simplicity, we stick with masking here.
        mask = torch.ones(kernel_size, kernel_size)
        mask[kernel_size//2+1:,:] = 0

        # For the very first convolution, we will also mask the center row
        if mask_center:
            mask[kernel_size//2,:] = 0

        super().__init__(c_in, c_out, mask, **kwargs)
```

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```
class HorizontalStackConvolution(MaskedConvolution):

    def __init__(self, c_in, c_out, kernel_size=3, mask_center=False, **kwargs):
        # Mask out all pixels on the left. Note that our kernel has a size of 1
        # in height because we only look at the pixel in the same row.
        mask = torch.ones(1,kernel_size)
        mask[0,kernel_size//2+1:] = 0

        # For the very first convolution, we will also mask the center pixel
        if mask_center:
            mask[0,kernel_size//2] = 0

        super().__init__(c_in, c_out, mask, **kwargs)
```

Note that we have an input argument called `mask_center`. Remember that the input to the model is the actual input image. Hence, the very first convolution we apply cannot use the center pixel as input, but must be masked. All consecutive convolutions, however, should use the center pixel as we otherwise lose the features of the previous layer. Hence, the input argument `mask_center` is True for the very first convolutions, and False for all others.

Visualizing the receptive field

To validate our implementation of masked convolutions, we can visualize the receptive field we obtain with such convolutions. We should see that with increasing number of convolutional layers, the receptive field grows in both vertical and horizontal direction, without the issue of a blind spot. The receptive field can be empirically measured by back-propagating an arbitrary loss for the output features of a speicifc pixel with respect to the input. We implement this idea below, and visualize the receptive field below.

[7]:
```
inp_img = torch.zeros(1, 1, 11, 11)
inp_img.requires_grad_()

def show_center_recep_field(img, out):
    """
    Calculates the gradients of the input with respect to the output center pixel,
    and visualizes the overall receptive field.
    Inputs:
        img - Input image for which we want to calculate the receptive field on.
        out - Output features/loss which is used for backpropagation, and should be
              the output of the network/computation graph.
    """
    # Determine gradients
    loss = out[0,:,img.shape[2]//2,img.shape[3]//2].sum() # L1 loss for simplicity
    loss.backward(retain_graph=True) # Retain graph as we want to stack multiple layers␣
↪and show the receptive field of all of them
    img_grads = img.grad.abs()
    img.grad.fill_(0) # Reset grads

    # Plot receptive field
    img = img_grads.squeeze().cpu().numpy()
    fig, ax = plt.subplots(1,2)
    pos = ax[0].imshow(img)
    ax[1].imshow(img>0)
```

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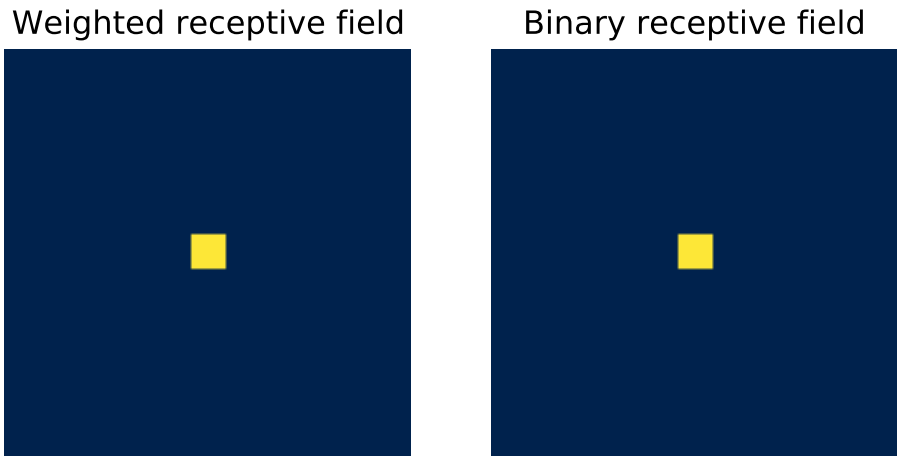
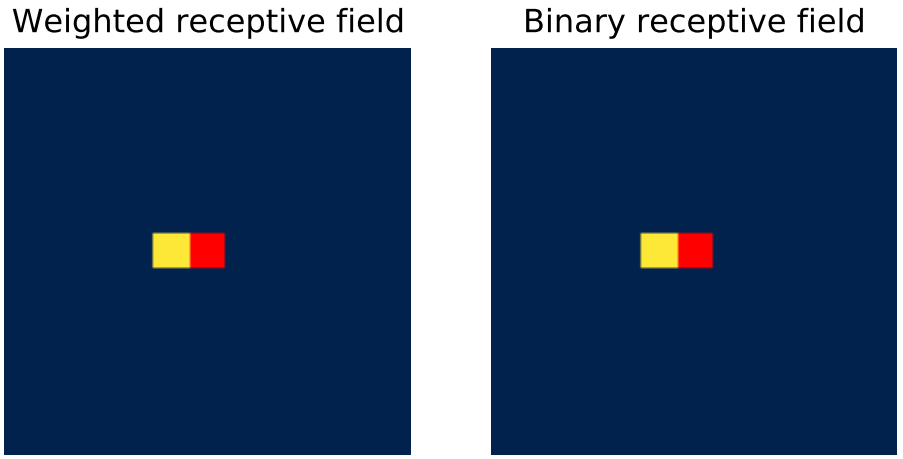
```
    # Mark the center pixel in red if it doesn't have any gradients (should be the case␣
↪for standard autoregressive models)
    show_center = (img[img.shape[0]//2,img.shape[1]//2] == 0)
    if show_center:
        center_pixel = np.zeros(img.shape + (4,))
        center_pixel[center_pixel.shape[0]//2,center_pixel.shape[1]//2,:] = np.array([1.
↪0, 0.0, 0.0, 1.0])
    for i in range(2):
        ax[i].axis('off')
        if show_center:
            ax[i].imshow(center_pixel)
    ax[0].set_title("Weighted receptive field")
    ax[1].set_title("Binary receptive field")
    plt.show()
    plt.close()

show_center_recep_field(inp_img, inp_img)
```



Let's first visualize the receptive field of a horizontal convolution without the center pixel. We use a small, arbitrary input image (11×11 pixels), and calculate the loss for the center pixel. For simplicity, we initialize all weights with 1 and the bias with 0, and use a single channel. This is sufficient for our visualization purposes.

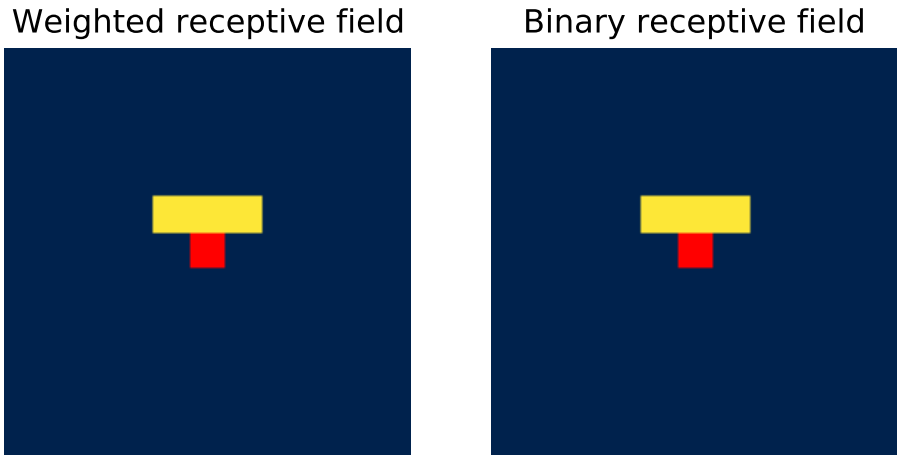
[8]:
```
horiz_conv = HorizontalStackConvolution(c_in=1, c_out=1, kernel_size=3, mask_center=True)
horiz_conv.conv.weight.data.fill_(1)
horiz_conv.conv.bias.data.fill_(0)
horiz_img = horiz_conv(inp_img)
show_center_recep_field(inp_img, horiz_img)
```



The receptive field is shown in yellow, the center pixel in red, and all other pixels outside of the receptive field are dark blue. As expected, the receptive field of a single horizontal convolution with the center pixel masked and a 3×3 kernel is only the pixel on the left. If we use a larger kernel size, more pixels would be taken into account on the left.

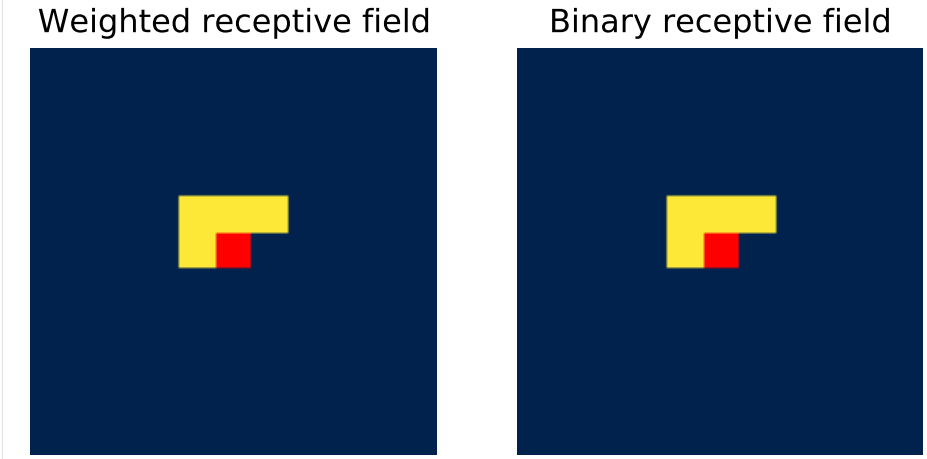
Next, let's take a look at the vertical convolution:

[9]:
```
vert_conv = VerticalStackConvolution(c_in=1, c_out=1, kernel_size=3, mask_center=True)
vert_conv.conv.weight.data.fill_(1)
vert_conv.conv.bias.data.fill_(0)
vert_img = vert_conv(inp_img)
show_center_recep_field(inp_img, vert_img)
```



The vertical convolution takes all pixels above into account. Combining these two, we get the L-shaped receptive field of the original masked convolution:

[10]:
```
horiz_img = vert_img + horiz_img
show_center_recep_field(inp_img, horiz_img)
```



If we stack multiple horizontal and vertical convolutions, we need to take two aspects into account:

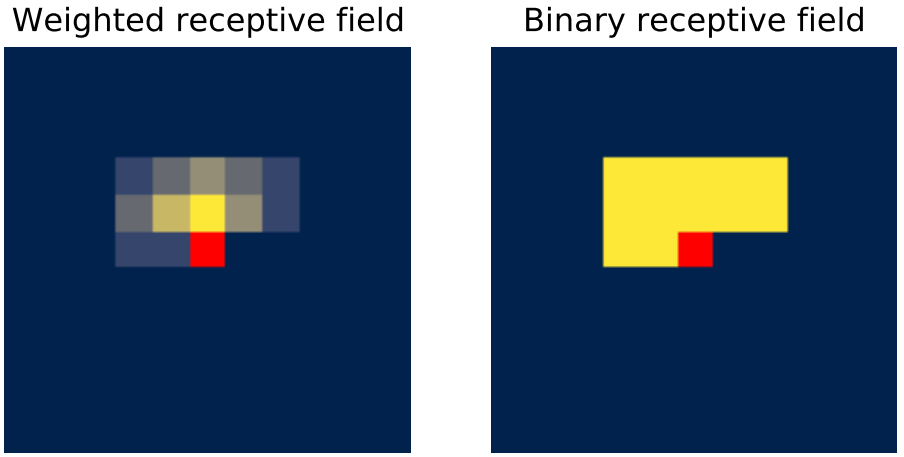
1. The center should not be masked anymore for the following convolutions as the features at the pixel's position are already independent of its actual value. If it is hard to imagine why we can do this, just change the value below to `mask_center=True` and see what happens.
2. The vertical convolution is not allowed to work on features from the horizontal convolution. In the feature map of the horizontal convolutions, a pixel contains information about all of the "true" pixels on the left. If we apply a vertical convolution which also uses features from the right, we effectively expand our receptive field to the true input which we want to prevent. Thus, the feature maps can only be merged for the horizontal convolution.

Using this, we can stack the convolutions in the following way. We have two feature streams: one for the vertical stack, and one for the horizontal stack. The horizontal convolutions can operate on the joint features of the previous horizontals and vertical convolutions, while the vertical stack only takes its own previous features as input. For a quick implementation, we can therefore sum the horizontal and vertical output features at each layer, and use those as final output features to calculate the loss on. An implementation of 4 consecutive layers is shown below. Note that we reuse the features from the other convolutions with `mask_center=True` from above.

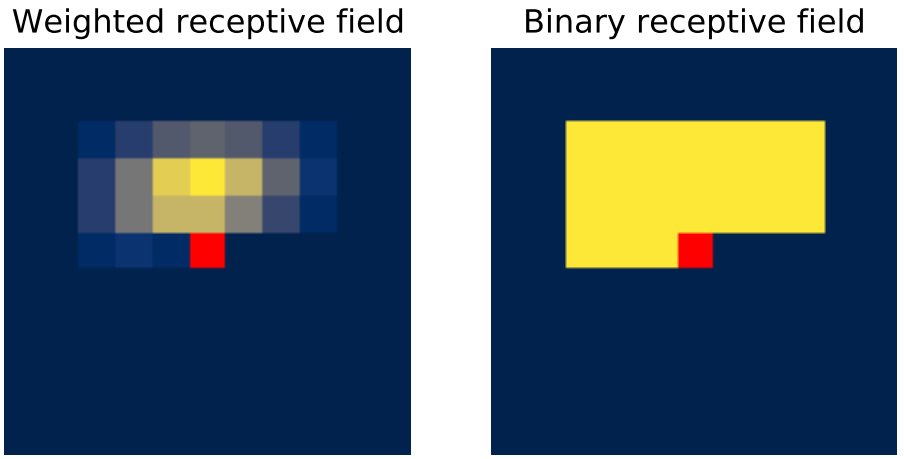
[11]:
```
# Initialize convolutions with equal weight to all input pixels
horiz_conv = HorizontalStackConvolution(c_in=1, c_out=1, kernel_size=3, mask_
↪center=False)
horiz_conv.conv.weight.data.fill_(1)
horiz_conv.conv.bias.data.fill_(0)
vert_conv = VerticalStackConvolution(c_in=1, c_out=1, kernel_size=3,mask_center=False)
vert_conv.conv.weight.data.fill_(1)
vert_conv.conv.bias.data.fill_(0)

# We reuse our convolutions for the 4 layers here. Note that in a standard network,
# we don't do that, and instead learn 4 separate convolution. As this cell is only for
# visualization purposes, we reuse the convolutions for all layers.
for l_idx in range(4):
    vert_img = vert_conv(vert_img)
    horiz_img = horiz_conv(horiz_img) + vert_img
    print(f"Layer {l_idx+2}")
    show_center_recep_field(inp_img, horiz_img)
```

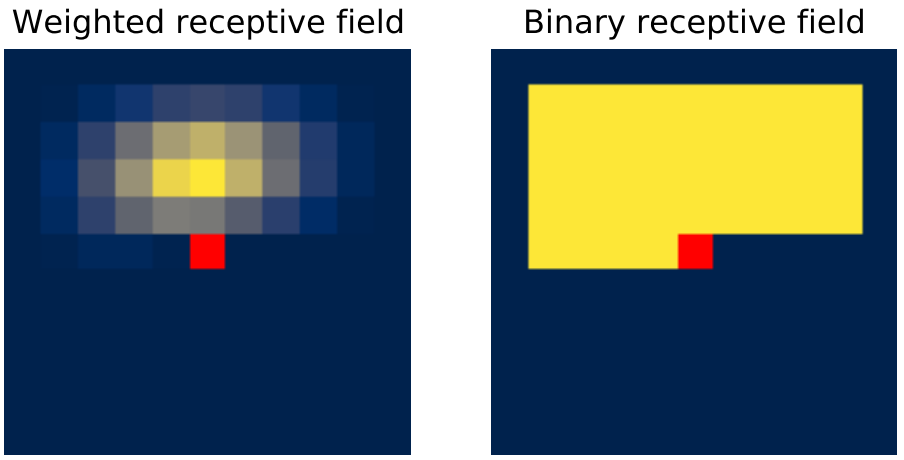
```
Layer 2
```



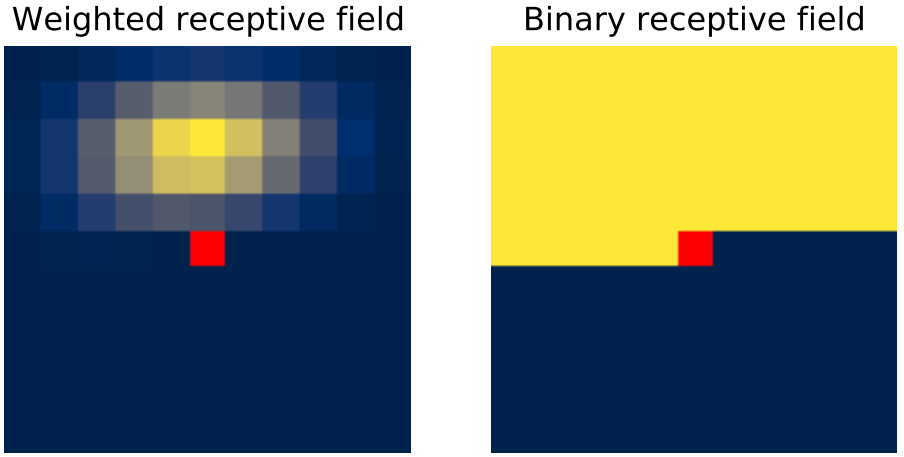
Layer 3



Layer 4



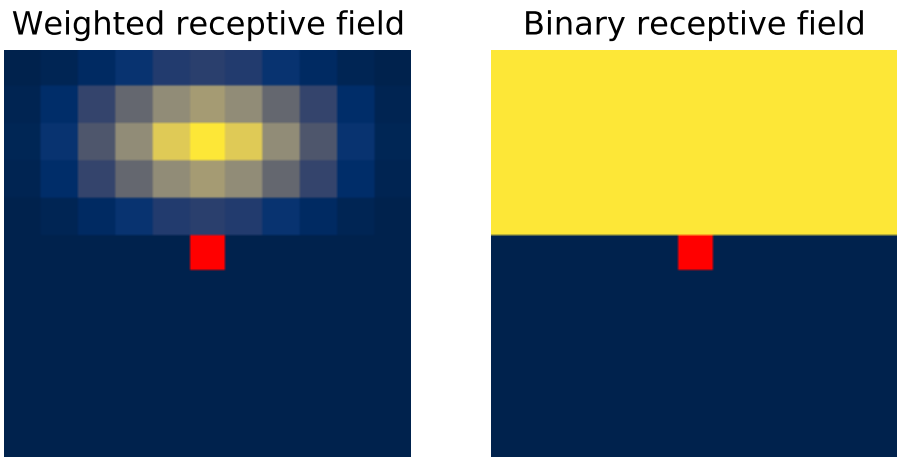
Layer 5



The receptive field above it visualized for the horizontal stack, which includes the features of the vertical convolutions. It grows over layers without any blind spot as we had before. The difference between "weighted" and "binary" receptive field is that for the latter, we check whether there are any gradients flowing back to this pixel. This indicates that the center pixel indeed can use information from this pixel. Nevertheless, due to the convolution weights, some pixels have a stronger effect on the prediction than others. This is visualized in the weighted receptive field by plotting the gradient magnitude for each pixel instead of a binary yes/no.

Another receptive field we can check is the one for the vertical stack as the one above is for the horizontal stack. Let's visualize it below:

[12]:
```
show_center_recep_field(inp_img, vert_img)
```



As we have discussed before, the vertical stack only looks at pixels above the one we want to predict. Hence, we can validate that our implementation works as we initially expected it to. As a final step, let's clean up the computation graph we still had kept in memory for the visualization of the receptive field:

[13]:
```
del inp_img, horiz_conv, vert_conv
```

4.26.2 Gated PixelCNN

In the next step, we will use the masked convolutions to build a full autoregressive model, called Gated PixelCNN. The difference between the original PixelCNN and Gated PixelCNN is the use of separate horizontal and vertical stacks. However, in literature, you often see that people refer to the Gated PixelCNN simply as "PixelCNN". Hence, in the following, if we say "PixelCNN", we usually mean the gated version. What "Gated" refers to in the model name is explained next.

Gated Convolutions

For visualizing the receptive field, we assumed a very simplified stack of vertical and horizontal convolutions. Obviously, there are more sophisticated ways of doing it, and PixelCNN uses gated convolutions for this. Specifically, the Gated Convolution block in PixelCNN looks as follows (figure credit - Aaron van den Oord et al.):

The left path is the vertical stack (the $N \times N$ convolution is masked correspondingly), and the right path is the horizontal stack. Gated convolutions are implemented by having a twice as large output channel size, and combine them by a element-wise multiplication of $\tanh$ and a sigmoid. For a linear layer, we can express a gated activation unit as follows:

$$\mathbf{y} = \tanh\left(\mathbf{W}_f \mathbf{x}\right) \odot \sigma\left(\mathbf{W}_g \mathbf{x}\right)$$

For simplicity, biases have been neglected and the linear layer split into two part, $\mathbf{W}_f$ and $\mathbf{W}_g$. This concept resembles the input and modulation gate in an LSTM, and has been used in many other architectures as well. The main motivation behind this gated activation is that it might allow to model more complex interactions and simplifies learning. But as in any other architecture, this is mostly a design choice and can be considered a hyperparameters.

Besides the gated convolutions, we also see that the horizontal stack uses a residual connection while the vertical stack does not. This is because we use the output of the horizontal stack for prediction. Each convolution in the vertical stack also receives a strong gradient signal as it is only two 1×1 convolutions away from the residual connection, and does not require another residual connection to all its earleri layers.

The implementation in PyTorch is fairly straight forward for this block, because the visualization above gives us a computation graph to follow:

[14]:
```
class GatedMaskedConv(nn.Module):

    def __init__(self, c_in, **kwargs):
        """
        Gated Convolution block implemented the computation graph shown above.
        """
        super().__init__()
        self.conv_vert = VerticalStackConvolution(c_in, c_out=2*c_in, **kwargs)
        self.conv_horiz = HorizontalStackConvolution(c_in, c_out=2*c_in, **kwargs)
        self.conv_vert_to_horiz = nn.Conv2d(2*c_in, 2*c_in, kernel_size=1, padding=0)
        self.conv_horiz_1x1 = nn.Conv2d(c_in, c_in, kernel_size=1, padding=0)

    def forward(self, v_stack, h_stack):
        # Vertical stack (left)
        v_stack_feat = self.conv_vert(v_stack)
        v_val, v_gate = v_stack_feat.chunk(2, dim=1)
        v_stack_out = torch.tanh(v_val) * torch.sigmoid(v_gate)

        # Horizontal stack (right)
```

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```
        h_stack_feat = self.conv_horiz(h_stack)
        h_stack_feat = h_stack_feat + self.conv_vert_to_horiz(v_stack_feat)
        h_val, h_gate = h_stack_feat.chunk(2, dim=1)
        h_stack_feat = torch.tanh(h_val) * torch.sigmoid(h_gate)
        h_stack_out = self.conv_horiz_1x1(h_stack_feat)
        h_stack_out = h_stack_out + h_stack

        return v_stack_out, h_stack_out
```

Building the model

Using the gated convolutions, we can now build our PixelCNN model. The architecture consists of multiple stacked GatedMaskedConv blocks, where we add an additional dilation factor to a few convolutions. This is used to increase the receptive field of the model and allows to take a larger context into accout during generation. As a reminder, dilation on a convolution works looks as follows (figure credit - Vincent Dumoulin and Francesco Visin):

Note that the smaller output size is only because the animation assumes no padding. In our implementation, we will pad the input image correspondingly. Alternatively to dilated convolutions, we could downsample the input and use a encoder-decoder architecture as in PixelCNN++ [3]. This is especially beneficial if we want to build a very deep autoregressive model. Nonetheless, as we seek to train a reasonably small model, dilated convolutions are the more efficient option to use here.

Below, we implement the PixelCNN model as a PyTorch Lightning module. Besides the stack of gated convolutions, we also have the initial horizontal and vertical convolutions which mask the center pixel, and a final 1×1 convolution which maps the output features to class predictions. To determine the likelihood of a batch of images, we first create our initial features using the masked horizontal and vertical input convolution. Next, we forward the features through the stack of gated convolutions. Finally, we take the output features of the horizontal stack, and apply the 1×1 convolution for classification. We use the bits per dimension metric for the likelihood, similarly to Tutorial 11 and assignment 3.

[15]:
```
class PixelCNN(pl.LightningModule):

    def __init__(self, c_in, c_hidden):
        super().__init__()
        self.save_hyperparameters()

        # Initial convolutions skipping the center pixel
        self.conv_vstack = VerticalStackConvolution(c_in, c_hidden, mask_center=True)
        self.conv_hstack = HorizontalStackConvolution(c_in, c_hidden, mask_center=True)
        # Convolution block of PixelCNN. We use dilation instead of downscaling
        self.conv_layers = nn.ModuleList([
            GatedMaskedConv(c_hidden),
            GatedMaskedConv(c_hidden, dilation=2),
            GatedMaskedConv(c_hidden),
            GatedMaskedConv(c_hidden, dilation=4),
            GatedMaskedConv(c_hidden),
            GatedMaskedConv(c_hidden, dilation=2),
            GatedMaskedConv(c_hidden)
        ])
        # Output classification convolution (1x1)
        self.conv_out = nn.Conv2d(c_hidden, c_in * 256, kernel_size=1, padding=0)
```

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```
        self.example_input_array = train_set[0][0][None]

    def forward(self, x):
        """
        Forward image through model and return logits for each pixel.
        Inputs:
            x - Image tensor with integer values between 0 and 255.
        """
        # Scale input from 0 to 255 back to -1 to 1
        x = (x.float() / 255.0) * 2 - 1

        # Initial convolutions
        v_stack = self.conv_vstack(x)
        h_stack = self.conv_hstack(x)
        # Gated Convolutions
        for layer in self.conv_layers:
            v_stack, h_stack = layer(v_stack, h_stack)
        # 1x1 classification convolution
        # Apply ELU before 1x1 convolution for non-linearity on residual connection
        out = self.conv_out(F.elu(h_stack))

        # Output dimensions: [Batch, Classes, Channels, Height, Width]
        out = out.reshape(out.shape[0], 256, out.shape[1]//256, out.shape[2], out.
↪shape[3])
        return out

    def calc_likelihood(self, x):
        # Forward pass with bpd likelihood calculation
        pred = self.forward(x)
        nll = F.cross_entropy(pred, x, reduction='none')
        bpd = nll.mean(dim=[1,2,3]) * np.log2(np.exp(1))
        return bpd.mean()

    @torch.no_grad()
    def sample(self, img_shape, img=None):
        """
        Sampling function for the autoregressive model.
        Inputs:
            img_shape - Shape of the image to generate (B,C,H,W)
            img (optional) - If given, this tensor will be used as
                             a starting image. The pixels to fill
                             should be -1 in the input tensor.
        """
        # Create empty image
        if img is None:
            img = torch.zeros(img_shape, dtype=torch.long).to(device) - 1
        # Generation loop
        for h in tqdm(range(img_shape[2]), leave=False):
            for w in range(img_shape[3]):
                for c in range(img_shape[1]):
                    # Skip if not to be filled (-1)
```

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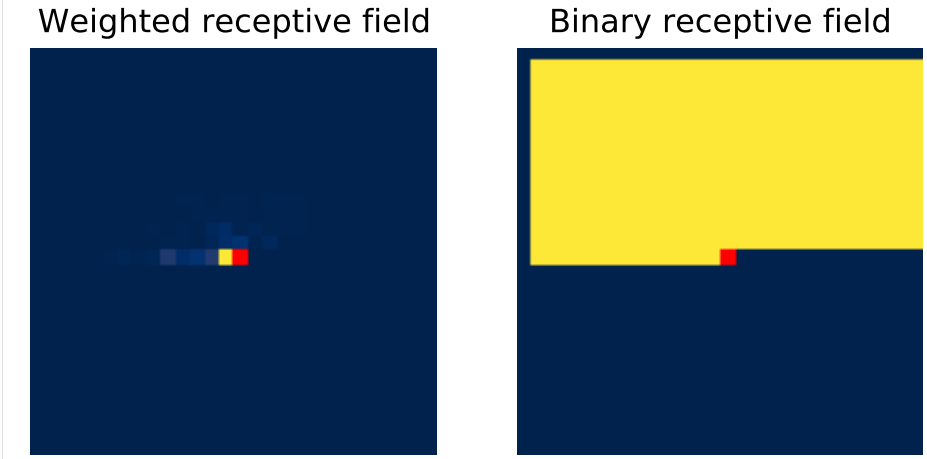
```
                    if (img[:,c,h,w] != -1).all().item():
                        continue
                    # For efficiency, we only have to input the upper part of the image
                    # as all other parts will be skipped by the masked convolutions␣
↪anyways
                    pred = self.forward(img[:,:,:h+1,:])
                    probs = F.softmax(pred[:,:,c,h,w], dim=-1)
                    img[:,c,h,w] = torch.multinomial(probs, num_samples=1).squeeze(dim=-
↪1)
        return img

    def configure_optimizers(self):
        optimizer = optim.Adam(self.parameters(), lr=1e-3)
        scheduler = optim.lr_scheduler.StepLR(optimizer, 1, gamma=0.99)
        return [optimizer], [scheduler]

    def training_step(self, batch, batch_idx):
        loss = self.calc_likelihood(batch[0])
        self.log('train_bpd', loss)
        return loss

    def validation_step(self, batch, batch_idx):
        loss = self.calc_likelihood(batch[0])
        self.log('val_bpd', loss)

    def test_step(self, batch, batch_idx):
        loss = self.calc_likelihood(batch[0])
        self.log('test_bpd', loss)
```

To sample from the autoregressive model, we need to iterate over all dimensions of the input. We start with an empty image, and fill the pixels one by one, starting from the upper left corner. Note that as for predicting x_i, all pixels below it have no influence on the prediction. Hence, we can cut the image in height without changing the prediction while increasing efficiency. Nevertheless, all the loops in the sampling function already show that it will take us quite some time to sample. A lot of computation could be reused across loop iterations as those the features on the already predicted pixels will not change over iterations. Nevertheless, this takes quite some effort to implement, and is often not done in implementations because in the end, autoregressive sampling remains sequential and slow. Hence, we settle with the default implementation here.

Before training the model, we can check the full receptive field of the model on an MNIST image of size 28×28:

[16]:
```
test_model = PixelCNN(c_in=1, c_hidden=64)
inp = torch.zeros(1,1,28,28)
inp.requires_grad_()
out = test_model(inp)
show_center_recep_field(inp, out.squeeze(dim=2))
del inp, out, test_model
```



The visualization shows that for predicting any pixel, we can take almost half of the image into account. However, keep in mind that this is the "theoretical" receptive field and not necessarily the effective receptive field, which is usually much smaller. For a stronger model, we should therefore try to increase the receptive field even further. Especially, for the pixel on the bottom right, the very last pixel, we would be allowed to take into account the whole image. However, our current receptive field only spans across 1/4 of the image. An encoder-decoder architecture can help with this, but it also shows that we require a much deeper, more complex network in autoregressive models than in VAEs or energy-based models.

Training loop

To train the model, we again can rely on PyTorch Lightning and write a function below for loading the pretrained model if it exists. To reduce the computational cost, we have saved the validation and test score in the checkpoint already:

[17]:
```
def train_model(**kwargs):
    # Create a PyTorch Lightning trainer with the generation callback
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, "PixelCNN"),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=150,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="min",␣
↪monitor="val_bpd"),
                                    LearningRateMonitor("epoch")])
    result = None
    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, "PixelCNN.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model, loading...")
        model = PixelCNN.load_from_checkpoint(pretrained_filename)
        ckpt = torch.load(pretrained_filename, map_location=device)
        result = ckpt.get("result", None)
    else:
        model = PixelCNN(**kwargs)
        trainer.fit(model, train_loader, val_loader)
    model = model.to(device)

    if result is None:
```

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```
        # Test best model on validation and test set
        val_result = trainer.test(model, val_loader, verbose=False)
        test_result = trainer.test(model, test_loader, verbose=False)
        result = {"test": test_result, "val": val_result}
    return model, result
```

Training the model is time consuming and we recommend using the provided pre-trained model for going through this notebook. However, feel free to play around with the hyperparameter like number of layers etc. if you want to get a feeling for those.

When calling the training function with a pre-trained model, we automatically load it and print its test performance:

[18]:
```
model, result = train_model(c_in=1, c_hidden=64)
test_res = result["test"][0]
print("Test bits per dimension: %4.3fbpd" % (test_res["test_loss"] if "test_loss" in␣
↪test_res else test_res["test_bpd"]))
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
```

```
Found pretrained model, loading...
Test bits per dimension: 0.808bpd
```

With a test performance of 0.809bpd, the PixelCNN significantly outperforms the normalizing flows we have seen in Tutorial 11. Considering image modeling as an autoregressive problem simplifies the learning process as predicting one pixel given the ground truth of all others is much easier than predicting all pixels at once. In addition, PixelCNN can explicitly predict the pixel values by a discrete softmax while Normalizing Flows have to learn transformations in continuous latent space. These two aspects allow the PixelCNN to achieve a notably better performance.

To fully compare the models, let's also measure the number of parameters of the PixelCNN:

[19]:
```
num_params = sum([np.prod(param.shape) for param in model.parameters()])
print("Number of parameters: {:,}".format(num_params))
```

```
Number of parameters: 852,160
```

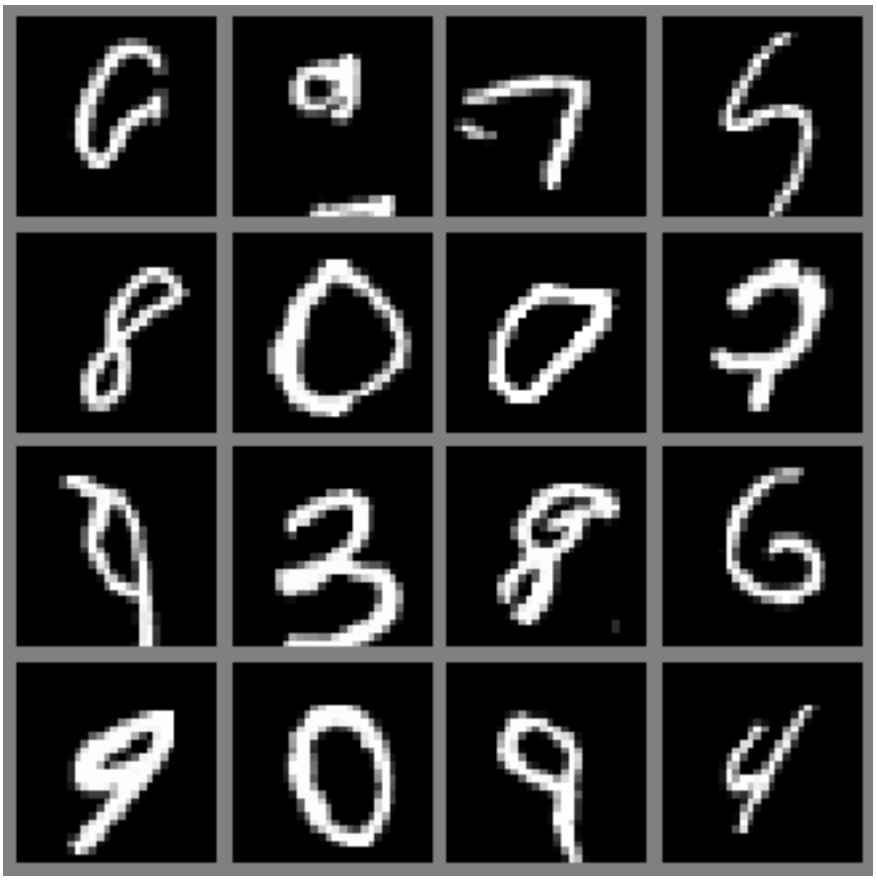
Compared to the multi-scale normalizing flows, the PixelCNN has considerably less parameters. Of course, the number of parameters depend on our hyperparameter choices. Nevertheless, in general, it can be said that autoregressive models require considerably less parameters than normalizing flows to reach good performance, based on the reasons stated above. Still, autoregressive models are much slower in sampling than normalizing flows, which limits their possible applications.

4.26.3 Sampling

One way of qualitatively analysing generative models is by looking at the actual samples. Let's therefore use our sampling function to generate a few digits:

[20]:
```
pl.seed_everything(1)
samples = model.sample(img_shape=(16,1,28,28))
show_imgs(samples.cpu())
```

```
HBox(children=(FloatProgress(value=0.0, max=28.0), HTML(value='')))
```



Most of the samples can be identified as digits, and overall we achieve a better quality than we had in normalizing flows. This goes along with the lower likelihood we achieved with autoregressive models. Nevertheless, we also see that there is still place for improvement as a considerable amount of samples cannot be identified (for example the first row). Deeper autoregressive models are expected to achieve better quality, as they can take more context into account for generating the pixels.

Note that on Google Colab, you might see different results, specifically with a white line at the top. After some debugging, it seemed that the difference occurs inside the dilated convolution, as it gives different results for different batch sizes. However, it is hard to debug this further as it might be a bug of the installed PyTorch version on Google Colab.

The trained model itself is not restricted to any specific image size. However, what happens if we actually sample a larger image than we had seen in our training dataset? Let's try below to sample images of size 64×64 instead of 28×28:

[21]:
```
pl.seed_everything(1)
samples = model.sample(img_shape=(8,1,64,64))
show_imgs(samples.cpu())
```

```
HBox(children=(FloatProgress(value=0.0, max=64.0), HTML(value='')))
```

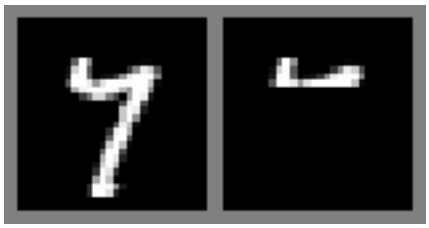
The larger images show that changing the size of the image during testing confuses the model and generates abstract figures (you can sometimes spot a digit in the upper left corner). In addition, sampling for images of 64x64 pixels take more than a minute on a GPU. Clearly, autoregressive models cannot be scaled to large images without changing the sampling procedure such as with forecasting. Our implementation is also not the most efficient as many computations can be stored and reused throughout the sampling process. Nevertheless, the sampling procedure stays sequential which is inherently slower than parallel generation like done in normalizing flows.

Autocompletion

One common application done with autoregressive models is auto-completing an image. As autoregressive models predict pixels one by one, we can set the first N pixels to predefined values and check how the model completes the image. For implementing this, we just need to skip the iterations in the sampling loop that already have a value unequals -1. See above in our PyTorch Lightning module for the specific implementation. In the cell below, we randomly take three images from the training set, mask about the lower half of the image, and let the model autocomplete it. To see the diversity of samples, we do this 12 times for each image:

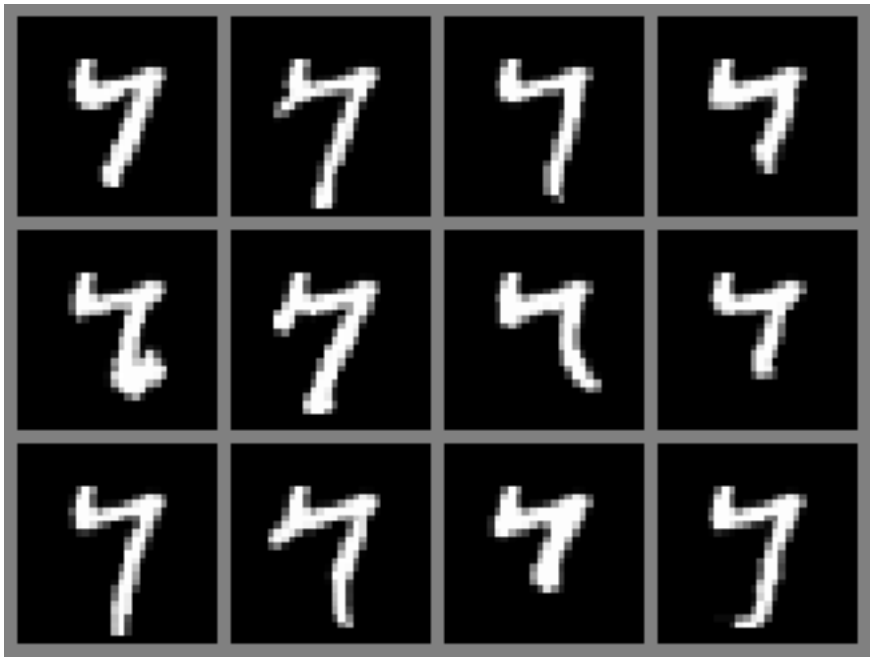
[22]:
```
def autocomplete_image(img):
    # Remove lower half of the image
    img_init = img.clone()
    img_init[:,10:,:] = -1
    print("Original image and input image to sampling:")
    show_imgs([img,img_init])
    # Generate 12 example completions
    img_init = img_init.unsqueeze(dim=0).expand(12,-1,-1,-1).to(device)
    pl.seed_everything(1)
    img_generated = model.sample(img_init.shape, img_init)
    print("Autocompletion samples:")
    show_imgs(img_generated)

for i in range(1,4):
    img = train_set[i][0]
    autocomplete_image(img)
```

```
Original image and input image to sampling:
```

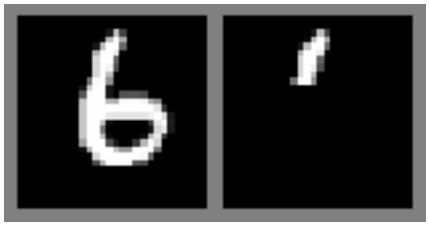


HBox(children=(FloatProgress(value=0.0, max=28.0), HTML(value='')))

Autocompletion samples:

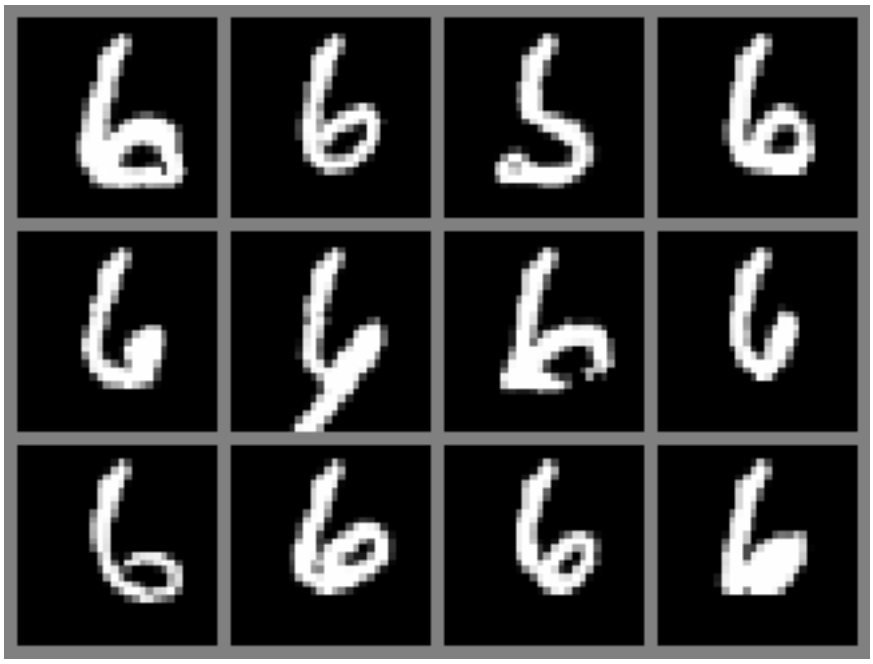


Original image and input image to sampling:

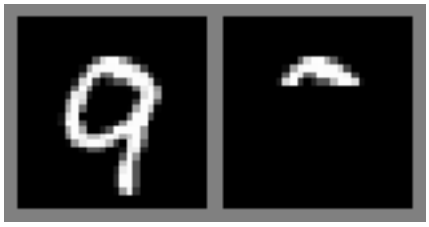


HBox(children=(FloatProgress(value=0.0, max=28.0), HTML(value='')))

Autocompletion samples:

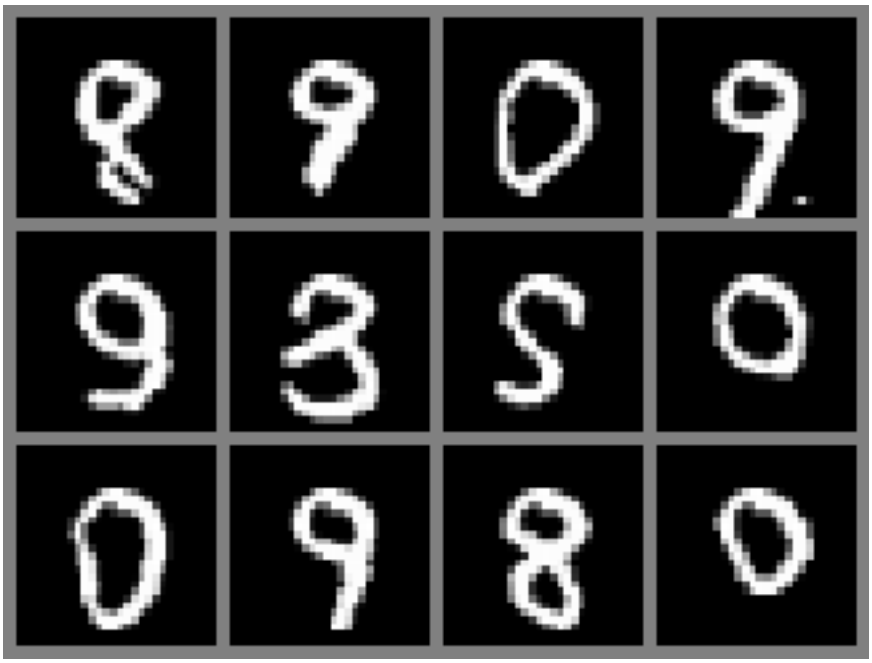


Original image and input image to sampling:



HBox(children=(FloatProgress(value=0.0, max=28.0), HTML(value='')))

Autocompletion samples:



For the first two digits (7 and 6), we see that the 12 samples all result in a shape which resemble the original digit. Nevertheless, there are some style difference in writing the 7, and some deformed sixes in the samples. When auto-completing the 9 below, we see that the model can fit multiple digits to it. We obtain diverse samples from 0, 3, 8 and 9. This shows that despite having no latent space, we can still obtain diverse samples from an autoregressive model.

Visualization of the predictive distribution (softmax)

Autoregressive models use a softmax over 256 values to predict the next pixel. This gives the model a large flexibility as the probabilities for each pixel value can be learned independently if necessary. However, the values are actually not independent because the values 32 and 33 are much closer than 32 and 255. In the following, we visualize the softmax distribution that the model predicts to gain insights how it has learned the relationships of close-by pixels.

To do this, we first run the model on a batch of images and store the output softmax distributions:

[23]:
```
det_loader = data.DataLoader(train_set, batch_size=128, shuffle=False, drop_last=False)
imgs,_ = next(iter(det_loader))
imgs = imgs.to(device)
with torch.no_grad():
    out = model(imgs)
    out = F.softmax(out, dim=1)
    mean_out = out.mean(dim=[0,2,3,4]).cpu().numpy()
    out = out.cpu().numpy()
```

Before diving into the model, let's visualize the distribution of the pixel values in the whole dataset:

[24]:
```
sns.set()
plot_args = {"color": to_rgb("C0")+(0.5,), "edgecolor": "C0", "linewidth": 0.5, "width":␣
↪1.0}
plt.hist(imgs.view(-1).cpu().numpy(), bins=256, density=True, **plot_args)
plt.yscale("log")
```

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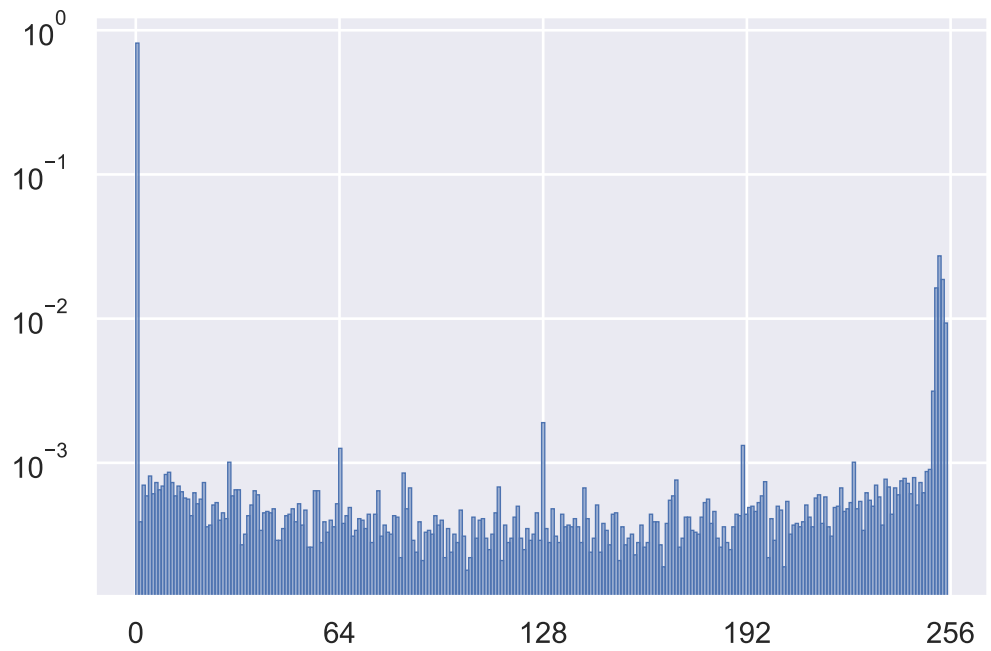
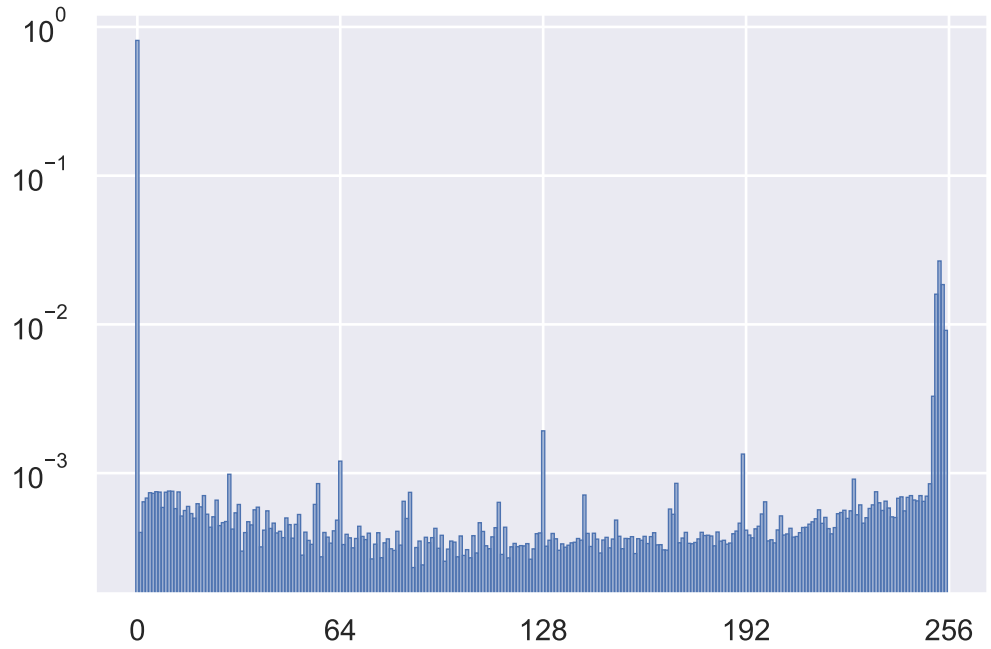
```
plt.xticks([0,64,128,192,256])
plt.show()
plt.close()
```



As we would expect from the seen images, the pixel value 0 (black) is the dominant value, followed by a batch of values between 250 and 255. Note that we use a log scale on the y-axis due to the big imbalance in the dataset. Interestingly, the pixel values 64, 128 and 191 also stand out which is likely due to the quantization used during the creation of the dataset. For RGB images, we would also see two peaks around 0 and 255, but the values in between would be much more frequent than in MNIST (see Figure 1 in the PixelCNN++ for a visualization on CIFAR10).

Next, we can visualize the distribution our model predicts (in average):

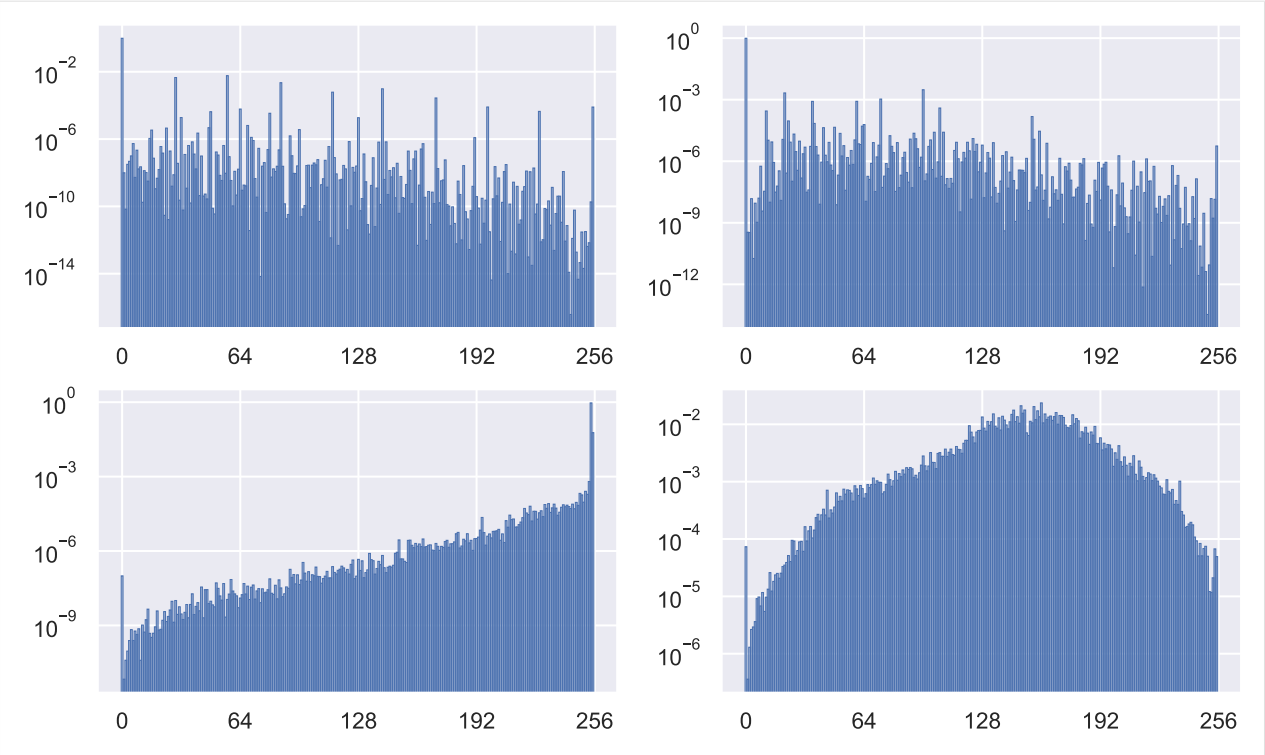
[25]:
```
plt.bar(np.arange(mean_out.shape[0]), mean_out, **plot_args)
plt.yscale("log")
plt.xticks([0,64,128,192,256])
plt.show()
plt.close()
```



This distribution is very close to the actual dataset distribution. This is in general a good sign, but we can see a slightly smoother histogram than above.

Finally, to take a closer look at learned value relations, we can visualize the distribution for individual pixel predictions to get a better intuition. For this, we pick 4 random images and pixels, and visualize their distribution below:

[26]:
```
fig, ax = plt.subplots(2,2, figsize=(10,6))
for i in range(4):
    ax_sub = ax[i//2][i%2]
    ax_sub.bar(np.arange(out.shape[1], dtype=np.int32), out[i+4,:,0,14,14], **plot_args)
    ax_sub.set_yscale("log")
    ax_sub.set_xticks([0,64,128,192,256])
plt.show()
plt.close()
```



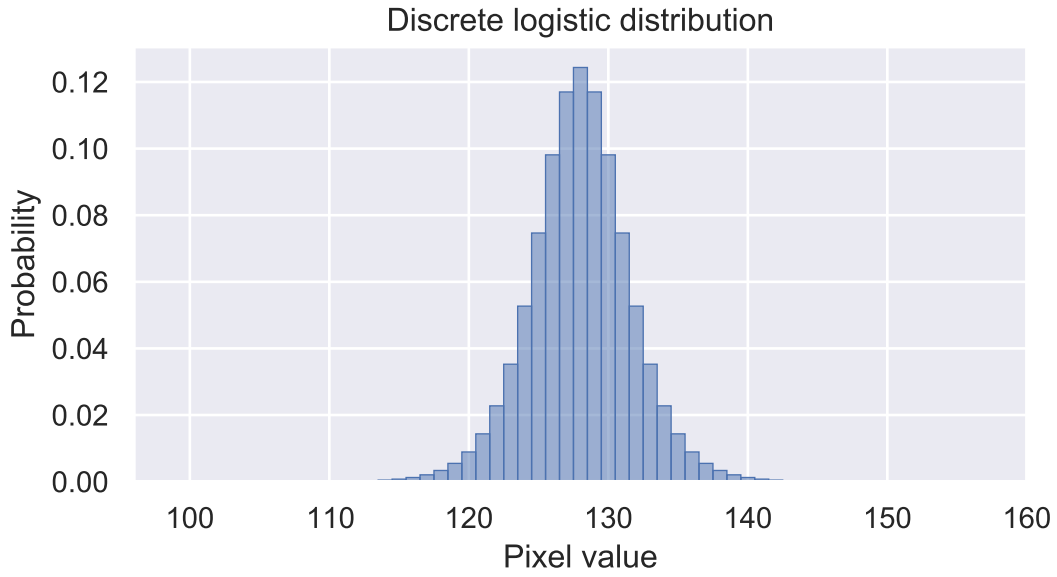
Overall we see a very diverse set of distributions, with a usual peak for 0 and close to 1. However, the distributions in the first row show a potentially undesirable behavior. For instance, the value 242 has a 1000x lower likelihood than 243 although they are extremely close and can often not be distinguished. This shows that the model might have not generlized well over pixel values. The better solution to this problem is to use discrete logitics mixtures instead of a softmax distribution. A discrete logistic distribution can be imagined as discretized, binned Gaussians. Using a mixture of discrete logistics instead of a softmax introduces an inductive bias to the model to assign close-by values similar likelihoods. We can visualize a discrete logistic below:

[27]:
```
mu = torch.Tensor([128])
sigma = torch.Tensor([2.0])

def discrete_logistic(x, mu, sigma):
    return torch.sigmoid((x+0.5-mu)/sigma) - torch.sigmoid((x-0.5-mu)/sigma)

x = torch.arange(256)
p = discrete_logistic(x, mu, sigma)

# Visualization
plt.figure(figsize=(6,3))
plt.bar(x.numpy(), p.numpy(), **plot_args)
plt.xlim(96,160)
plt.title("Discrete logistic distribution")
plt.xlabel("Pixel value")
plt.ylabel("Probability")
plt.show()
plt.close()
```



Instead of the softmax, the model would output mean and standard deviations for the K logistics we use in the mixture. This is one of the improvements in autoregressive models that PixelCNN++ [3] has introduced compared to the original PixelCNN.

4.26.4 Conclusion

In this tutorial, we have looked at autoregressive image modeling, and implemented the PixelCNN architecture. With the usage of masked convolutions, we are able to apply a convolutional network in which a pixel is only influenced by all its predecessors. Separating the masked convolution into a horizontal and vertical stack allowed us to remove the known blind spot on the right upper row of a pixel. In experiments, autoregressive models outperformed normalizing flows in terms of bits per dimension, but are much slower to sample from. Improvements, that we have not implemented ourselves here, are discrete logistic mixtures, a downsampling architecture, and changing the pixel order in a diagonal fashion (see PixelSNAIL). Overall, autoregressive models are another, strong family of generative models, which however are mostly used in sequence tasks because of their linear scaling in sampling time than quadratic as on images.

4.26.5 References

[1] van den Oord, A., et al. "Pixel Recurrent Neural Networks." arXiv preprint arXiv:1601.06759 (2016). Link

[2] van den Oord, A., et al. "Conditional Image Generation with PixelCNN Decoders." In Advances in Neural Information Processing Systems 29, pp. 4790–4798 (2016). Link

[3] Salimans, Tim, et al. "PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications." arXiv preprint arXiv:1701.05517 (2017). Link

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If you found this tutorial helpful, consider -ing our repository.

For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.27 Tutorial 15: Vision Transformers

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will take a closer look at a recent new trend: Transformers for Computer Vision. Since Alexey Dosovitskiy et al. successfully applied a Transformer on a variety of image recognition benchmarks, there have been an incredible amount of follow-up works showing that CNNs might not be optimal architecture for Computer Vision anymore. But how do Vision Transformers work exactly, and what benefits and drawbacks do they offer in contrast to CNNs? We will answer these questions by implementing a Vision Transformer ourselves and train it on the popular, small dataset CIFAR10. We will compare these results to the convolutional architectures of Tutorial 5.

If you are not familiar with Transformers yet, take a look at Tutorial 6 where we discuss the fundamentals of Multi-Head Attention and Transformers. As in many previous tutorials, we will use PyTorch Lightning again (introduced in Tutorial 5). Let's start with importing our standard set of libraries.

[1]:
```
## Standard libraries
import os
import numpy as np
import random
import math
import json
from functools import partial
from PIL import Image

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## tqdm for loading bars
from tqdm.notebook import tqdm
```

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```
## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim

## Torchvision
import torchvision
from torchvision.datasets import CIFAR10
from torchvision import transforms

# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Import tensorboard
%load_ext tensorboard

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial15"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)
```

```
Global seed set to 42
```

```
Device: cuda:0
```

We provide a pre-trained Vision Transformer which we download in the next cell. However, Vision Transformers can be relatively quickly trained on CIFAR10 with an overall training time of less than an hour on an NVIDIA TitanRTX. Feel free to experiment with training your own Transformer once you went through the whole notebook.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/"
# Files to download
```

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```
pretrained_files = ["tutorial15/ViT.ckpt", "tutorial15/tensorboards/ViT/events.out.
↪tfevents.ViT",
                    "tutorial5/tensorboards/ResNet/events.out.tfevents.resnet"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name.split("/",1)[1])
    if "/" in file_name.split("/",1)[1]:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

We load the CIFAR10 dataset below. We use the same setup of the datasets and data augmentations as for the CNNs in Tutorial 5 to keep a fair comparison. The constants in the `transforms.Normalize` correspond to the values that scale and shift the data to a zero mean and standard deviation of one.

[3]:
```
test_transform = transforms.Compose([transforms.ToTensor(),
                                     transforms.Normalize([0.49139968, 0.48215841, 0.
↪44653091], [0.24703223, 0.24348513, 0.26158784])
                                     ])
# For training, we add some augmentation. Networks are too powerful and would overfit.
train_transform = transforms.Compose([transforms.RandomHorizontalFlip(),
                                      transforms.RandomResizedCrop((32,32),scale=(0.8,1.
↪0),ratio=(0.9,1.1)),
                                      transforms.ToTensor(),
                                      transforms.Normalize([0.49139968, 0.48215841, 0.
↪44653091], [0.24703223, 0.24348513, 0.26158784])
                                     ])
# Loading the training dataset. We need to split it into a training and validation part
# We need to do a little trick because the validation set should not use the␣
↪augmentation.
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=train_transform,␣
↪download=True)
val_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=test_transform,␣
↪download=True)
pl.seed_everything(42)
train_set, _ = torch.utils.data.random_split(train_dataset, [45000, 5000])
pl.seed_everything(42)
_, val_set = torch.utils.data.random_split(val_dataset, [45000, 5000])

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=test_transform,␣
↪download=True)
```

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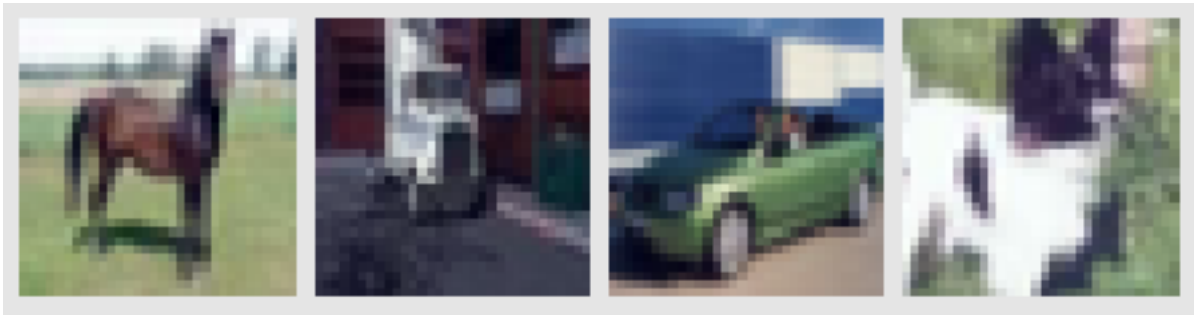
```
# We define a set of data loaders that we can use for various purposes later.
train_loader = data.DataLoader(train_set, batch_size=128, shuffle=True, drop_last=True,␣
↪pin_memory=True, num_workers=4)
val_loader = data.DataLoader(val_set, batch_size=128, shuffle=False, drop_last=False,␣
↪num_workers=4)
test_loader = data.DataLoader(test_set, batch_size=128, shuffle=False, drop_last=False,␣
↪num_workers=4)

# Visualize some examples
NUM_IMAGES = 4
CIFAR_images = torch.stack([val_set[idx][0] for idx in range(NUM_IMAGES)], dim=0)
img_grid = torchvision.utils.make_grid(CIFAR_images, nrow=4, normalize=True, pad_value=0.
↪9)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Image examples of the CIFAR10 dataset")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

```
Files already downloaded and verified
Files already downloaded and verified
```

```
Global seed set to 42
Global seed set to 42
```

```
Files already downloaded and verified
```



4.27.1 Transformers for image classification

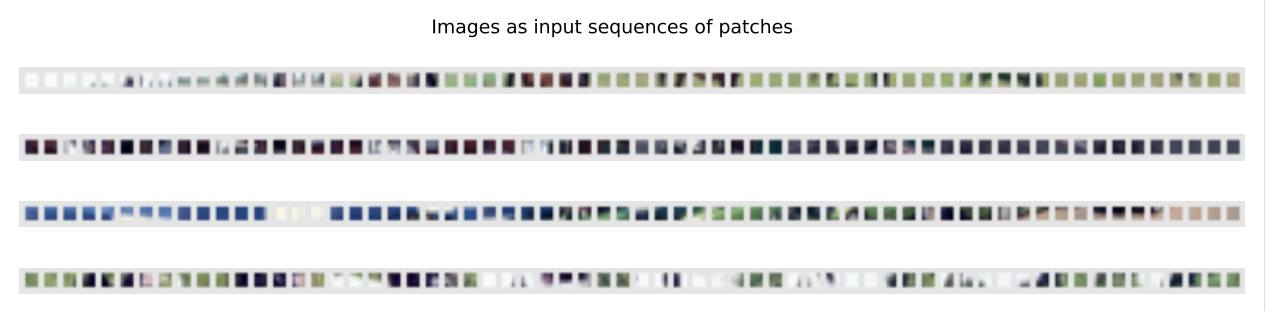
Transformers have been originally proposed to process sets since it is a permutation-equivariant architecture, i.e., producing the same output permuted if the input is permuted. To apply Transformers to sequences, we have simply added a positional encoding to the input feature vectors, and the model learned by itself what to do with it. So, why not do the same thing on images? This is exactly what Alexey Dosovitskiy et al. proposed in their paper "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale". Specifically, the Vision Transformer is a model for image classification that views images as sequences of smaller patches. As a preprocessing step, we split an image of, for example, 48×48 pixels into 9 16×16 patches. Each of those patches is considered to be a "word"/"token" and projected to a feature space. With adding positional encodings and a token for classification on top, we can apply a Transformer as usual to this sequence and start training it for our task. A nice GIF visualization of the architecture is shown below (figure credit - Phil Wang):

We will walk step by step through the Vision Transformer, and implement all parts by ourselves. First, let's implement the image preprocessing: an image of size $N \times N$ has to be split into $(N/M)^2$ patches of size $M \times M$. These represent the input words to the Transformer.

[4]:
```
def img_to_patch(x, patch_size, flatten_channels=True):
    """
    Inputs:
        x - torch.Tensor representing the image of shape [B, C, H, W]
        patch_size - Number of pixels per dimension of the patches (integer)
        flatten_channels - If True, the patches will be returned in a flattened format
                           as a feature vector instead of a image grid.
    """
    B, C, H, W = x.shape
    x = x.reshape(B, C, H//patch_size, patch_size, W//patch_size, patch_size)
    x = x.permute(0, 2, 4, 1, 3, 5) # [B, H', W', C, p_H, p_W]
    x = x.flatten(1,2)              # [B, H'*W', C, p_H, p_W]
    if flatten_channels:
        x = x.flatten(2,4)          # [B, H'*W', C*p_H*p_W]
    return x
```

Let's take a look at how that works for our CIFAR examples above. For our images of size 32×32, we choose a patch size of 4. Hence, we obtain sequences of 64 patches of size 4×4. We visualize them below:

[5]:
```
img_patches = img_to_patch(CIFAR_images, patch_size=4, flatten_channels=False)

fig, ax = plt.subplots(CIFAR_images.shape[0], 1, figsize=(14,3))
fig.suptitle("Images as input sequences of patches")
for i in range(CIFAR_images.shape[0]):
    img_grid = torchvision.utils.make_grid(img_patches[i], nrow=64, normalize=True, pad_
↪value=0.9)
    img_grid = img_grid.permute(1, 2, 0)
    ax[i].imshow(img_grid)
    ax[i].axis('off')
plt.show()
plt.close()
```



Compared to the original images, it is much harder to recognize the objects from those patch lists now. Still, this is the input we provide to the Transformer for classifying the images. The model has to learn itself how it has to combine the patches to recognize the objects. The inductive bias in CNNs that an image is a grid of pixels, is lost in this input format.

After we have looked at the preprocessing, we can now start building the Transformer model. Since we have discussed the fundamentals of Multi-Head Attention in Tutorial 6, we will use the PyTorch module `nn.MultiheadAttention` (docs) here. Further, we use the Pre-Layer Normalization version of the Transformer blocks proposed by Ruibin Xiong et al. in 2020. The idea is to apply Layer Normalization not in between residual blocks, but instead as a first layer in the residual blocks. This reorganization of the layers supports better gradient flow and removes the necessity of a warm-up stage. A visualization of the difference between the standard Post-LN and the Pre-LN version is shown below.

The implementation of the Pre-LN attention block looks as follows:

[6]:
```
class AttentionBlock(nn.Module):

    def __init__(self, embed_dim, hidden_dim, num_heads, dropout=0.0):
        """
        Inputs:
            embed_dim - Dimensionality of input and attention feature vectors
            hidden_dim - Dimensionality of hidden layer in feed-forward network
                         (usually 2-4x larger than embed_dim)
            num_heads - Number of heads to use in the Multi-Head Attention block
            dropout - Amount of dropout to apply in the feed-forward network
        """
        super().__init__()

        self.layer_norm_1 = nn.LayerNorm(embed_dim)
        self.attn = nn.MultiheadAttention(embed_dim, num_heads,
                                          dropout=dropout)
        self.layer_norm_2 = nn.LayerNorm(embed_dim)
        self.linear = nn.Sequential(
            nn.Linear(embed_dim, hidden_dim),
            nn.GELU(),
            nn.Dropout(dropout),
            nn.Linear(hidden_dim, embed_dim),
            nn.Dropout(dropout)
        )


    def forward(self, x):
        inp_x = self.layer_norm_1(x)
```

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```
        x = x + self.attn(inp_x, inp_x, inp_x)[0]
        x = x + self.linear(self.layer_norm_2(x))
        return x
```

Now we have all modules ready to build our own Vision Transformer. Besides the Transformer encoder, we need the following modules:

- A **linear projection** layer that maps the input patches to a feature vector of larger size. It is implemented by a simple linear layer that takes each $M \times M$ patch independently as input.
- A **classification token** that is added to the input sequence. We will use the output feature vector of the classification token (CLS token in short) for determining the classification prediction.
- Learnable **positional encodings** that are added to the tokens before being processed by the Transformer. Those are needed to learn position-dependent information, and convert the set to a sequence. Since we usually work with a fixed resolution, we can learn the positional encodings instead of having the pattern of sine and cosine functions.
- An **MLP head** that takes the output feature vector of the CLS token, and maps it to a classification prediction. This is usually implemented by a small feed-forward network or even a single linear layer.

With those components in mind, let's implement the full Vision Transformer below:

[7]:
```
class VisionTransformer(nn.Module):

    def __init__(self, embed_dim, hidden_dim, num_channels, num_heads, num_layers, num_
↪classes, patch_size, num_patches, dropout=0.0):
        """
        Inputs:
            embed_dim - Dimensionality of the input feature vectors to the Transformer
            hidden_dim - Dimensionality of the hidden layer in the feed-forward networks
                         within the Transformer
            num_channels - Number of channels of the input (3 for RGB)
            num_heads - Number of heads to use in the Multi-Head Attention block
            num_layers - Number of layers to use in the Transformer
            num_classes - Number of classes to predict
            patch_size - Number of pixels that the patches have per dimension
            num_patches - Maximum number of patches an image can have
            dropout - Amount of dropout to apply in the feed-forward network and
                      on the input encoding
        """
        super().__init__()

        self.patch_size = patch_size

        # Layers/Networks
        self.input_layer = nn.Linear(num_channels*(patch_size**2), embed_dim)
        self.transformer = nn.Sequential(*[AttentionBlock(embed_dim, hidden_dim, num_
↪heads, dropout=dropout) for _ in range(num_layers)])
        self.mlp_head = nn.Sequential(
            nn.LayerNorm(embed_dim),
            nn.Linear(embed_dim, num_classes)
        )
        self.dropout = nn.Dropout(dropout)
```

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```
        # Parameters/Embeddings
        self.cls_token = nn.Parameter(torch.randn(1,1,embed_dim))
        self.pos_embedding = nn.Parameter(torch.randn(1,1+num_patches,embed_dim))


    def forward(self, x):
        # Preprocess input
        x = img_to_patch(x, self.patch_size)
        B, T, _ = x.shape
        x = self.input_layer(x)

        # Add CLS token and positional encoding
        cls_token = self.cls_token.repeat(B, 1, 1)
        x = torch.cat([cls_token, x], dim=1)
        x = x + self.pos_embedding[:,:T+1]

        # Apply Transforrmer
        x = self.dropout(x)
        x = x.transpose(0, 1)
        x = self.transformer(x)

        # Perform classification prediction
        cls = x[0]
        out = self.mlp_head(cls)
        return out
```

Finally, we can put everything into a PyTorch Lightning Module as usual. We use `torch.optim.AdamW` as the optimizer, which is Adam with a corrected weight decay implementation. Since we use the Pre-LN Transformer version, we do not need to use a learning rate warmup stage anymore. Instead, we use the same learning rate scheduler as the CNNs in our previous tutorial on image classification.

[8]:
```
class ViT(pl.LightningModule):

    def __init__(self, model_kwargs, lr):
        super().__init__()
        self.save_hyperparameters()
        self.model = VisionTransformer(**model_kwargs)
        self.example_input_array = next(iter(train_loader))[0]

    def forward(self, x):
        return self.model(x)

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(), lr=self.hparams.lr)
        lr_scheduler = optim.lr_scheduler.MultiStepLR(optimizer, milestones=[100,150],␣
↪gamma=0.1)
        return [optimizer], [lr_scheduler]

    def _calculate_loss(self, batch, mode="train"):
        imgs, labels = batch
        preds = self.model(imgs)
        loss = F.cross_entropy(preds, labels)
```

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```
        acc = (preds.argmax(dim=-1) == labels).float().mean()

        self.log(f'{mode}_loss', loss)
        self.log(f'{mode}_acc', acc)
        return loss

    def training_step(self, batch, batch_idx):
        loss = self._calculate_loss(batch, mode="train")
        return loss

    def validation_step(self, batch, batch_idx):
        self._calculate_loss(batch, mode="val")

    def test_step(self, batch, batch_idx):
        self._calculate_loss(batch, mode="test")
```

4.27.2 Experiments

Commonly, Vision Transformers are applied to large-scale image classification benchmarks such as ImageNet to leverage their full potential. However, here we take a step back and ask: can Vision Transformer also succeed on classical, small benchmarks such as CIFAR10? To find this out, we train a Vision Transformer from scratch on the CIFAR10 dataset. Let's first create a training function for our PyTorch Lightning module which also loads the pre-trained model if you have downloaded it above.

[9]:
```
def train_model(**kwargs):
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, "ViT"),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=180,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc"),
                                    LearningRateMonitor("epoch")])
    trainer.logger._log_graph = True         # If True, we plot the computation graph in␣
↪tensorboard
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, "ViT.ckpt")
    if os.path.isfile(pretrained_filename):
        print(f"Found pretrained model at {pretrained_filename}, loading...")
        model = ViT.load_from_checkpoint(pretrained_filename) # Automatically loads the␣
↪model with the saved hyperparameters
    else:
        pl.seed_everything(42) # To be reproducable
        model = ViT(**kwargs)
        trainer.fit(model, train_loader, val_loader)
        model = ViT.load_from_checkpoint(trainer.checkpoint_callback.best_model_path) #␣
↪Load best checkpoint after training

    # Test best model on validation and test set
```

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```
    val_result = trainer.test(model, val_loader, verbose=False)
    test_result = trainer.test(model, test_loader, verbose=False)
    result = {"test": test_result[0]["test_acc"], "val": val_result[0]["test_acc"]}

    return model, result
```

Now, we can already start training our model. As seen in our implementation, we have a couple of hyperparameters that we have to set. When creating this notebook, we have performed a small grid search over hyperparameters and listed the best hyperparameters in the cell below. Nevertheless, it is worth discussing the influence that each hyperparameter has, and what intuition we have for choosing its value.

First, let's consider the patch size. The smaller we make the patches, the longer the input sequences to the Transformer become. While in general, this allows the Transformer to model more complex functions, it requires a longer computation time due to its quadratic memory usage in the attention layer. Furthermore, small patches can make the task more difficult since the Transformer has to learn which patches are close-by, and which are far away. We experimented with patch sizes of 2, 4, and 8 which gives us the input sequence lengths of 256, 64, and 16 respectively. We found 4 to result in the best performance and hence pick it below.

Next, the embedding and hidden dimensionality have a similar impact on a Transformer as to an MLP. The larger the sizes, the more complex the model becomes, and the longer it takes to train. In Transformers, however, we have one more aspect to consider: the query-key sizes in the Multi-Head Attention layers. Each key has the feature dimensionality of `embed_dim/num_heads`. Considering that we have an input sequence length of 64, a minimum reasonable size for the key vectors is 16 or 32. Lower dimensionalities can restrain the possible attention maps too much. We observed that more than 8 heads are not necessary for the Transformer, and therefore pick an embedding dimensionality of `256`. The hidden dimensionality in the feed-forward networks is usually 2-4x larger than the embedding dimensionality, and thus we pick `512`.

Finally, the learning rate for Transformers is usually relatively small, and in papers, a common value to use is 3e-5. However, since we work with a smaller dataset and have a potentially easier task, we found that we are able to increase the learning rate to 3e-4 without any problems. To reduce overfitting, we use a dropout value of 0.2. Remember that we also use small image augmentations as regularization during training.

Feel free to explore the hyperparameters yourself by changing the values below. In general, the Vision Transformer did not show to be too sensitive to the hyperparameter choices on the CIFAR10 dataset.

[10]:
```
model, results = train_model(model_kwargs={
                                'embed_dim': 256,
                                'hidden_dim': 512,
                                'num_heads': 8,
                                'num_layers': 6,
                                'patch_size': 4,
                                'num_channels': 3,
                                'num_patches': 64,
                                'num_classes': 10,
                                'dropout': 0.2
                            },
                            lr=3e-4)
print("ViT results", results)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
```

```
Found pretrained model at ../saved_models/tutorial15/ViT.ckpt, loading...
```

```
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
HBox(children=(HTML(value='Testing'), FloatProgress(value=1.0, bar_style='info',␣
↪layout=Layout(flex='2'), max=...
```

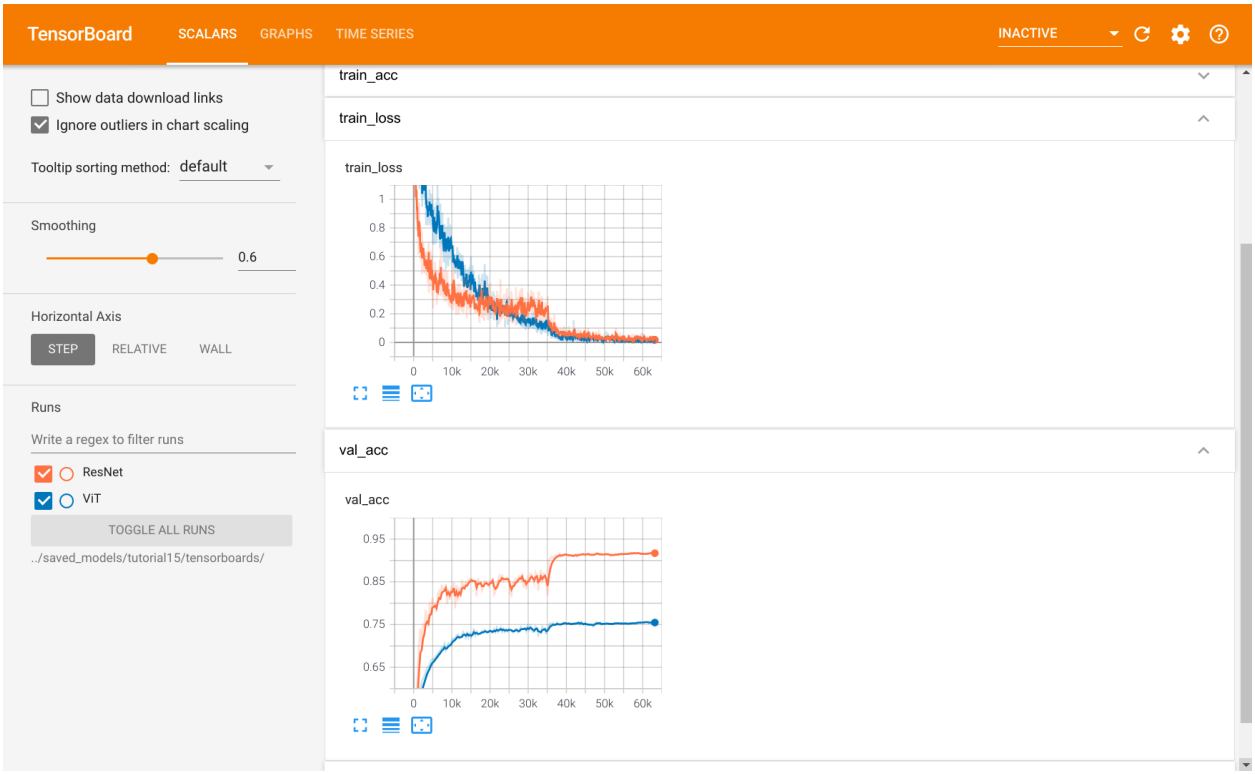
```
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
HBox(children=(HTML(value='Testing'), FloatProgress(value=1.0, bar_style='info',␣
↪layout=Layout(flex='2'), max=...
```

```
ViT results {'test': 0.7559000253677368, 'val': 0.7563999891281128}
```

The Vision Transformer achieves a validation and test performance of about 75%. In comparison, almost all CNN architectures that we have tested in Tutorial 5 obtained a classification performance of around 90%. This is a considerable gap and shows that although Vision Transformers perform strongly on ImageNet with potential pretraining, they cannot come close to simple CNNs on CIFAR10 when being trained from scratch. The differences between a CNN and Transformer can be well observed in the training curves. Let's look at them in a tensorboard below:

[11]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH!
%tensorboard --logdir ../saved_models/tutorial15/tensorboards/
```



The tensorboard compares the Vision Transformer to a ResNet trained on CIFAR10. When looking at the training losses, we see that the ResNet learns much more quickly in the first iterations. While the learning rate might have an influence on the initial learning speed, we see the same trend in the validation accuracy. The ResNet achieves the best performance of the Vision Transformer after just 5 epochs (2000 iterations). Further, while the ResNet training loss and validation accuracy have a similar trend, the validation performance of the Vision Transformers only marginally changes after 10k iterations while the training loss has almost just started going down. Yet, the Vision Transformer is also able to achieve close to 100% accuracy on the training set.

All those observed phenomenons can be explained with a concept that we have visited before: inductive biases. Convolutional Neural Networks have been designed with the assumption that images are translation invariant. Hence, we

apply convolutions with shared filters across the image. Furthermore, a CNN architecture integrates the concept of distance in an image: two pixels that are close to each other are more related than two distant pixels. Local patterns are combined into larger patterns until we perform our classification prediction. All those aspects are inductive biases of a CNN. In contrast, a Vision Transformer does not know which two pixels are close to each other, and which are far apart. It has to learn this information solely from the sparse learning signal of the classification task. This is a huge disadvantage when we have a small dataset since such information is crucial for generalizing to an unseen test dataset. With large enough datasets and/or good pre-training, a Transformer can learn this information without the need for inductive biases, and instead is more flexible than a CNN. Especially long-distance relations between local patterns can be difficult to process in CNNs, while in Transformers, all patches have the distance of one. This is why Vision Transformers are so strong on large-scale datasets such as ImageNet but underperform a lot when being applied to a small dataset such as CIFAR10.

4.27.3 Conclusion

In this tutorial, we have implemented our own Vision Transformer from scratch and applied it to the task of image classification. Vision Transformers work by splitting an image into a sequence of smaller patches, use those as input to a standard Transformer encoder. While Vision Transformers achieved outstanding results on large-scale image recognition benchmarks such as ImageNet, they considerably underperform when being trained from scratch on small-scale datasets like CIFAR10. The reason is that in contrast to CNNs, Transformers do not have the inductive biases of translation invariance and the feature hierarchy (i.e. larger patterns consist of many smaller patterns). However, these aspects can be learned when enough data is provided, or the model has been pre-trained on other large-scale tasks. Considering that Vision Transformers have just been proposed end of 2020, there is likely a lot more to come on Transformers for Computer Vision.

References

Dosovitskiy, Alexey, et al. "An image is worth 16x16 words: Transformers for image recognition at scale." International Conference on Learning Representations (2021). link

Chen, Xiangning, et al. "When Vision Transformers Outperform ResNets without Pretraining or Strong Data Augmentations." arXiv preprint arXiv:2106.01548 (2021). link

Tolstikhin, Ilya, et al. "MLP-mixer: An all-MLP Architecture for Vision." arXiv preprint arXiv:2105.01601 (2021). link

Xiong, Ruibin, et al. "On layer normalization in the transformer architecture." International Conference on Machine Learning. PMLR, 2020. link

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If you found this tutorial helpful, consider -ing our repository.

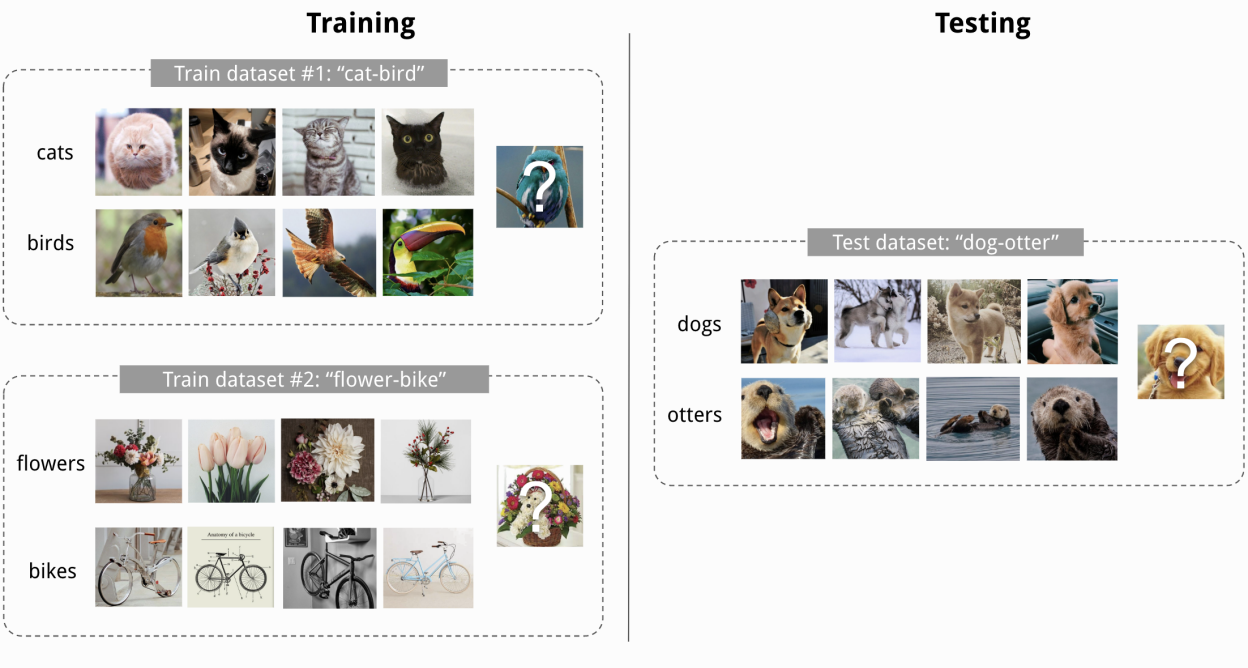
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.28 Tutorial 16: Meta-Learning - Learning to Learn

Filled notebook:
Pre-trained models:
Recordings:
Author: Phillip Lippe

In this tutorial, we will discuss algorithms that learn models which can quickly adapt to new classes and/or tasks with few samples. This area of machine learning is called *Meta-Learning* aiming at "learning to learn". Learning from very few examples is a natural task for humans. In contrast to current deep learning models, we need to see only a few examples of a police car or firetruck to recognize them in daily traffic. This is a crucial ability since, in real-world applications, it is rarely the case that the data stays static and does not change over time. For example, an object detection system for mobile phones trained on data from 2000 will have trouble detecting today's common mobile phones, and thus, needs to adapt to new data without excessive label effort. The optimization techniques we have discussed so far struggle with this because they only aim at obtaining a good performance on a test set that had similar data. However, what if the test set has classes that we do not have in the training set? Or what if we want to test the model on a completely different task?

Meta-Learning offers solutions to these situations, and we will discuss three popular algorithms: **Prototypical Networks** (Snell et al., 2017), **Model-Agnostic Meta-Learning / MAML** (Finn et al., 2017), and **Proto-MAML** (Triantafillou et al., 2020). We will focus on the task of few-shot classification where the training and test set have distinct sets of classes. For instance, we would train the model on the binary classifications of cats-birds and flowers-bikes, but during test time, the model would need to learn from 4 examples each the difference between dogs and otters, two classes we have not seen during training (Figure credit - Lilian Weng).



A different setup, which is very common in Reinforcement Learning and recently Natural Language Processing, is to aim at few-shot learning of a completely new task. For example, a robot agent that learned to run, jump and pick up boxes, should quickly adapt to collecting and stacking boxes. In NLP, we can think of a model which was trained

in sentiment classification, hate speech detection, and sarcasm classification, to adapt to classifying the emotion of a text. All methods we will discuss in this notebook can be easily applied to these settings since we only use a different definition of a 'task'. For few-shot classification, we consider a task to distinguish between M novel classes. Here, we would not only have novel classes, but also a completely different dataset.

First of all, let's start with importing our standard libraries. We will again be using PyTorch Lightning.

[1]:
```
## Standard libraries
import os
import numpy as np
import random
import json
from PIL import Image
from collections import defaultdict
from statistics import mean, stdev
from copy import deepcopy

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## tqdm for loading bars
from tqdm.auto import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim

## Torchvision
import torchvision
from torchvision.datasets import CIFAR100, SVHN
from torchvision import transforms

# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Import tensorboard
%load_ext tensorboard
```

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```
# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial16"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)
```

```
Global seed set to 42
```

```
Device: cuda:0
```

Training the models in this notebook can take between 2 and 8 hours, and the evaluation time of some algorithms is in the span of couples of minutes. Hence, we download pre-trained models and results below.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial16/"
# Files to download
pretrained_files = ["ProtoNet.ckpt", "ProtoMAML.ckpt",
                    "tensorboards/ProtoNet/events.out.tfevents.ProtoNet",
                    "tensorboards/ProtoMAML/events.out.tfevents.ProtoMAML",
                    "protomaml_fewshot.json",
                    "protomaml_svhn_fewshot.json"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.28.1 Few-shot classification

We start our implementation by discussing the dataset setup. In this notebook, we will use CIFAR100 which we have already seen in Tutorial 6. CIFAR100 has 100 classes each with 600 images of size 32×32 pixels. Instead of splitting the training, validation, and test set over examples, we will split them over classes: we will use 80 classes for training, and 10 for validation, and 10 for testing. Our overall goal is to obtain a model that can distinguish between the 10 test classes with seeing very few examples. First, let's load the dataset and visualize some examples.

[3]:
```
# Loading CIFAR100 dataset
CIFAR_train_set = CIFAR100(root=DATASET_PATH, train=True, download=True,␣
↪transform=transforms.ToTensor())
CIFAR_test_set = CIFAR100(root=DATASET_PATH, train=False, download=True,␣
↪transform=transforms.ToTensor())
```

```
Files already downloaded and verified
Files already downloaded and verified
```

[4]:
```
# Visualize some examples
NUM_IMAGES = 12
CIFAR_images = torch.stack([CIFAR_train_set[np.random.randint(len(CIFAR_train_set))][0]␣
↪for idx in range(NUM_IMAGES)], dim=0)
img_grid = torchvision.utils.make_grid(CIFAR_images, nrow=6, normalize=True, pad_value=0.
↪9)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Image examples of the CIFAR100 dataset")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

Data preprocessing

Next, we need to prepare the dataset in the training, validation and test split as mentioned before. The torchvision package gives us the training and test set as two separate dataset objects. The next code cells will merge the original training and test set, and then create the new train-val-test split.

[5]:
```
# Merging original training and test set
CIFAR_all_images = np.concatenate([CIFAR_train_set.data, CIFAR_test_set.data], axis=0)
CIFAR_all_targets = torch.LongTensor(CIFAR_train_set.targets + CIFAR_test_set.targets)
```

To have an easier time handling the dataset, we define our own, simple dataset class below. It takes a set of images, labels/targets, and image transformations, and returns the corresponding images and labels element-wise.

[6]:
```
class ImageDataset(data.Dataset):

    def __init__(self, imgs, targets, img_transform=None):
        """
        Inputs:
            imgs - Numpy array of shape [N,32,32,3] containing all images.
            targets - PyTorch array of shape [N] containing all labels.
            img_transform - A torchvision transformation that should be applied
                            to the images before returning. If none, no transformation
                            is applied.
        """
        super().__init__()
        self.img_transform = img_transform
        self.imgs = imgs
        self.targets = targets

    def __getitem__(self, idx):
        img, target = self.imgs[idx], self.targets[idx]
        img = Image.fromarray(img)

        if self.img_transform is not None:
            img = self.img_transform(img)

        return img, target

    def __len__(self):
        return self.imgs.shape[0]
```

Now, we can create the class splits. We will assign the classes randomly to training, validation and test, and use a 80%-10%-10% split.

[7]:
```
torch.manual_seed(0)           # Set seed for reproducibility
classes = torch.randperm(100)  # Returns random permutation of numbers 0 to 99
train_classes, val_classes, test_classes = classes[:80], classes[80:90], classes[90:]
```

To get an intuition of the validation and test classes, we print the class names below:

[8]:
```
# Printing validation and test classes
idx_to_class = {val: key for key, val in CIFAR_train_set.class_to_idx.items()}
print("Validation classes:", [idx_to_class[c.item()] for c in val_classes])
print("Test classes:", [idx_to_class[c.item()] for c in test_classes])
```

```
Validation classes: ['caterpillar', 'castle', 'skunk', 'ray', 'bus', 'motorcycle',
↪'keyboard', 'chimpanzee', 'possum', 'tiger']
Test classes: ['kangaroo', 'crocodile', 'butterfly', 'shark', 'forest', 'pickup_truck',
↪'telephone', 'lion', 'worm', 'mushroom']
```

As we can see, the classes have quite some variety and some classes might be easier to distinguish than others. For instance, in the test classes, 'pickup_truck' is the only vehicle while the classes 'mushroom', 'worm' and 'forest' might be harder to keep apart. Remember that we want to learn the classification of those ten classes from 80 other classes in our training set, and few examples from the actual test classes. We will experiment with the number of examples per class.

Finally, we can create the training, validation and test dataset according to our split above. For this, we create dataset objects of our previously defined class `ImageDataset`.

[9]:
```
def dataset_from_labels(imgs, targets, class_set, **kwargs):
    class_mask = (targets[:,None] == class_set[None,:]).any(dim=-1)
    return ImageDataset(imgs=imgs[class_mask],
                        targets=targets[class_mask],
                        **kwargs)
```

As in our experiments before on CIFAR in Tutorial 5, 6 and 9, we normalize the dataset. Additionally, we use small augmentations during training to prevent overfitting.

[10]:
```
# Pre-computed statistics from the new train set
DATA_MEANS = torch.Tensor([0.5183975 , 0.49192241, 0.44651328])
DATA_STD = torch.Tensor([0.26770132, 0.25828985, 0.27961241])

test_transform = transforms.Compose([transforms.ToTensor(),
                                     transforms.Normalize(
                                         DATA_MEANS, DATA_STD)
                                     ])
# For training, we add some augmentation.
train_transform = transforms.Compose([transforms.RandomHorizontalFlip(),
                                      transforms.RandomResizedCrop(
                                          (32, 32), scale=(0.8, 1.0), ratio=(0.9, 1.1)),
                                      transforms.ToTensor(),
                                      transforms.Normalize(
                                          DATA_MEANS, DATA_STD)
                                      ])

train_set = dataset_from_labels(
    CIFAR_all_images, CIFAR_all_targets, train_classes, img_transform=train_transform)
val_set = dataset_from_labels(
    CIFAR_all_images, CIFAR_all_targets, val_classes, img_transform=test_transform)
test_set = dataset_from_labels(
    CIFAR_all_images, CIFAR_all_targets, test_classes, img_transform=test_transform)
```

Data sampling

The strategy of how to use the available training data for learning few-shot adaptation is crucial in meta-learning. All three algorithms that we discuss here have a similar idea: simulate few-shot learning during training. Specifically, at each training step, we randomly select a small number of classes and sample a small number of examples for each class. This represents our few-shot training batch, which we also refer to as **support set**. Additionally, we sample a second set of examples from the same classes and refer to this batch as **query set**. Our training objective is to classify the query set correctly from seeing the support set and its corresponding labels. The main difference between our three methods (ProtoNet, MAML, and Proto-MAML) is in how they use the support set to adapt to the training classes.

This subsection summarizes the code that is needed to create such training batches. In PyTorch, we can specify the data sampling procedure by so-called `Sampler` (documentation). Samplers are iterable objects that return indices in the order in which the data elements should be sampled. In our previous notebooks, we usually used the option `shuffle=True` in the `data.DataLoader` objects which creates a sampler returning the data indices in random order. Here, we focus on samplers that return batches of indices that correspond to support and query set batches. Below, we implement such a sampler.

[11]:
```
class FewShotBatchSampler(object):

    def __init__(self, dataset_targets, N_way, K_shot, include_query=False, shuffle=True,
↪ shuffle_once=False):
        """
        Inputs:
            dataset_targets - PyTorch tensor of the labels of the data elements.
            N_way - Number of classes to sample per batch.
            K_shot - Number of examples to sample per class in the batch.
            include_query - If True, returns batch of size N_way*K_shot*2, which
                            can be split into support and query set. Simplifies
                            the implementation of sampling the same classes but
                            distinct examples for support and query set.
            shuffle - If True, examples and classes are newly shuffled in each
                      iteration (for training)
            shuffle_once - If True, examples and classes are shuffled once in
                           the beginning, but kept constant across iterations
                           (for validation)
        """
        super().__init__()
        self.dataset_targets = dataset_targets
        self.N_way = N_way
        self.K_shot = K_shot
        self.shuffle = shuffle
        self.include_query = include_query
        if self.include_query:
            self.K_shot *= 2
        self.batch_size = self.N_way * self.K_shot  # Number of overall images per batch

        # Organize examples by class
        self.classes = torch.unique(self.dataset_targets).tolist()
        self.num_classes = len(self.classes)
        self.indices_per_class = {}
        self.batches_per_class = {}  # Number of K-shot batches that each class can␣
↪provide
        for c in self.classes:
            self.indices_per_class[c] = torch.where(self.dataset_targets == c)[0]
```

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```
            self.batches_per_class[c] = self.indices_per_class[c].shape[0] // self.K_shot

        # Create a list of classes from which we select the N classes per batch
        self.iterations = sum(self.batches_per_class.values()) // self.N_way
        self.class_list = [c for c in self.classes for _ in range(self.batches_per_
↪class[c])]
        if shuffle_once or self.shuffle:
            self.shuffle_data()
        else:
            # For testing, we iterate over classes instead of shuffling them
            sort_idxs = [i+p*self.num_classes for i,
                         c in enumerate(self.classes) for p in range(self.batches_per_
↪class[c])]
            self.class_list = np.array(self.class_list)[np.argsort(sort_idxs)].tolist()

    def shuffle_data(self):
        # Shuffle the examples per class
        for c in self.classes:
            perm = torch.randperm(self.indices_per_class[c].shape[0])
            self.indices_per_class[c] = self.indices_per_class[c][perm]
        # Shuffle the class list from which we sample. Note that this way of shuffling
        # does not prevent to choose the same class twice in a batch. However, for
        # training and validation, this is not a problem.
        random.shuffle(self.class_list)

    def __iter__(self):
        # Shuffle data
        if self.shuffle:
            self.shuffle_data()

        # Sample few-shot batches
        start_index = defaultdict(int)
        for it in range(self.iterations):
            class_batch = self.class_list[it*self.N_way:(it+1)*self.N_way]  # Select N␣
↪classes for the batch
            index_batch = []
            for c in class_batch:  # For each class, select the next K examples and add␣
↪them to the batch
                index_batch.extend(self.indices_per_class[c][start_index[c]:start_
↪index[c]+self.K_shot])
                start_index[c] += self.K_shot
            if self.include_query:  # If we return support+query set, sort them so that␣
↪they are easy to split
                index_batch = index_batch[::2] + index_batch[1::2]
            yield index_batch

    def __len__(self):
        return self.iterations
```

Note that this sampler eventually allows the sampling of batches where we use a class twice due to a simpler shuffling function (`shuffle_data`). In other words, during training or validation, if we sample batches for a 5-class 4-shot training setting, it can occasionally happen that we get a batch where 2 of the 5 classes are identical. Since we have 80 classes to choose from, this however happens relatively rarely. Further, it actually does not constitute any issue if

the code for the meta-learning methods support variable number of classes and shots per class. Nonetheless, when the number of classes/tasks is smaller, it is recommended to replace the `shuffle_data` method with a sampler that prevents picking the same class twice in a batch.

Now, we can create our intended data loaders by passing an object of `FewShotBatchSampler` as `batch_sampler=...` input to the PyTorch data loader object. For our experiments, we will use a 5-class 4-shot training setting. This means that each support set contains 5 classes with 4 examples each, i.e., 20 images overall. Usually, it is good to keep the number of shots equal to the number that you aim to test on. However, we will experiment later with a different number of shots, and hence, we pick 4 as a compromise for now. To get the best-performing model, it is recommended to consider the number of training shots as hyperparameters in a grid search.

[12]:
```
N_WAY = 5
K_SHOT = 4
train_data_loader = data.DataLoader(train_set,
                                    batch_sampler=FewShotBatchSampler(train_set.targets,
                                                                      include_query=True,
                                                                      N_way=N_WAY,
                                                                      K_shot=K_SHOT,
                                                                      shuffle=True),
                                    num_workers=4)
val_data_loader = data.DataLoader(val_set,
                                  batch_sampler=FewShotBatchSampler(val_set.targets,
                                                                    include_query=True,
                                                                    N_way=N_WAY,
                                                                    K_shot=K_SHOT,
                                                                    shuffle=False,
                                                                    shuffle_once=True),
                                  num_workers=4)
```

For simplicity, we implemented the sampling of a support and query set as sampling a support set with twice the number of examples. After sampling a batch from the data loader, we need to split it into a support and query set. We can summarize this step in the following function:

[13]:
```
def split_batch(imgs, targets):
    support_imgs, query_imgs = imgs.chunk(2, dim=0)
    support_targets, query_targets = targets.chunk(2, dim=0)
    return support_imgs, query_imgs, support_targets, query_targets
```

Finally, to ensure that our implementation of the data sampling process is correct, we can sample a batch and visualize its support and query set. What we would like to see is that the support and query set have the same classes, but distinct examples.

[14]:
```
imgs, targets = next(iter(val_data_loader))  # We use the validation set since it does␣
↪not apply augmentations
support_imgs, query_imgs, _, _ = split_batch(imgs, targets)
support_grid = torchvision.utils.make_grid(support_imgs, nrow=K_SHOT, normalize=True,␣
↪pad_value=0.9)
support_grid = support_grid.permute(1, 2, 0)
query_grid = torchvision.utils.make_grid(query_imgs, nrow=K_SHOT, normalize=True, pad_
↪value=0.9)
query_grid = query_grid.permute(1, 2, 0)

fig, ax = plt.subplots(1, 2, figsize=(8, 5))
ax[0].imshow(support_grid)
```

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```
ax[0].set_title("Support set")
ax[0].axis('off')
ax[1].imshow(query_grid)
ax[1].set_title("Query set")
ax[1].axis('off')
plt.suptitle("Few Shot Batch", weight='bold')
plt.show()
plt.close()
```

As we can see, the support and query set have the same five classes, but different examples. The models will be tasked to classify the examples in the query set by learning from the support set and its labels. With the data sampling in place, we can now start to implement our first meta-learning model: Prototypical Networks.

4.28.2 Prototypical Networks

The Prototypical Network, or ProtoNet for short, is a metric-based meta-learning algorithm that operates similarly to the nearest neighbor classification. Metric-based meta-learning methods classify a new example $\mathbf{x}$ based on some distance function d_φ between x and all elements in the support set. ProtoNets implements this idea with the concept of prototypes in a learned feature space. First, ProtoNet uses an embedding function f_θ to encode each input in the support set into a L-dimensional feature vector. Next, for each class c, we collect the feature vectors of all examples with label c and average their feature vectors. Formally, we can define this as:

$$\mathbf{v}_c = \frac{1}{|S_c|} \sum_{(\mathbf{x}_i, y_i) \in S_c} f_\theta(\mathbf{x}_i)$$

where S_c is the part of the support set S for which $y_i = c$, and $\mathbf{v}_c$ represents the *prototype* of class c. The prototype calculation is visualized below for a 2-dimensional feature space and 3 classes (Figure credit - Snell et al.). The colored dots represent encoded support elements with the color-corresponding class labels, and the black dots next to the class label are the averaged prototypes.

Based on these prototypes, we want to classify a new example. Remember that since we want to learn the encoding function f_θ, this classification must be differentiable, and hence, we need to define a probability distribution across classes. For this, we will make use of the distance function d_φ: the closer a new example $\mathbf{x}$ is to a prototype $\mathbf{v}_c$, the higher the probability for $\mathbf{x}$ belonging to class c. Formally, we can simply use a softmax over the distances of $\mathbf{x}$ to all class prototypes:

$$p(y = c|\mathbf{x}) = \text{softmax}(-d_\varphi(f_\theta(\mathbf{x}), \mathbf{v}_c)) = \frac{\exp\left(-d_\varphi(f_\theta(\mathbf{x}), \mathbf{v}_c)\right)}{\sum_{c' \in \mathcal{C}} \exp\left(-d_\varphi(f_\theta(\mathbf{x}), \mathbf{v}_{c'})\right)}$$

Note that the negative sign is necessary since we want to increase the probability for close-by vectors and have a low probability for distant vectors. We train the network f_θ based on the cross-entropy error of the training query set examples. Thereby, the gradient flows through both the prototypes $\mathbf{v}_c$ and the query set encodings $f_\theta(\mathbf{x})$. For the distance function d_φ, we can choose any function as long as it is differentiable concerning both of its inputs. The most common function, which we also use here, is the squared euclidean distance, but there have been several works on different distance functions as well.

ProtoNet implementation

Now that we know how a ProtoNet works in principle, let's look at how we can apply it to our specific problem of few-shot image classification, and implement it below. First, we need to define the encoder function f_θ. Since we work with CIFAR images, we can take a look back at Tutorial 5 where we compared common Computer Vision architectures, and choose one of the best-performing ones. Here, we go with a DenseNet since it is in general more parameter efficient than ResNet. Luckily, we do not need to implement DenseNet ourselves again and can rely on torchvision's model package instead. We use common hyperparameters of 64 initial feature channels, add 32 per block, and use a bottleneck size of 64 (i.e. 2 times the growth rate). We use 4 stages of 6 layers each, which results in overall about 1 million parameters. Note that the torchvision package assumes that the last layer is used for classification and hence calls its output size `num_classes`. However, we can instead just use it as the feature space of ProtoNet and choose an arbitrary dimensionality. We will use the same network for other algorithms in this notebook to ensure a fair comparison.

[15]:
```
def get_convnet(output_size):
    convnet = torchvision.models.DenseNet(growth_rate=32,
                                           block_config=(6, 6, 6, 6),
                                           bn_size=2,
                                           num_init_features=64,
                                           num_classes=output_size  # Output␣
↪dimensionality
                                          )
    return convnet
```

Next, we can look at implementing ProtoNet. We will define it as PyTorch Lightning module to use all functionalities of PyTorch Lightning. The first step during training is to encode all images in a batch with our network. Next, we calculate the class prototypes from the support set (function `calculate_prototypes`), and classify the query set examples according to the prototypes (function `classify_feats`). Keep in mind that we use the data sampling described before, such that the support and query set are stacked together in the batch. Thus, we use our previously defined function `split_batch` to split them apart. The full code can be found below.

[16]:
```
class ProtoNet(pl.LightningModule):
```

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```
    def __init__(self, proto_dim, lr):
        """
        Inputs
            proto_dim - Dimensionality of prototype feature space
            lr - Learning rate of Adam optimizer
        """
        super().__init__()
        self.save_hyperparameters()
        self.model = get_convnet(output_size=self.hparams.proto_dim)

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(), lr=self.hparams.lr)
        scheduler = optim.lr_scheduler.MultiStepLR(
            optimizer, milestones=[140, 180], gamma=0.1)
        return [optimizer], [scheduler]

    @staticmethod
    def calculate_prototypes(features, targets):
        # Given a stack of features vectors and labels, return class prototypes
        # features - shape [N, proto_dim], targets - shape [N]
        classes, _ = torch.unique(targets).sort()  # Determine which classes we have
        prototypes = []
        for c in classes:
            p = features[torch.where(targets == c)[0]].mean(dim=0)  # Average class␣
↪feature vectors
            prototypes.append(p)
        prototypes = torch.stack(prototypes, dim=0)
        # Return the 'classes' tensor to know which prototype belongs to which class
        return prototypes, classes

    def classify_feats(self, prototypes, classes, feats, targets):
        # Classify new examples with prototypes and return classification error
        dist = torch.pow(prototypes[None, :] - feats[:, None], 2).sum(dim=2)  # Squared␣
↪euclidean distance
        preds = F.log_softmax(-dist, dim=1)
        labels = (classes[None, :] == targets[:, None]).long().argmax(dim=-1)
        acc = (preds.argmax(dim=1) == labels).float().mean()
        return preds, labels, acc

    def calculate_loss(self, batch, mode):
        # Determine training loss for a given support and query set
        imgs, targets = batch
        features = self.model(imgs)  # Encode all images of support and query set
        support_feats, query_feats, support_targets, query_targets = split_
↪batch(features, targets)
        prototypes, classes = ProtoNet.calculate_prototypes(support_feats, support_
↪targets)
        preds, labels, acc = self.classify_feats(prototypes, classes, query_feats, query_
↪targets)
        loss = F.cross_entropy(preds, labels)

        self.log(f"{mode}_loss", loss)
```

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```
        self.log(f"{mode}_acc", acc)
        return loss

    def training_step(self, batch, batch_idx):
        return self.calculate_loss(batch, mode="train")

    def validation_step(self, batch, batch_idx):
        _ = self.calculate_loss(batch, mode="val")
```

For validation, we use the same principle as training and sample support and query sets from the hold-out 10 classes. However, this gives us noisy scores depending on which query sets are chosen to which support sets. This is why we will use a different strategy during testing. For validation, our training strategy is sufficient since it is much faster than testing, and gives a good estimate of the training generalization as long as we keep the support-query sets constant across validation iterations.

Training

After implementing the model, we can already start training it. We use our common PyTorch Lightning training function, and train the model for 200 epochs. The training function takes `model_class` as input argument, i.e. the PyTorch Lightning module class that should be trained, since we will reuse this function for other algorithms as well.

[17]:
```
def train_model(model_class, train_loader, val_loader, **kwargs):
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, model_class.__
↪name__),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=200,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc"),
                                    LearningRateMonitor("epoch")],
                         enable_progress_bar=False)
    trainer.logger._default_hp_metric = None

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(
        CHECKPOINT_PATH, model_class.__name__ + ".ckpt")
    if os.path.isfile(pretrained_filename):
        print(f"Found pretrained model at {pretrained_filename}, loading...")
        # Automatically loads the model with the saved hyperparameters
        model = model_class.load_from_checkpoint(pretrained_filename)
    else:
        pl.seed_everything(42)  # To be reproducable
        model = model_class(**kwargs)
        trainer.fit(model, train_loader, val_loader)
        model = model_class.load_from_checkpoint(
            trainer.checkpoint_callback.best_model_path)  # Load best checkpoint after␣
↪training

    return model
```

Below is the training call for our ProtoNet. We use a 64-dimensional feature space. Larger feature spaces showed to give noisier results since the squared euclidean distance becomes proportionally larger in expectation, and smaller

feature spaces might not allow for enough flexibility. We recommend to load the pre-trained model here at first, but feel free to play around with the hyperparameters yourself.

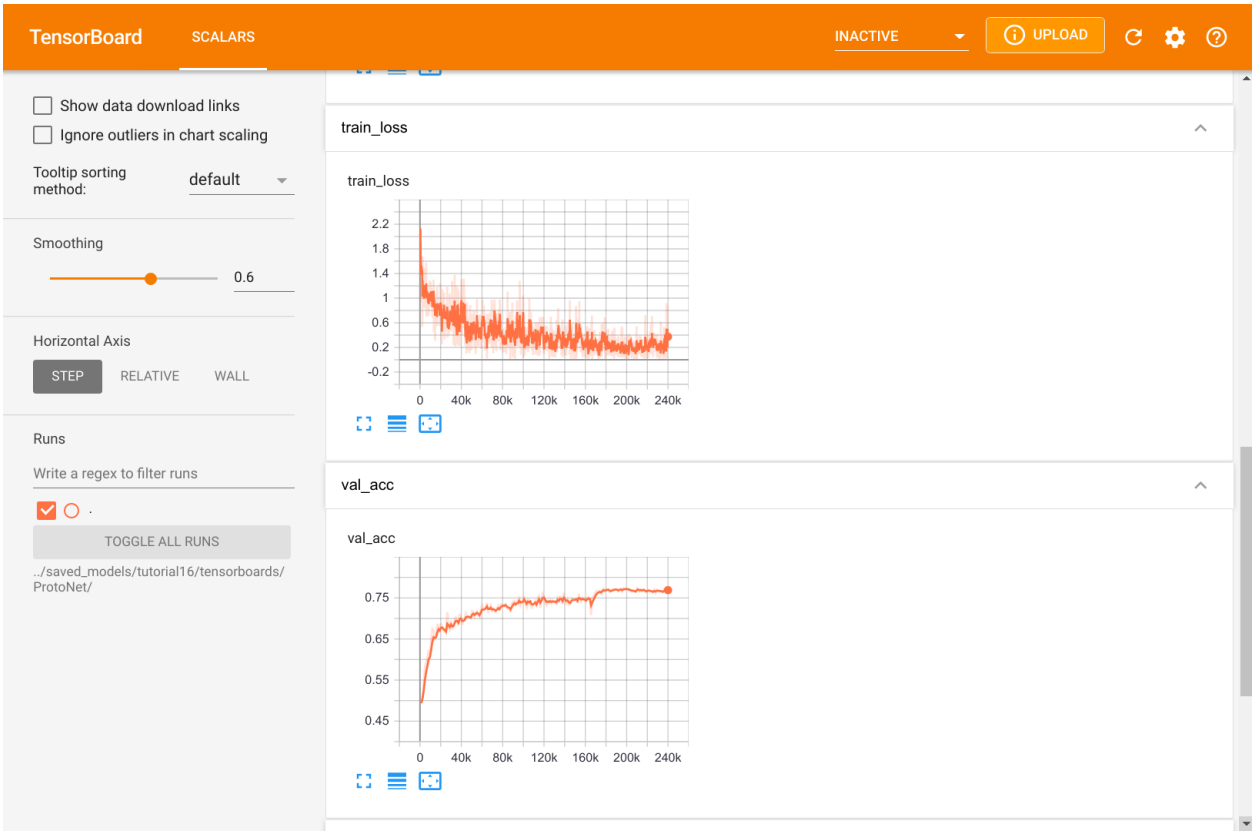
[18]:
```
protonet_model = train_model(ProtoNet,
                             proto_dim=64,
                             lr=2e-4,
                             train_loader=train_data_loader,
                             val_loader=val_data_loader)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
```

```
Found pretrained model at ../saved_models/tutorial16/ProtoNet.ckpt, loading...
```

We can also take a closer look at the TensorBoard below.

[19]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH if needed
%tensorboard --logdir ../saved_models/tutorial16/tensorboards/ProtoNet/
```



In contrast to standard supervised learning, we see that ProtoNet does not overfit as much as we would expect. The validation accuracy is of course lower than the average training, but the training loss does not stick close to zero. This is because no training batch is as the other, and we also mix new examples in the support set and query set. This gives us slightly different prototypes in every iteration and makes it harder for the network to fully overfit.

Testing

Our goal of meta-learning is to obtain a model that can quickly adapt to a new task, or in this case, new classes to distinguish between. To test this, we will use our trained ProtoNet and adapt it to the 10 test classes. Thereby, we pick k examples per class from which we determine the prototypes and test the classification accuracy on all other examples. This can be seen as using the k examples per class as a support set, and the rest of the dataset as a query set. We iterate through the dataset such that each example has been once included in a support set. The average performance across all support sets tells us how well we can expect ProtoNet to perform when seeing only k examples per class. During training, we used $k = 4$. In testing, we will experiment with $k = \{2, 4, 8, 16, 32\}$ to get a better sense of how k influences the results. We would expect that we achieve higher accuracies the more examples we have in the support set, but we don't know how it scales. Hence, let's first implement a function that executes the testing procedure for a given k:

[20]:
```
@torch.no_grad()
def test_proto_net(model, dataset, data_feats=None, k_shot=4):
    """
    Inputs
        model - Pretrained ProtoNet model
        dataset - The dataset on which the test should be performed.
                  Should be instance of ImageDataset
        data_feats - The encoded features of all images in the dataset.
                     If None, they will be newly calculated, and returned
                     for later usage.
        k_shot - Number of examples per class in the support set.
    """
    model = model.to(device)
    model.eval()
    num_classes = dataset.targets.unique().shape[0]
    exmps_per_class = dataset.targets.shape[0]//num_classes  # We assume uniform example␣
↪distribution here

    # The encoder network remains unchanged across k-shot settings. Hence, we only need
    # to extract the features for all images once.
    if data_feats is None:
        # Dataset preparation
        dataloader = data.DataLoader(dataset, batch_size=128, num_workers=4,␣
↪shuffle=False, drop_last=False)

        img_features = []
        img_targets = []
        for imgs, targets in tqdm(dataloader, "Extracting image features", leave=False):
            imgs = imgs.to(device)
            feats = model.model(imgs)
            img_features.append(feats.detach().cpu())
            img_targets.append(targets)
        img_features = torch.cat(img_features, dim=0)
        img_targets = torch.cat(img_targets, dim=0)
        # Sort by classes, so that we obtain tensors of shape [num_classes, exmps_per_
↪class, ...]
        # Makes it easier to process later
        img_targets, sort_idx = img_targets.sort()
        img_targets = img_targets.reshape(num_classes, exmps_per_class).transpose(0, 1)
        img_features = img_features[sort_idx].reshape(num_classes, exmps_per_class, -1).
↪transpose(0, 1)
```

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```
    else:
        img_features, img_targets = data_feats

    # We iterate through the full dataset in two manners. First, to select the k-shot␣
↪batch.
    # Second, the evaluate the model on all other examples
    accuracies = []
    for k_idx in tqdm(range(0, img_features.shape[0], k_shot), "Evaluating prototype␣
↪classification", leave=False):
        # Select support set and calculate prototypes
        k_img_feats, k_targets = img_features[k_idx:k_idx+k_shot].flatten(0,1), img_
↪targets[k_idx:k_idx+k_shot].flatten(0,1)
        prototypes, proto_classes = model.calculate_prototypes(k_img_feats, k_targets)
        # Evaluate accuracy on the rest of the dataset
        batch_acc = 0
        for e_idx in range(0, img_features.shape[0], k_shot):
            if k_idx == e_idx:  # Do not evaluate on the support set examples
                continue
            e_img_feats, e_targets = img_features[e_idx:e_idx+k_shot].flatten(0,1), img_
↪targets[e_idx:e_idx+k_shot].flatten(0,1)
            _, _, acc = model.classify_feats(prototypes, proto_classes, e_img_feats, e_
↪targets)
            batch_acc += acc.item()
        batch_acc /= img_features.shape[0]//k_shot-1
        accuracies.append(batch_acc)

    return (mean(accuracies), stdev(accuracies)), (img_features, img_targets)
```

Testing ProtoNet is relatively quick if we have processed all images once. Hence, we can do in this notebook:

[21]:
```
protonet_accuracies = dict()
data_feats = None
for k in [2, 4, 8, 16, 32]:
    protonet_accuracies[k], data_feats = test_proto_net(protonet_model, test_set, data_
↪feats=data_feats, k_shot=k)
    print(f"Accuracy for k={k}: {100.0*protonet_accuracies[k][0]:4.2f}% (+-{100*protonet_
↪accuracies[k][1]:4.2f}%)")
```

```
HBox(children=(HTML(value='Extracting image features'), FloatProgress(value=0.0, max=47.
↪0), HTML(value='')))
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/torch/nn/functional.py:
↪718: UserWarning: Named tensors and all their associated APIs are an experimental␣
↪feature and subject to change. Please do not use them for anything important until␣
↪they are released as stable. (Triggered internally at  /opt/conda/conda-bld/pytorch_
↪1623448265233/work/c10/core/TensorImpl.h:1156.)
  return torch.max_pool2d(input, kernel_size, stride, padding, dilation, ceil_mode)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=300.0), HTML(va...
```

```
Accuracy for k=2: 44.30% (+-3.63%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=150.0), HTML(va...
```

```
Accuracy for k=4: 52.07% (+-2.27%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=75.0), HTML(val...
```

```
Accuracy for k=8: 57.59% (+-1.30%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=38.0), HTML(val...
```

```
Accuracy for k=16: 62.56% (+-1.02%)
```

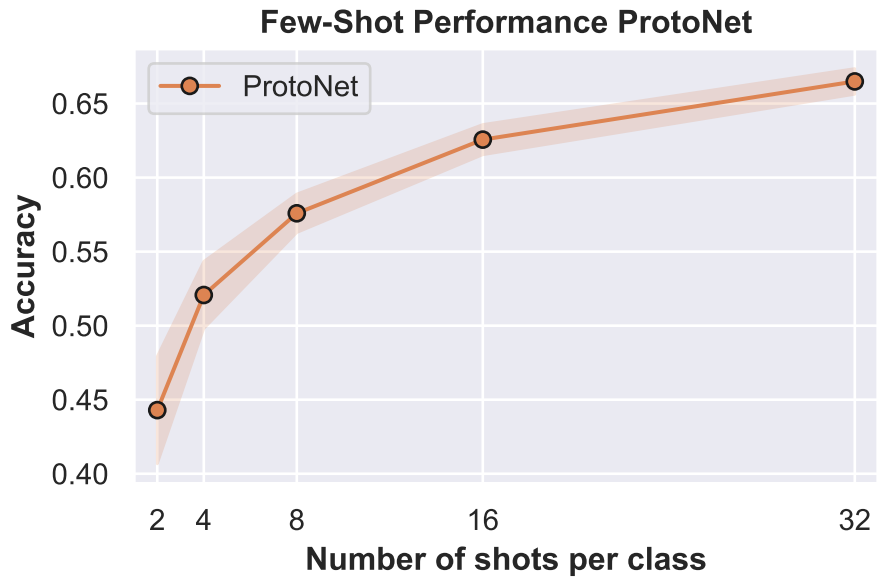
```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=19.0), HTML(val...
```

```
Accuracy for k=32: 66.49% (+-0.87%)
```

Before discussing the results above, let's first plot the accuracies over number of examples in the support set:

[22]:
```
def plot_few_shot(acc_dict, name, color=None, ax=None):
    sns.set()
    if ax is None:
        fig, ax = plt.subplots(1,1,figsize=(5,3))
    ks = sorted(list(acc_dict.keys()))
    mean_accs = [acc_dict[k][0] for k in ks]
    std_accs = [acc_dict[k][1] for k in ks]
    ax.plot(ks, mean_accs, marker='o', markeredgecolor='k', markersize=6, label=name,␣
↪color=color)
    ax.fill_between(ks, [m-s for m,s in zip(mean_accs, std_accs)], [m+s for m,s in␣
↪zip(mean_accs, std_accs)], alpha=0.2, color=color)
    ax.set_xticks(ks)
    ax.set_xlim([ks[0]-1, ks[-1]+1])
    ax.set_xlabel("Number of shots per class", weight='bold')
    ax.set_ylabel("Accuracy", weight='bold')
    if len(ax.get_title()) == 0:
        ax.set_title("Few-Shot Performance " + name, weight='bold')
    else:
        ax.set_title(ax.get_title() + " and " + name, weight='bold')
    ax.legend()
    return ax
```

[23]:
```
ax = plot_few_shot(protonet_accuracies, name="ProtoNet", color="C1")
plt.show()
plt.close()
```



As we initially expected, the performance of ProtoNet indeed increases the more samples we have. However, even with just two samples per class, we classify almost half of the images correctly, which is well above random accuracy (10%). The curve shows an exponentially dampend trend, meaning that adding 2 extra examples to $k = 2$ has a much higher impact than adding 2 extra samples if we already have $k = 16$. Nonetheless, we can say that ProtoNet adapts fairly well to new classes.

4.28.3 MAML and ProtoMAML

The second meta-learning algorithm we will look at is MAML, short for Model-Agnostic Meta-Learning. MAML is an optimization-based meta-learning algorithm, which means that it tries to adjust the standard optimization procedure to a few-shot setting. The idea of MAML is relatively simple: given a model, support, and query set during training, we optimize the model for m steps on the support set and evaluate the gradients of the query loss with respect to the original model's parameters. For the same model, we do it for a few different support-query sets and accumulate the gradients. This results in learning a model that provides a good initialization for being quickly adapted to the training tasks. If we denote the model parameters with θ, we can visualize the procedure as follows (Figure credit - Finn et al.).

The full algorithm of MAML is therefore as follows. At each training step, we sample a batch of tasks, i.e., a batch of support-query set pairs. For each task $\mathcal{T}_i$, we optimize a model f_θ on the support set via SGD, and denote this model as $f_{\theta_i'}$. We refer to this optimization as *inner loop*. Using this new model, we calculate the gradients of the original parameters, θ, with respect to the query loss on $f_{\theta_i'}$. These gradients are accumulated over all tasks and used to update θ. This is called *outer loop* since we iterate over tasks. The full MAML algorithm is summarized below (Figure credit - Finn et al.).

To obtain gradients for the initial parameters θ from the optimized model $f_{\theta_i'}$, we actually need second-order gradients, i.e. gradients of gradients, as the support set gradients depend on θ as well. This makes MAML computationally expensive, especially when using multiple inner loop steps. A simpler, yet almost equally well-performing alternative is First-Order MAML (FOMAML) which only uses first-order gradients. This means that the second-order gradients are ignored, and we can calculate the outer loop gradients (line 10 in algorithm 2) simply by calculating the gradients

with respect to θ_i' and use those as an update to θ. Hence, the new update rule becomes:

$$\theta \leftarrow \theta - \beta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \nabla_{\theta_i'} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'})$$

Note the change of θ to θ_i' for ∇.

ProtoMAML

A problem of MAML is how to design the output classification layer. In case all tasks have a different number of classes, we need to initialize the output layer with zeros or randomly in every iteration. Even if we always have the same number of classes, we just start from random predictions. This requires several inner loop steps to reach a reasonable classification result. To overcome this problem, Triantafillou et al. (2020) propose to combine the merits of Prototypical Networks and MAML. Specifically, we can use prototypes to initialize our output layer to have a strong initialization. Thereby, it can be shown that the softmax over euclidean distances can be reformulated as a linear layer with softmax. To see this, let's first write out the negative Euclidean distance between a feature vector $f_\theta(\mathbf{x}^*)$ of a new data point $\mathbf{x}^*$ to a prototype $\mathbf{v}_c$ of class c:

$$-||f_\theta(\mathbf{x}^*) - \mathbf{v}_c||^2 = -f_\theta(\mathbf{x}^*)^T f_\theta(\mathbf{x}^*) + 2\mathbf{v}_c^T f_\theta(\mathbf{x}^*) - \mathbf{v}_c^T \mathbf{v}_c$$

We perform the classification across all classes $c \in \mathcal{C}$ and take a softmax on the distance. Hence, any term that is the same for all classes can be removed without changing the output probabilities. In the equation above, this is true for $-f_\theta(\mathbf{x}^*)^T f_\theta(\mathbf{x}^*)$ since it is independent of any class prototype. Thus, we can write:

$$-||f_\theta(\mathbf{x}^*) - \mathbf{v}_c||^2 = 2\mathbf{v}_c^T f_\theta(\mathbf{x}^*) - ||\mathbf{v}_c||^2 + \text{constant}$$

Taking a second look at the equation above, it looks a lot like a linear layer. For this, we use $\mathbf{W}_{c,\cdot} = 2\mathbf{v}_c$ and $b_c = -||\mathbf{v}_c||^2$ which gives us the linear layer $\mathbf{W} f_\theta(\mathbf{x}^*) + \mathbf{b}$. Hence, if we initialize the output weight with twice the prototypes, and the biases by the negative squared L2 norm of the prototypes, we start with a Prototypical Network. MAML allows us to adapt this layer and the rest of the network further.

In the following, we will implement First-Order ProtoMAML for few-shot classification. The implementation of MAML would be the same except for the output layer initialization.

ProtoMAML implementation

For implementing ProtoMAML, we can follow Algorithm 2 with minor modifications. At each training step, we first sample a batch of tasks, and a support and query set for each task. In our case of few-shot classification, this means that we simply sample multiple support-query set pairs from our sampler. For each task, we finetune our current model on the support set. However, since we need to remember the original parameters for the other tasks, the outer loop gradient update, and future training steps, we need to create a copy of our model and finetune only the copy. We can copy a model by using standard Python functions like `deepcopy`. The inner loop is implemented in the function `adapt_few_shot` in the PyTorch Lightning module below.

After finetuning the model, we apply it to the query set and calculate the first-order gradients with respect to the original parameters θ. In contrast to simple MAML, we also have to consider the gradients with respect to the output layer initialization, i.e. the prototypes, since they directly rely on θ. To realize this efficiently, we take two steps. First, we calculate the prototypes by applying the original model, i.e. not the copied model, on the support elements. When initializing the output layer, we detach the prototypes to stop the gradients. This is because, in the inner loop itself, we do not want to consider gradients through the prototypes back to the original model. However, after the inner loop is finished, we re-attach the computation graph of the prototypes by writing `output_weight = (output_weight - init_weight).detach() + init_weight`. While this line does not change the value of the variable `output_weight`, it adds its dependency on the prototype initialization `init_weight`. Thus, if we call `.backward` on `output_weight`, we will automatically calculate the first-order gradients with respect to the prototype initialization in the original model.

After calculating all gradients and summing them together in the original model, we can take a standard optimizer step. PyTorch Lightning's method is however designed to return a loss-tensor on which we call `.backward` first. Since this is not possible here, we need to perform the optimization step ourselves. All details can be found in the code below.

For implementing (Proto-)MAML with second-order gradients, it is recommended to use libraries such as *:math:*nabla`higher <https://github.com/facebookresearch/higher>`__ from Facebook AI Research. For simplicity, we stick with first-order methods here.

[24]:
```
class ProtoMAML(pl.LightningModule):

    def __init__(self, proto_dim, lr, lr_inner, lr_output, num_inner_steps):
        """
        Inputs
            proto_dim - Dimensionality of prototype feature space
            lr - Learning rate of the outer loop Adam optimizer
            lr_inner - Learning rate of the inner loop SGD optimizer
            lr_output - Learning rate for the output layer in the inner loop
            num_inner_steps - Number of inner loop updates to perform
        """
        super().__init__()
        self.save_hyperparameters()
        self.model = get_convnet(output_size=self.hparams.proto_dim)

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(), lr=self.hparams.lr)
        scheduler = optim.lr_scheduler.MultiStepLR(optimizer, milestones=[140,180],␣
↪gamma=0.1)
        return [optimizer], [scheduler]

    def run_model(self, local_model, output_weight, output_bias, imgs, labels):
        # Execute a model with given output layer weights and inputs
        feats = local_model(imgs)
        preds = F.linear(feats, output_weight, output_bias)
        loss = F.cross_entropy(preds, labels)
        acc = (preds.argmax(dim=1) == labels).float()
        return loss, preds, acc

    def adapt_few_shot(self, support_imgs, support_targets):
        # Determine prototype initialization
        support_feats = self.model(support_imgs)
        prototypes, classes = ProtoNet.calculate_prototypes(support_feats, support_
↪targets)
        support_labels = (classes[None,:] == support_targets[:,None]).long().argmax(dim=-
↪1)
        # Create inner-loop model and optimizer
        local_model = deepcopy(self.model)
        local_model.train()
        local_optim = optim.SGD(local_model.parameters(), lr=self.hparams.lr_inner)
        local_optim.zero_grad()
        # Create output layer weights with prototype-based initialization
        init_weight = 2 * prototypes
        init_bias = -torch.norm(prototypes, dim=1)**2
        output_weight = init_weight.detach().requires_grad_()
        output_bias = init_bias.detach().requires_grad_()
```

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```
        # Optimize inner loop model on support set
        for _ in range(self.hparams.num_inner_steps):
            # Determine loss on the support set
            loss, _, _ = self.run_model(local_model, output_weight, output_bias, support_
↪imgs, support_labels)
            # Calculate gradients and perform inner loop update
            loss.backward()
            local_optim.step()
            # Update output layer via SGD
            # (https://discuss.pytorch.org/t/the-difference-between-torch-tensor-data-
↪and-torch-tensor/25995/4):
            with torch.no_grad():
                output_weight.copy_(output_weight - self.hparams.lr_output * output_
↪weight.grad)
                output_bias.copy_(output_bias - self.hparams.lr_output * output_bias.
↪grad)

            # Reset gradients
            local_optim.zero_grad()
            output_weight.grad.fill_(0)
            output_bias.grad.fill_(0)

        # Re-attach computation graph of prototypes
        output_weight = (output_weight - init_weight).detach() + init_weight
        output_bias = (output_bias - init_bias).detach() + init_bias

        return local_model, output_weight, output_bias, classes

    def outer_loop(self, batch, mode="train"):
        accuracies = []
        losses = []
        self.model.zero_grad()

        # Determine gradients for batch of tasks
        for task_batch in batch:
            imgs, targets = task_batch
            support_imgs, query_imgs, support_targets, query_targets = split_batch(imgs,␣
↪targets)
            # Perform inner loop adaptation
            local_model, output_weight, output_bias, classes = self.adapt_few_
↪shot(support_imgs, support_targets)
            # Determine loss of query set
            query_labels = (classes[None,:] == query_targets[:,None]).long().argmax(dim=-
↪1)
            loss, preds, acc = self.run_model(local_model, output_weight, output_bias,␣
↪query_imgs, query_labels)
            # Calculate gradients for query set loss
            if mode == "train":
                loss.backward()

                for p_global, p_local in zip(self.model.parameters(), local_model.
↪parameters()):
```

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```
                    p_global.grad += p_local.grad  # First-order approx. -> add␣
↪gradients of finetuned and base model

                accuracies.append(acc.mean().detach())
                losses.append(loss.detach())

            # Perform update of base model
            if mode == "train":
                opt = self.optimizers()
                opt.step()
                opt.zero_grad()

            self.log(f"{mode}_loss", sum(losses) / len(losses))
            self.log(f"{mode}_acc", sum(accuracies) / len(accuracies))

        def training_step(self, batch, batch_idx):
            self.outer_loop(batch, mode="train")
            return None  # Returning None means we skip the default training optimizer steps␣
↪by PyTorch Lightning

        def validation_step(self, batch, batch_idx):
            # Validation requires to finetune a model, hence we need to enable gradients
            torch.set_grad_enabled(True)
            self.outer_loop(batch, mode="val")
            torch.set_grad_enabled(False)
```

Training

To train ProtoMAML, we need to change our sampling slightly. Instead of a single support-query set batch, we need to sample multiple. To implement this, we yet use another Sampler that combines multiple batches from a `FewShotBatchSampler` and returns it afterward. Additionally, we define a `collate_fn` for our data loader which takes the stack of support-query set images and returns the tasks as a list. This makes it easier to process in our PyTorch Lightning module before. The implementation of the sampler can be found below.

[25]:
```
class TaskBatchSampler(object):

    def __init__(self, dataset_targets, batch_size, N_way, K_shot, include_query=False,␣
↪shuffle=True):
        """
        Inputs:
            dataset_targets - PyTorch tensor of the labels of the data elements.
            batch_size - Number of tasks to aggregate in a batch
            N_way - Number of classes to sample per batch.
            K_shot - Number of examples to sample per class in the batch.
            include_query - If True, returns batch of size N_way*K_shot*2, which
                            can be split into support and query set. Simplifies
                            the implementation of sampling the same classes but
                            distinct examples for support and query set.
            shuffle - If True, examples and classes are newly shuffled in each
                      iteration (for training)
        """
```

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```
        super().__init__()
        self.batch_sampler = FewShotBatchSampler(dataset_targets, N_way, K_shot, include_
↪query, shuffle)
        self.task_batch_size = batch_size
        self.local_batch_size = self.batch_sampler.batch_size

    def __iter__(self):
        # Aggregate multiple batches before returning the indices
        batch_list = []
        for batch_idx, batch in enumerate(self.batch_sampler):
            batch_list.extend(batch)
            if (batch_idx+1) % self.task_batch_size == 0:
                yield batch_list
                batch_list = []

    def __len__(self):
        return len(self.batch_sampler)//self.task_batch_size

    def get_collate_fn(self):
        # Returns a collate function that converts one big tensor into a list of task-
↪specific tensors
        def collate_fn(item_list):
            imgs = torch.stack([img for img, target in item_list], dim=0)
            targets = torch.stack([target for img, target in item_list], dim=0)
            imgs = imgs.chunk(self.task_batch_size, dim=0)
            targets = targets.chunk(self.task_batch_size, dim=0)
            return list(zip(imgs, targets))
        return collate_fn
```

The creation of the data loaders is with this sampler straight-forward. Note that since many images need to loaded for a training batch, it is recommended to use less workers than usual.

[26]:
```
# Training constant (same as for ProtoNet)
N_WAY = 5
K_SHOT = 4

# Training set
train_protomaml_sampler = TaskBatchSampler(train_set.targets,
                                           include_query=True,
                                           N_way=N_WAY,
                                           K_shot=K_SHOT,
                                           batch_size=16)
train_protomaml_loader = data.DataLoader(train_set,
                                         batch_sampler=train_protomaml_sampler,
                                         collate_fn=train_protomaml_sampler.get_collate_
↪fn(),
                                         num_workers=2)

# Validation set
val_protomaml_sampler = TaskBatchSampler(val_set.targets,
                                         include_query=True,
                                         N_way=N_WAY,
```

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```
                                        K_shot=K_SHOT,
                                        batch_size=1,  # We do not update the␣
↪parameters, hence the batch size is irrelevant here
                                        shuffle=False)
val_protomaml_loader = data.DataLoader(val_set,
                                       batch_sampler=val_protomaml_sampler,
                                       collate_fn=val_protomaml_sampler.get_collate_fn(),
                                       num_workers=2)
```

Now, we are ready to train our ProtoMAML. We use the same feature space size as for ProtoNet but can use a higher learning rate since the outer loop gradients are accumulated over 16 batches. The inner loop learning rate is set to 0.1, which is much higher than the outer loop learning rate because we use SGD in the inner loop instead of Adam. Commonly, the learning rate for the output layer is higher than the base model if the base model is very deep or pre-trained. However, for our setup, we observed no noticeable impact of using a different learning rate than the base model. The number of inner loop updates is another crucial hyperparameter and depends on the similarity of our training tasks. Since all tasks are on images from the same dataset, we notice that a single inner loop update achieves similar performance as 3 or 5 while training considerably faster. However, especially in RL and NLP, a larger number of inner loop steps are often needed.

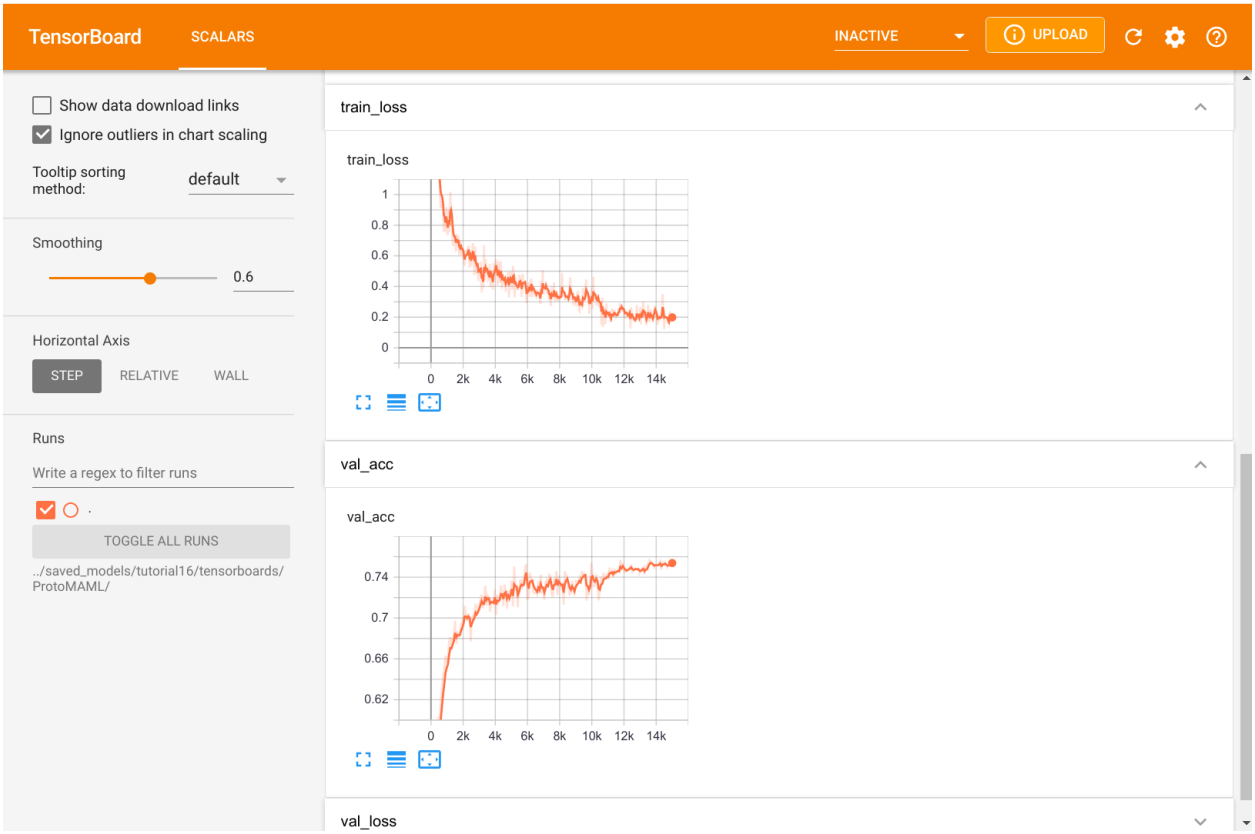
[27]:
```
protomaml_model = train_model(ProtoMAML,
                              proto_dim=64,
                              lr=1e-3,
                              lr_inner=0.1,
                              lr_output=0.1,
                              num_inner_steps=1,  # Often values between 1 and 10
                              train_loader=train_protomaml_loader,
                              val_loader=val_protomaml_loader)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
```

```
Found pretrained model at ../saved_models/tutorial16/ProtoMAML.ckpt, loading...
```

Let's have a look at the training TensorBoard.

[28]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH if needed
%tensorboard --logdir ../saved_models/tutorial16/tensorboards/ProtoMAML/
```



One obvious difference to ProtoNet is that the loss curves look much less noisy. This is because we average the outer loop gradients over multiple tasks, and thus have a smoother training curve. Additionally, we only have 15k training iterations after 200 epochs. This is again because of the task batches, which cause 16 times fewer iterations. However, each iteration has seen 16 times more data in this experiment. Thus, we still have a fair comparison between ProtoMAML and ProtoNet. At first sight on the validation accuracy, one would assume that ProtoNet performs superior to ProtoMAML, but we have to verify that with proper testing below.

Testing

We test ProtoMAML in the same manner as ProtoNet, namely by picking random examples in the test set as support sets and use the rest of the dataset as the query set. Instead of just calculating the prototypes for all examples, we need to finetune a separate model for each support set. This is why this process is more expensive than ProtoNet, and in our case, testing $k = \{2, 4, 8, 16, 32\}$ can take almost an hour. Hence, we provide evaluation files besides the pretrained models.

[29]:
```
def test_protomaml(model, dataset, k_shot=4):
    pl.seed_everything(42)
    model = model.to(device)
    num_classes = dataset.targets.unique().shape[0]
    exmps_per_class = dataset.targets.shape[0]//num_classes

    # Data loader for full test set as query set
    full_dataloader = data.DataLoader(dataset,
                                      batch_size=128,
                                      num_workers=4,
                                      shuffle=False,
```

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```
                                        drop_last=False)
    # Data loader for sampling support sets
    sampler = FewShotBatchSampler(dataset.targets,
                                  include_query=False,
                                  N_way=num_classes,
                                  K_shot=k_shot,
                                  shuffle=False,
                                  shuffle_once=False)
    sample_dataloader = data.DataLoader(dataset,
                                        batch_sampler=sampler,
                                        num_workers=2)

    # We iterate through the full dataset in two manners. First, to select the k-shot␣
↪batch.
    # Second, the evaluate the model on all other examples
    accuracies = []
    for (support_imgs, support_targets), support_indices in tqdm(zip(sample_dataloader,␣
↪sampler), "Performing few-shot finetuning"):
        support_imgs = support_imgs.to(device)
        support_targets = support_targets.to(device)
        # Finetune new model on support set
        local_model, output_weight, output_bias, classes = model.adapt_few_shot(support_
↪imgs, support_targets)
        with torch.no_grad():  # No gradients for query set needed
            local_model.eval()
            batch_acc = torch.zeros((0,), dtype=torch.float32, device=device)
            # Evaluate all examples in test dataset
            for query_imgs, query_targets in full_dataloader:
                query_imgs = query_imgs.to(device)
                query_targets = query_targets.to(device)
                query_labels = (classes[None,:] == query_targets[:,None]).long().
↪argmax(dim=-1)
                _, _, acc = model.run_model(local_model, output_weight, output_bias,␣
↪query_imgs, query_labels)
                batch_acc = torch.cat([batch_acc, acc.detach()], dim=0)
            # Exclude support set elements
            for s_idx in support_indices:
                batch_acc[s_idx] = 0
            batch_acc = batch_acc.sum().item() / (batch_acc.shape[0] - len(support_
↪indices))
            accuracies.append(batch_acc)
    return mean(accuracies), stdev(accuracies)
```

In contrast to training, it is recommended to use many more inner loop updates during testing. During training, we are not interested in getting the best model from the inner loop, but the model which can provide the best gradients. Hence, one update might be already sufficient in training, but for testing, it was often observed that a larger number of updates can give a considerable performance boost. Thus, we change the inner loop updates to 200 before testing.

[30]:
```
protomaml_model.hparams.num_inner_steps = 200
```

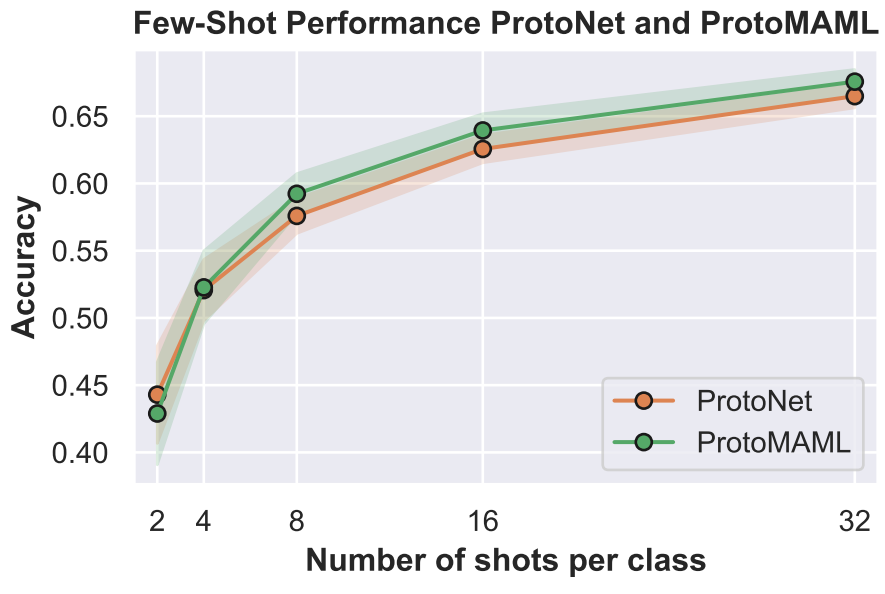
Now, we can test our model. For the pre-trained models, we provide a json file with the results to reduce evaluation time.

[31]:
```
protomaml_result_file = os.path.join(CHECKPOINT_PATH, "protomaml_fewshot.json")

if os.path.isfile(protomaml_result_file):
    # Load pre-computed results
    with open(protomaml_result_file, 'r') as f:
        protomaml_accuracies = json.load(f)
    protomaml_accuracies = {int(k): v for k, v in protomaml_accuracies.items()}
else:
    # Perform same experiments as for ProtoNet
    protomaml_accuracies = dict()
    for k in [2, 4, 8, 16, 32]:
        protomaml_accuracies[k] = test_protomaml(protomaml_model, test_set, k_shot=k)
    # Export results
    with open(protomaml_result_file, 'w') as f:
        json.dump(protomaml_accuracies, f, indent=4)

for k in protomaml_accuracies:
    print(f"Accuracy for k={k}: {100.0*protomaml_accuracies[k][0]:4.2f}% (+-{100.
↪0*protomaml_accuracies[k][1]:4.2f}%)")
```

```
Accuracy for k=2: 42.89% (+-3.82%)
Accuracy for k=4: 52.27% (+-2.72%)
Accuracy for k=8: 59.23% (+-1.50%)
Accuracy for k=16: 63.94% (+-1.24%)
Accuracy for k=32: 67.57% (+-0.90%)
```

Again, let's plot the results in our plot from before.

[32]:
```
ax = plot_few_shot(protonet_accuracies, name="ProtoNet", color="C1")
plot_few_shot(protomaml_accuracies, name="ProtoMAML", color="C2", ax=ax)
plt.show()
plt.close()
```



We can observe that ProtoMAML is indeed able to outperform ProtoNet for $k > 4$. This is because, with more samples, it becomes more relevant to also adapt the base model's parameters. Meanwhile, for $k = 2$, ProtoMAML

achieves lower performance than ProtoNet. This is likely also related to choosing 200 inner loop updates since with more updates, there exists the risk of overfitting. Nonetheless, the high standard deviation for $k = 2$ makes it hard to take any statistically valid conclusion.

Overall, we can conclude that ProtoMAML slightly outperforms ProtoNet for larger shot counts. However, one disadvantage of ProtoMAML is its much longer training and testing time. ProtoNet provides a simple, efficient, yet strong baseline for ProtoMAML, and might be the better solution in situations where limited resources are available.

4.28.4 Domain adaptation

So far, we have evaluated our meta-learning algorithms on the same dataset on which we have trained them. However, meta-learning algorithms are especially interesting when we want to move from one to another dataset. So, what happens if we apply them on a quite different dataset than CIFAR? This is what we try out below, and evaluate ProtoNet and ProtoMAML on the SVHN dataset.

SVHN dataset

The Street View House Numbers (SVHN) dataset is a real-world image dataset for house number detection. It is similar to MNIST by having the classes 0 to 9, but is more difficult due to its real-world setting and possible distracting numbers left and right. Let's first load the dataset, and visualize some images to get an impression of the dataset.

[33]:
```
SVHN_test_dataset = SVHN(root=DATASET_PATH, split='test', download=True,␣
↪transform=transforms.ToTensor())
```

```
Using downloaded and verified file: ../data/test_32x32.mat
```

[34]:
```
# Visualize some examples
NUM_IMAGES = 12
SVHN_images = torch.stack([SVHN_test_dataset[np.random.randint(len(SVHN_test_
↪dataset))][0] for idx in range(NUM_IMAGES)], dim=0)
img_grid = torchvision.utils.make_grid(SVHN_images, nrow=6, normalize=True, pad_value=0.
↪9)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Image examples of the SVHN dataset")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

Each image is labeled with one class between 0 and 9 representing the main digit in the image. Can our ProtoNet and ProtoMAML learn to classify the digits from only a few examples? This is what we will test out below. The images have the same size as CIFAR, so that we can use the images without changes. We first prepare the dataset, for which we take the first 500 images per class. For this dataset, we use our test functions as before to get an estimated performance for different number of shots.

[35]:
```
imgs = np.transpose(SVHN_test_dataset.data, (0,2,3,1))
targets = SVHN_test_dataset.labels
min_label_count = min(500, np.bincount(SVHN_test_dataset.labels).min())  # Limit number␣
↪of examples to 500 to reduce test time

idxs = np.concatenate([np.where(targets==c)[0][:min_label_count] for c in␣
↪range(1+targets.max())], axis=0)
imgs = imgs[idxs]
targets = torch.from_numpy(targets[idxs]).long()

svhn_fewshot_dataset = ImageDataset(imgs, targets, img_transform=test_transform)
svhn_fewshot_dataset.imgs.shape
```

[35]:
```
(5000, 32, 32, 3)
```

Experiments

First, we can apply ProtoNet to the SVHN dataset:

[36]:
```
protonet_svhn_accuracies = dict()
data_feats = None
for k in [2, 4, 8, 16, 32]:
    protonet_svhn_accuracies[k], data_feats = test_proto_net(protonet_model, svhn_
↪fewshot_dataset, data_feats=data_feats, k_shot=k)
    print(f"Accuracy for k={k}: {100.0*protonet_svhn_accuracies[k][0]:4.2f}% (+-
↪{100*protonet_svhn_accuracies[k][1]:4.2f}%)")
```

```
HBox(children=(HTML(value='Extracting image features'), FloatProgress(value=0.0, max=40.
↪0), HTML(value='')))
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=250.0), HTML(va...
```

```
Accuracy for k=2: 18.82% (+-2.28%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=125.0), HTML(va...
```

```
Accuracy for k=4: 21.94% (+-2.09%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=63.0), HTML(val...
```

```
Accuracy for k=8: 25.59% (+-1.76%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=32.0), HTML(val...
```

```
Accuracy for k=16: 29.06% (+-1.84%)
```

```
HBox(children=(HTML(value='Evaluating prototype classification'), FloatProgress(value=0.
↪0, max=16.0), HTML(val...
```

```
Accuracy for k=32: 32.93% (+-1.33%)
```

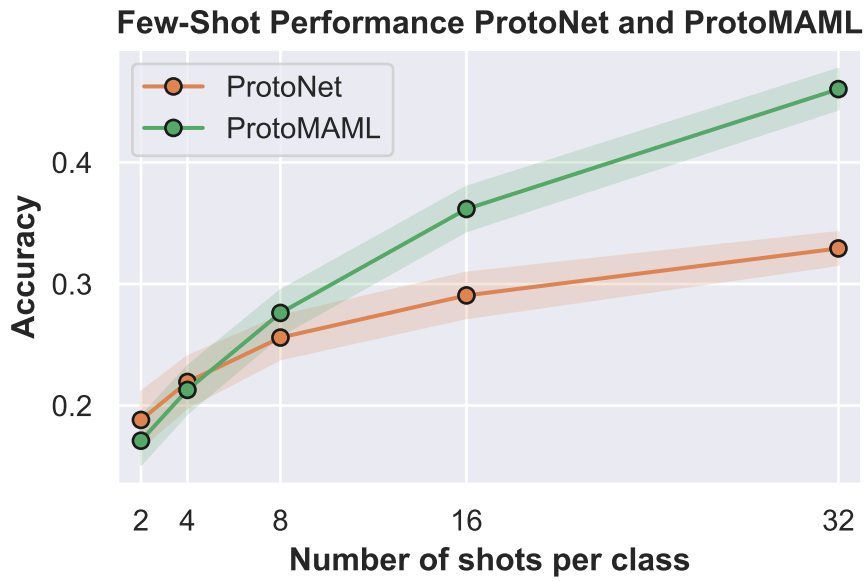
It becomes clear that the results are much lower than the ones on CIFAR, and just slightly above random for $k = 2$. How about ProtoMAML? We provide again evaluation files since the evaluation can take several minutes to complete.

[37]:
```
protomaml_result_file = os.path.join(CHECKPOINT_PATH, "protomaml_svhn_fewshot.json")

if os.path.isfile(protomaml_result_file):
    # Load pre-computed results
    with open(protomaml_result_file, 'r') as f:
        protomaml_svhn_accuracies = json.load(f)
    protomaml_svhn_accuracies = {int(k): v for k, v in protomaml_svhn_accuracies.items()}
else:
    # Perform same experiments as for ProtoNet
    protomaml_svhn_accuracies = dict()
    for k in [2, 4, 8, 16, 32]:
        protomaml_svhn_accuracies[k] = test_protomaml(protomaml_model, svhn_fewshot_
↪dataset, k_shot=k)
    # Export results
    with open(protomaml_result_file, 'w') as f:
        json.dump(protomaml_svhn_accuracies, f, indent=4)

for k in protomaml_svhn_accuracies:
    print(f"Accuracy for k={k}: {100.0*protomaml_svhn_accuracies[k][0]:4.2f}% (+-{100.
↪0*protomaml_svhn_accuracies[k][1]:4.2f}%)")
```

```
Accuracy for k=2: 17.11% (+-1.95%)
Accuracy for k=4: 21.29% (+-1.92%)
Accuracy for k=8: 27.62% (+-1.84%)
Accuracy for k=16: 36.17% (+-1.80%)
Accuracy for k=32: 46.03% (+-1.65%)
```

While ProtoMAML shows similar performance than ProtoNet for $k \leq 4$, it considerably outperforms ProtoNet for more than 8 shots. This is because we can adapt the base model, which is crucial when the data does not fit the original training data. For $k = 32$, ProtoMAML achieves 13% higher classification accuracy than ProtoNet which already starts to flatten out. We can see the trend more clearly in our plot below.

[38]:
```
ax = plot_few_shot(protonet_svhn_accuracies, name="ProtoNet", color="C1")
plot_few_shot(protomaml_svhn_accuracies, name="ProtoMAML", color="C2", ax=ax)
plt.show()
plt.close()
```



4.28.5 Conclusion

In this notebook, we have discussed meta-learning algorithms that learn to adapt to new classes and/or tasks with just a few samples. We have discussed three popular algorithms, namely ProtoNet, MAML, and ProtoMAML. On the few-shot image classification task of CIFAR100, ProtoNet and ProtoMAML showed to perform similarly well, with slight benefits of ProtoMAML for larger shot sizes. However, for out-of-distribution data (SVHN), the ability to optimize the base model showed to be crucial and gave ProtoMAML considerable performance gains over ProtoNet. Nonetheless, ProtoNet offers other advantages compared to ProtoMAML, namely a very cheap training and test cost as well as a simpler implementation. Hence, it is recommended to consider whether the additional complexity of ProtoMAML is worth the extra training computation cost, or whether ProtoNet is already sufficient for the task at hand.

References

[1] Snell, Jake, Kevin Swersky, and Richard S. Zemel. "Prototypical networks for few-shot learning." NeurIPS 2017. (link)

[2] Chelsea Finn, Pieter Abbeel, Sergey Levine. "Model-Agnostic Meta-Learning for Fast Adaptation of Deep Networks." ICML 2017. (link)

[3] Triantafillou, Eleni, Tyler Zhu, Vincent Dumoulin, Pascal Lamblin, Utku Evci, Kelvin Xu, Ross Goroshin et al. "Meta-dataset: A dataset of datasets for learning to learn from few examples." ICLR 2020. (link)

If you found this tutorial helpful, consider -ing our repository.

For any questions, typos, or bugs that you found, please raise an issue on GitHub.

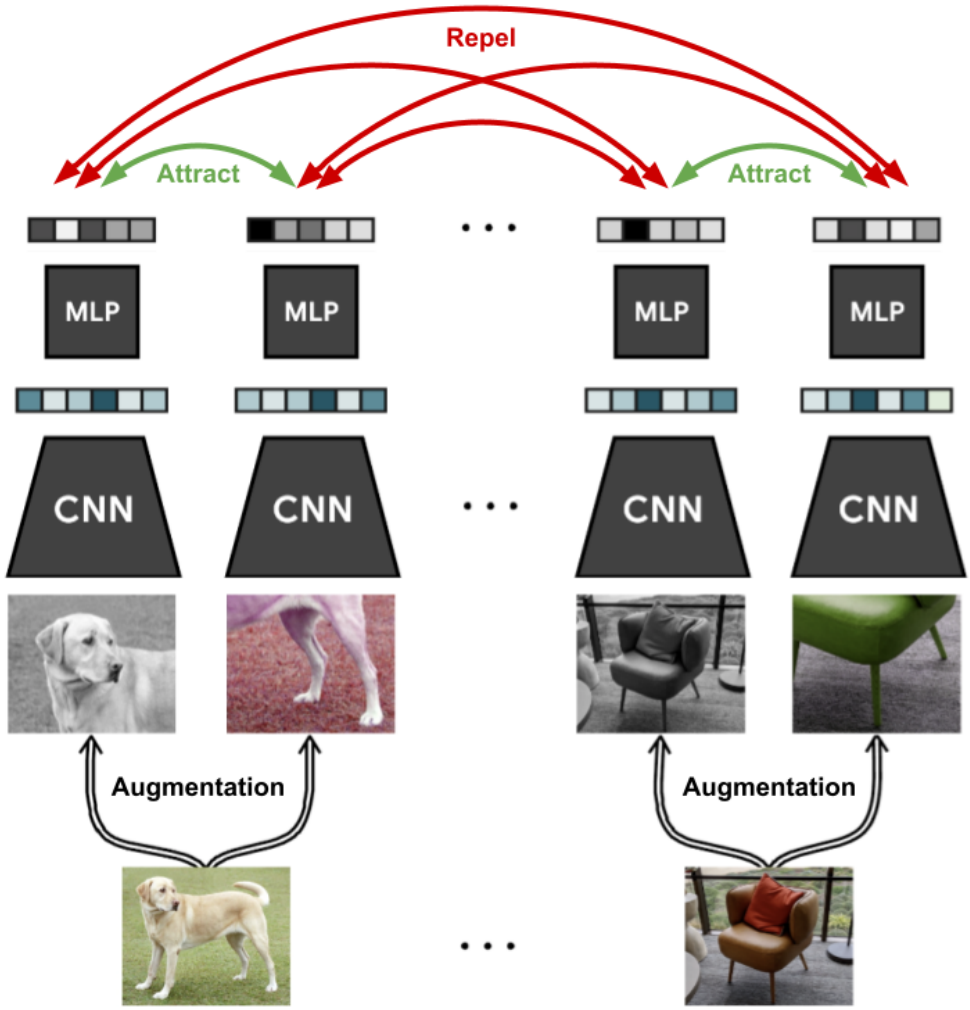
4.29 Tutorial 17: Self-Supervised Contrastive Learning with SimCLR

Filled notebook:
Pre-trained models:
Recordings:
JAX+Flax version:
Author: Phillip Lippe

Note: Interested in JAX? Check out our JAX+Flax version of this tutorial!

In this tutorial, we will take a closer look at self-supervised contrastive learning. Self-supervised learning, or also sometimes called unsupervised learning, describes the scenario where we have given input data, but no accompanying labels to train in a classical supervised way. However, this data still contains a lot of information from which we can learn: how are the images different from each other? What patterns are descriptive for certain images? Can we cluster the images? And so on. Methods for self-supervised learning try to learn as much as possible from the data alone, so it can quickly be finetuned for a specific classification task. The benefit of self-supervised learning is that a large dataset can often easily be obtained. For instance, if we want to train a vision model on semantic segmentation for autonomous driving, we can collect large amounts of data by simply installing a camera in a car, and driving through a city for an hour. In contrast, if we would want to do supervised learning, we would have to manually label all those images before training a model. This is extremely expensive, and would likely take a couple of months to manually label the same amount of data. Further, self-supervised learning can provide an alternative to transfer learning from models pretrained on ImageNet since we could pretrain a model on a specific dataset/situation, e.g. traffic scenarios for autonomous driving.

Within the last two years, a lot of new approaches have been proposed for self-supervised learning, in particular for images, that have resulted in great improvements over supervised models when few labels are available. The subfield that we will focus on in this tutorial is contrastive learning. Contrastive learning is motivated by the question mentioned above: how are images different from each other? Specifically, contrastive learning methods train a model to cluster an image and its slightly augmented version in latent space, while the distance to other images should be maximized. A very recent and simple method for this is SimCLR, which is visualized below (figure credit - Ting Chen et al.).



The general setup is that we are given a dataset of images without any labels, and want to train a model on this data such that it can quickly adapt to any image recognition task afterward. During each training iteration, we sample a batch of images as usual. For each image, we create two versions by applying data augmentation techniques like cropping, Gaussian noise, blurring, etc. An example of such is shown on the left with the image of the dog. We will go into the details and effects of the chosen augmentation techniques later. On those images, we apply a CNN like ResNet and obtain as output a 1D feature vector on which we apply a small MLP. The output features of the two augmented images are then trained to be close to each other, while all other images in that batch should be as different as possible. This way, the model has to learn to recognize the content of the image that remains unchanged under the data augmentations, such as objects which we usually care about in supervised tasks.

We will now implement this framework ourselves and discuss further details along the way. Let's first start with importing our standard libraries below:

[1]:
```
## Standard libraries
import os
from copy import deepcopy

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
```

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```
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.set()

## tqdm for loading bars
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.utils.data as data
import torch.optim as optim

## Torchvision
import torchvision
from torchvision.datasets import STL10
from torchvision import transforms

# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint

# Import tensorboard
%load_ext tensorboard

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../saved_models/tutorial17"
# In this notebook, we use data loaders with heavier computational processing. It is␣
↪recommended to use as many
# workers as possible in a data loader, which corresponds to the number of CPU cores
NUM_WORKERS = os.cpu_count()

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)
```

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```
print("Number of workers:", NUM_WORKERS)
```

```
Global seed set to 42
```

```
Device: cuda:0
Number of workers: 16
```

As in many tutorials before, we provide pre-trained models. Note that those models are slightly larger as normal (~100MB overall) since we use the default ResNet-18 architecture. If you are running this notebook locally, make sure to have sufficient disk space available.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/tutorial17/"
# Files to download
pretrained_files = ["SimCLR.ckpt", "ResNet.ckpt",
                    "tensorboards/SimCLR/events.out.tfevents.SimCLR",
                    "tensorboards/classification/ResNet/events.out.tfevents.ResNet"]
pretrained_files += [f"LogisticRegression_{size}.ckpt" for size in [10, 20, 50, 100, 200,
↪ 500]]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.29.1 SimCLR

We will start our exploration of contrastive learning by discussing the effect of different data augmentation techniques, and how we can implement an efficient data loader for such. Next, we implement SimCLR with PyTorch Lightning, and finally train it on a large, unlabeled dataset.

Data Augmentation for Contrastive Learning

To allow efficient training, we need to prepare the data loading such that we sample two different, random augmentations for each image in the batch. The easiest way to do this is by creating a transformation that, when being called, applies a set of data augmentations to an image twice. This is implemented in the class `ContrastiveTransformations` below:

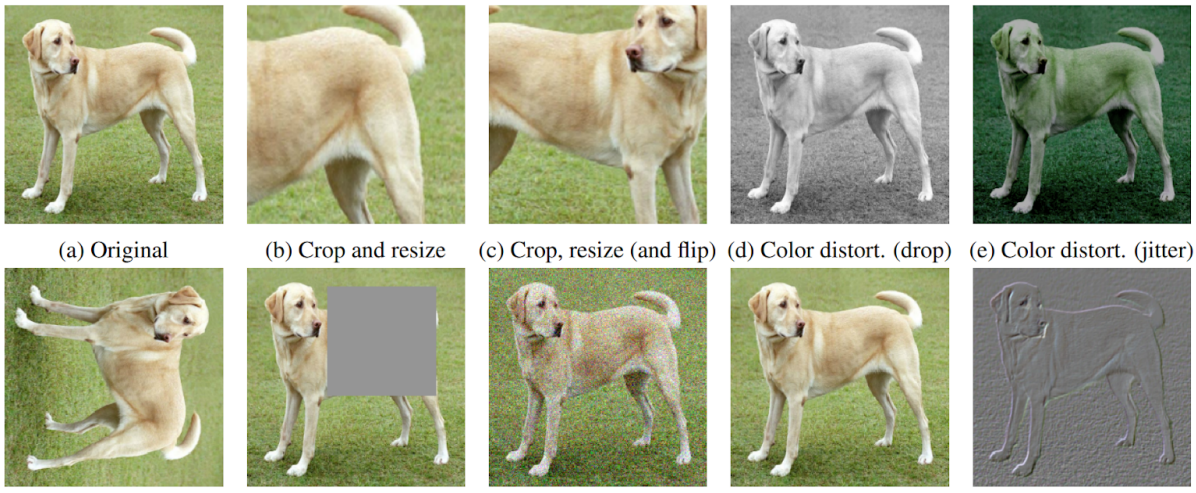
[3]:
```
class ContrastiveTransformations(object):

    def __init__(self, base_transforms, n_views=2):
        self.base_transforms = base_transforms
        self.n_views = n_views

    def __call__(self, x):
        return [self.base_transforms(x) for i in range(self.n_views)]
```

The contrastive learning framework can easily be extended to have more *positive* examples by sampling more than two augmentations of the same image. However, the most efficient training is usually obtained by using only two.

Next, we can look at the specific augmentations we want to apply. The choice of the data augmentation to use is the most crucial hyperparameter in SimCLR since it directly affects how the latent space is structured, and what patterns might be learned from the data. Let's first take a look at some of the most popular data augmentations (figure credit - Ting Chen and Geoffrey Hinton):



(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

(f) Rotate $\{90°, 180°, 270°\}$ (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

All of them can be used, but it turns out that two augmentations stand out in their importance: crop-and-resize, and color distortion. Interestingly, however, they only lead to strong performance if they have been used together as discussed by Ting Chen et al. in their SimCLR paper. When performing randomly cropping and resizing, we can distinguish between two situations: (a) cropped image A provides a local view of cropped image B, or (b) cropped images C and D show neighboring views of the same image (figure credit - Ting Chen and Geoffrey Hinton).

While situation (a) requires the model to learn some sort of scale invariance to make crops A and B similar in latent space, situation (b) is more challenging since the model needs to recognize an object beyond its limited view. However, without color distortion, there is a loophole that the model can exploit, namely that different crops of the same image usually look very similar in color space. Consider the picture of the dog above. Simply from the color of the fur and the green color tone of the background, you can reason that two patches belong to the same image without actually recognizing the dog in the picture. In this case, the model might end up focusing only on the color histograms of the images, and ignore other more generalizable features. If, however, we distort the colors in the two patches randomly

and independently of each other, the model cannot rely on this simple feature anymore. Hence, by combining random cropping and color distortions, the model can only match two patches by learning generalizable representations.

Overall, for our experiments, we apply a set of 5 transformations following the original SimCLR setup: random horizontal flip, crop-and-resize, color distortion, random grayscale, and gaussian blur. In comparison to the original implementation, we reduce the effect of the color jitter slightly (0.5 instead of 0.8 for brightness, contrast, and saturation, and 0.1 instead of 0.2 for hue). In our experiments, this setting obtained better performance and was faster and more stable to train. If, for instance, the brightness scale highly varies in a dataset, the original settings can be more beneficial since the model can't rely on this information anymore to distinguish between images.

[4]:
```
contrast_transforms = transforms.Compose([transforms.RandomHorizontalFlip(),
                                          transforms.RandomResizedCrop(size=96),
                                          transforms.RandomApply([
                                              transforms.ColorJitter(brightness=0.5,
                                                                     contrast=0.5,
                                                                     saturation=0.5,
                                                                     hue=0.1)
                                          ], p=0.8),
                                          transforms.RandomGrayscale(p=0.2),
                                          transforms.GaussianBlur(kernel_size=9),
                                          transforms.ToTensor(),
                                          transforms.Normalize((0.5,), (0.5,))
                                         ])
```

After discussing the data augmentation techniques, we can now focus on the dataset. In this tutorial, we will use the STL10 dataset, which, similarly to CIFAR10, contains images of 10 classes: airplane, bird, car, cat, deer, dog, horse, monkey, ship, truck. However, the images have a higher resolution, namely 96×96 pixels, and we are only provided with 500 labeled images per class. Additionally, we have a much larger set of $100,000$ unlabeled images which are similar to the training images but are sampled from a wider range of animals and vehicles. This makes the dataset ideal to showcase the benefits that self-supervised learning offers.

Luckily, the STL10 dataset is provided through torchvision. Keep in mind, however, that since this dataset is relatively large and has a considerably higher resolution than CIFAR10, it requires more disk space (~3GB) and takes a bit of time to download. For our initial discussion of self-supervised learning and SimCLR, we will create two data loaders with our contrastive transformations above: the `unlabeled_data` will be used to train our model via contrastive learning, and `train_data_contrast` will be used as a validation set in contrastive learning.

[5]:
```
unlabeled_data = STL10(root=DATASET_PATH, split='unlabeled', download=True,
                       transform=ContrastiveTransformations(contrast_transforms, n_
↪views=2))
train_data_contrast = STL10(root=DATASET_PATH, split='train', download=True,
                            transform=ContrastiveTransformations(contrast_transforms, n_
↪views=2))
```

```
Files already downloaded and verified
Files already downloaded and verified
```

Finally, before starting with our implementation of SimCLR, let's look at some example image pairs sampled with our augmentations:

[6]:
```
# Visualize some examples
pl.seed_everything(42)
NUM_IMAGES = 6
imgs = torch.stack([img for idx in range(NUM_IMAGES) for img in unlabeled_data[idx][0]],␣
↪dim=0)
```

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```
img_grid = torchvision.utils.make_grid(imgs, nrow=6, normalize=True, pad_value=0.9)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(10,5))
plt.title('Augmented image examples of the STL10 dataset')
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

```
Global seed set to 42
```

We see the wide variety of our data augmentation, including randomly cropping, grayscaling, gaussian blur, and color distortion. Thus, it remains a challenging task for the model to match two, independently augmented patches of the same image.

SimCLR implementation

Using the data loader pipeline above, we can now implement SimCLR. At each iteration, we get for every image x two differently augmented versions, which we refer to as $\tilde{x}_i$ and $\tilde{x}_j$. Both of these images are encoded into a one-dimensional feature vector, between which we want to maximize similarity which minimizes it to all other images in the batch. The encoder network is split into two parts: a base encoder network $f(\cdot)$, and a projection head $g(\cdot)$. The base network is usually a deep CNN as we have seen in e.g. Tutorial 5 before, and is responsible for extracting a representation vector from the augmented data examples. In our experiments, we will use the common ResNet-18 architecture as $f(\cdot)$, and refer to the output as $f(\tilde{x}_i) = h_i$. The projection head $g(\cdot)$ maps the representation h into a space where we apply the contrastive loss, i.e., compare similarities between vectors. It is often chosen to be a small MLP with non-linearities, and for simplicity, we follow the original SimCLR paper setup by defining it as a two-layer MLP with ReLU activation in the hidden layer. Note that in the follow-up paper, SimCLRv2, the authors mention that larger/wider MLPs can boost the performance considerably. This is why we apply an MLP with four times larger hidden dimensions, but deeper MLPs showed to overfit on the given dataset. The general setup is visualized below (figure credit - Ting Chen et al.):

After finishing the training with contrastive learning, we will remove the projection head $g(\cdot)$, and use $f(\cdot)$ as a pre-trained feature extractor. The representations z that come out of the projection head $g(\cdot)$ have been shown to perform worse than those of the base network $f(\cdot)$ when finetuning the network for a new task. This is likely because the representations z are trained to become invariant to many features like the color that can be important for downstream tasks.

Thus, $g(\cdot)$ is only needed for the contrastive learning stage.

Now that the architecture is described, let's take a closer look at how we train the model. As mentioned before, we want to maximize the similarity between the representations of the two augmented versions of the same image, i.e., z_i and z_j in the figure above, while minimizing it to all other examples in the batch. SimCLR thereby applies the InfoNCE loss, originally proposed by Aaron van den Oord et al. for contrastive learning. In short, the InfoNCE loss compares the similarity of z_i and z_j to the similarity of z_i to any other representation in the batch by performing a softmax over the similarity values. The loss can be formally written as:

$$\ell_{i,j} = -\log \frac{\exp(\text{sim}(z_i, z_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k\neq i]} \exp(\text{sim}(z_i, z_k)/\tau)} = -\text{sim}(z_i, z_j)/\tau + \log \left[\sum_{k=1}^{2N} \mathbb{1}_{[k\neq i]} \exp(\text{sim}(z_i, z_k)/\tau)\right]$$

The function sim is a similarity metric, and the hyperparameter τ is called temperature determining how peaked the distribution is. Since many similarity metrics are bounded, the temperature parameter allows us to balance the influence of many dissimilar image patches versus one similar patch. The similarity metric that is used in SimCLR is cosine similarity, as defined below:

$$\text{sim}(z_i, z_j) = \frac{z_i^\top \cdot z_j}{||z_i|| \cdot ||z_j||}$$

The maximum cosine similarity possible is 1, while the minimum is -1. In general, we will see that the features of two different images will converge to a cosine similarity around zero since the minimum, -1, would require z_i and z_j to be in the exact opposite direction in all feature dimensions, which does not allow for great flexibility.

Finally, now that we have discussed all details, let's implement SimCLR below as a PyTorch Lightning module:

[7]:
```
class SimCLR(pl.LightningModule):

    def __init__(self, hidden_dim, lr, temperature, weight_decay, max_epochs=500):
        super().__init__()
        self.save_hyperparameters()
        assert self.hparams.temperature > 0.0, 'The temperature must be a positive float!
↪'
        # Base model f(.)
        self.convnet = torchvision.models.resnet18(num_classes=4*hidden_dim)  # Output␣
↪of last linear layer
        # The MLP for g(.) consists of Linear->ReLU->Linear
        self.convnet.fc = nn.Sequential(
            self.convnet.fc,  # Linear(ResNet output, 4*hidden_dim)
            nn.ReLU(inplace=True),
            nn.Linear(4*hidden_dim, hidden_dim)
        )

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(),
                                lr=self.hparams.lr,
                                weight_decay=self.hparams.weight_decay)
        lr_scheduler = optim.lr_scheduler.CosineAnnealingLR(optimizer,
                                                            T_max=self.hparams.max_
↪epochs,
                                                            eta_min=self.hparams.lr/50)
        return [optimizer], [lr_scheduler]

    def info_nce_loss(self, batch, mode='train'):
        imgs, _ = batch
```

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```
        imgs = torch.cat(imgs, dim=0)

        # Encode all images
        feats = self.convnet(imgs)
        # Calculate cosine similarity
        cos_sim = F.cosine_similarity(feats[:,None,:], feats[None,:,:], dim=-1)
        # Mask out cosine similarity to itself
        self_mask = torch.eye(cos_sim.shape[0], dtype=torch.bool, device=cos_sim.device)
        cos_sim.masked_fill_(self_mask, -9e15)
        # Find positive example -> batch_size//2 away from the original example
        pos_mask = self_mask.roll(shifts=cos_sim.shape[0]//2, dims=0)
        # InfoNCE loss
        cos_sim = cos_sim / self.hparams.temperature
        nll = -cos_sim[pos_mask] + torch.logsumexp(cos_sim, dim=-1)
        nll = nll.mean()

        # Logging loss
        self.log(mode+'_loss', nll)
        # Get ranking position of positive example
        comb_sim = torch.cat([cos_sim[pos_mask][:,None],  # First position positive␣
↪example
                              cos_sim.masked_fill(pos_mask, -9e15)],
                             dim=-1)
        sim_argsort = comb_sim.argsort(dim=-1, descending=True).argmin(dim=-1)
        # Logging ranking metrics
        self.log(mode+'_acc_top1', (sim_argsort == 0).float().mean())
        self.log(mode+'_acc_top5', (sim_argsort < 5).float().mean())
        self.log(mode+'_acc_mean_pos', 1+sim_argsort.float().mean())

        return nll

    def training_step(self, batch, batch_idx):
        return self.info_nce_loss(batch, mode='train')

    def validation_step(self, batch, batch_idx):
        self.info_nce_loss(batch, mode='val')
```

Alternatively to performing the validation on the contrastive learning loss as well, we could also take a simple, small downstream task, and track the performance of the base network $f(\cdot)$ on that. However, in this tutorial, we will restrict ourselves to the STL10 dataset where we use the task of image classification on STL10 as our test task.

Training

Now that we have implemented SimCLR and the data loading pipeline, we are ready to train the model. We will use the same training function setup as usual. For saving the best model checkpoint, we track the metric `val_acc_top5`, which describes how often the correct image patch is within the top-5 most similar examples in the batch. This is usually less noisy than the top-1 metric, making it a better metric to choose the best model from.

[8]:
```
def train_simclr(batch_size, max_epochs=500, **kwargs):
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, 'SimCLR'),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
```

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```
                         devices=1,
                         max_epochs=max_epochs,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode='max',␣
↪monitor='val_acc_top5'),
                                    LearningRateMonitor('epoch')])
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, 'SimCLR.ckpt')
    if os.path.isfile(pretrained_filename):
        print(f'Found pretrained model at {pretrained_filename}, loading...')
        model = SimCLR.load_from_checkpoint(pretrained_filename) # Automatically loads␣
↪the model with the saved hyperparameters
    else:
        train_loader = data.DataLoader(unlabeled_data, batch_size=batch_size,␣
↪shuffle=True,
                                       drop_last=True, pin_memory=True, num_workers=NUM_
↪WORKERS)
        val_loader = data.DataLoader(train_data_contrast, batch_size=batch_size,␣
↪shuffle=False,
                                     drop_last=False, pin_memory=True, num_workers=NUM_
↪WORKERS)
        pl.seed_everything(42) # To be reproducable
        model = SimCLR(max_epochs=max_epochs, **kwargs)
        trainer.fit(model, train_loader, val_loader)
        model = SimCLR.load_from_checkpoint(trainer.checkpoint_callback.best_model_path)
↪# Load best checkpoint after training

    return model
```

A common observation in contrastive learning is that the larger the batch size, the better the models perform. A larger batch size allows us to compare each image to more negative examples, leading to overall smoother loss gradients. However, in our case, we experienced that a batch size of 256 was sufficient to get good results.

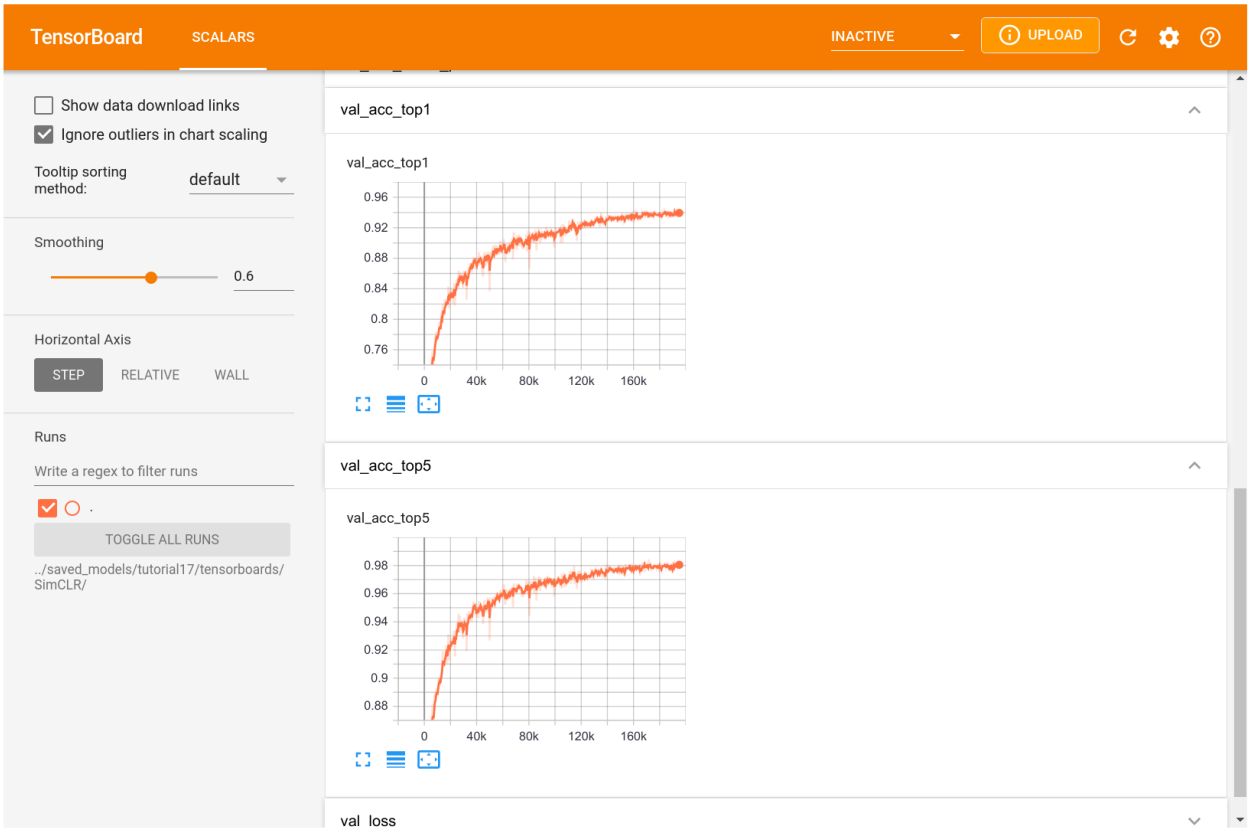
[9]:
```
simclr_model = train_simclr(batch_size=256,
                            hidden_dim=128,
                            lr=5e-4,
                            temperature=0.07,
                            weight_decay=1e-4,
                            max_epochs=500)
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
```

```
Found pretrained model at ../saved_models/tutorial17/SimCLR.ckpt, loading...
```

To get an intuition of how training with contrastive learning behaves, we can take a look at the TensorBoard below:

[10]:
```
%tensorboard --logdir ../saved_models/tutorial17/tensorboards/SimCLR/
```



One thing to note is that contrastive learning benefits a lot from long training. The shown plot above is from a training that took approx. 1 day on a NVIDIA TitanRTX. Training the model for even longer might reduce its loss further, but we did not experience any gains from it for the downstream task on image classification. In general, contrastive learning can also benefit from using larger models, if sufficient unlabeled data is available.

4.29.2 Logistic Regression

After we have trained our model via contrastive learning, we can deploy it on downstream tasks and see how well it performs with little data. A common setup, which also verifies whether the model has learned generalized representations, is to perform Logistic Regression on the features. In other words, we learn a single, linear layer that maps the representations to a class prediction. Since the base network $f(\cdot)$ is not changed during the training process, the model can only perform well if the representations of h describe all features that might be necessary for the task. Further, we do not have to worry too much about overfitting since we have very few parameters that are trained. Hence, we might expect that the model can perform well even with very little data.

First, let's implement a simple Logistic Regression setup for which we assume that the images already have been encoded in their feature vectors. If very little data is available, it might be beneficial to dynamically encode the images during training so that we can also apply data augmentations. However, the way we implement it here is much more efficient and can be trained within a few seconds. Further, using data augmentations did not show any significant gain in this simple setup.

[11]:
```
class LogisticRegression(pl.LightningModule):

    def __init__(self, feature_dim, num_classes, lr, weight_decay, max_epochs=100):
        super().__init__()
        self.save_hyperparameters()
```

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```
        # Mapping from representation h to classes
        self.model = nn.Linear(feature_dim, num_classes)

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(),
                                lr=self.hparams.lr,
                                weight_decay=self.hparams.weight_decay)
        lr_scheduler = optim.lr_scheduler.MultiStepLR(optimizer,
                                                      milestones=[int(self.hparams.max_
↪epochs*0.6),
                                                                  int(self.hparams.max_
↪epochs*0.8)],
                                                      gamma=0.1)
        return [optimizer], [lr_scheduler]

    def _calculate_loss(self, batch, mode='train'):
        feats, labels = batch
        preds = self.model(feats)
        loss = F.cross_entropy(preds, labels)
        acc = (preds.argmax(dim=-1) == labels).float().mean()

        self.log(mode + '_loss', loss)
        self.log(mode + '_acc', acc)
        return loss

    def training_step(self, batch, batch_idx):
        return self._calculate_loss(batch, mode='train')

    def validation_step(self, batch, batch_idx):
        self._calculate_loss(batch, mode='val')

    def test_step(self, batch, batch_idx):
        self._calculate_loss(batch, mode='test')
```

The data we use is the training and test set of STL10. The training contains 500 images per class, while the test set has 800 images per class.

[12]:
```
img_transforms = transforms.Compose([transforms.ToTensor(),
                                     transforms.Normalize((0.5,), (0.5,))])

train_img_data = STL10(root=DATASET_PATH, split='train', download=True,
                       transform=img_transforms)
test_img_data = STL10(root=DATASET_PATH, split='test', download=True,
                      transform=img_transforms)

print("Number of training examples:", len(train_img_data))
print("Number of test examples:", len(test_img_data))
```

```
Files already downloaded and verified
Files already downloaded and verified
Number of training examples: 5000
Number of test examples: 8000
```

Next, we implement a small function to encode all images in our datasets. The output representations are then used as inputs to the Logistic Regression model.

[13]:
```
@torch.no_grad()
def prepare_data_features(model, dataset):
    # Prepare model
    network = deepcopy(model.convnet)
    network.fc = nn.Identity()  # Removing projection head g(.)
    network.eval()
    network.to(device)

    # Encode all images
    data_loader = data.DataLoader(dataset, batch_size=64, num_workers=NUM_WORKERS,␣
↪shuffle=False, drop_last=False)
    feats, labels = [], []
    for batch_imgs, batch_labels in tqdm(data_loader):
        batch_imgs = batch_imgs.to(device)
        batch_feats = network(batch_imgs)
        feats.append(batch_feats.detach().cpu())
        labels.append(batch_labels)

    feats = torch.cat(feats, dim=0)
    labels = torch.cat(labels, dim=0)

    # Sort images by labels
    labels, idxs = labels.sort()
    feats = feats[idxs]

    return data.TensorDataset(feats, labels)
```

Let's apply the function to both training and test set below.

[14]:
```
train_feats_simclr = prepare_data_features(simclr_model, train_img_data)
test_feats_simclr = prepare_data_features(simclr_model, test_img_data)
```

```
  0%|          | 0/79 [00:00<?, ?it/s]
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/torch/nn/functional.py:
↪718: UserWarning: Named tensors and all their associated APIs are an experimental␣
↪feature and subject to change. Please do not use them for anything important until␣
↪they are released as stable. (Triggered internally at  /opt/conda/conda-bld/pytorch_
↪1623448265233/work/c10/core/TensorImpl.h:1156.)
  return torch.max_pool2d(input, kernel_size, stride, padding, dilation, ceil_mode)
```

```
  0%|          | 0/125 [00:00<?, ?it/s]
```

Finally, we can write a training function as usual. We evaluate the model on the test set every 10 epochs to allow early stopping, but the low frequency of the validation ensures that we do not overfit too much on the test set.

[15]:
```
def train_logreg(batch_size, train_feats_data, test_feats_data, model_suffix, max_
↪epochs=100, **kwargs):
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH,
↪"LogisticRegression"),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
```

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```
                         max_epochs=max_epochs,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode='max',␣
↪monitor='val_acc'),
                                    LearningRateMonitor("epoch")],
                         enable_progress_bar=False,
                         check_val_every_n_epoch=10)
    trainer.logger._default_hp_metric = None

    # Data loaders
    train_loader = data.DataLoader(train_feats_data, batch_size=batch_size, shuffle=True,
                                   drop_last=False, pin_memory=True, num_workers=0)
    test_loader = data.DataLoader(test_feats_data, batch_size=batch_size, shuffle=False,
                                  drop_last=False, pin_memory=True, num_workers=0)

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, f"LogisticRegression_{model_
↪suffix}.ckpt")
    if os.path.isfile(pretrained_filename):
        print(f"Found pretrained model at {pretrained_filename}, loading...")
        model = LogisticRegression.load_from_checkpoint(pretrained_filename)
    else:
        pl.seed_everything(42)  # To be reproducable
        model = LogisticRegression(**kwargs)
        trainer.fit(model, train_loader, test_loader)
        model = LogisticRegression.load_from_checkpoint(trainer.checkpoint_callback.best_
↪model_path)

    # Test best model on train and validation set
    train_result = trainer.test(model, train_loader, verbose=False)
    test_result = trainer.test(model, test_loader, verbose=False)
    result = {"train": train_result[0]["test_acc"], "test": test_result[0]["test_acc"]}

    return model, result
```

Despite the training dataset of STL10 already only having 500 labeled images per class, we will perform experiments with even smaller datasets. Specifically, we train a Logistic Regression model for datasets with only 10, 20, 50, 100, 200, and all 500 examples per class. This gives us an intuition on how well the representations learned by contrastive learning can be transfered to a image recognition task like this classification. First, let's define a function to create the intended sub-datasets from the full training set:

[16]:
```
def get_smaller_dataset(original_dataset, num_imgs_per_label):
    new_dataset = data.TensorDataset(
        *[t.unflatten(0, (10, -1))[:,:num_imgs_per_label].flatten(0, 1) for t in␣
↪original_dataset.tensors]
    )
    return new_dataset
```

Next, let's run all models. Despite us training 6 models, this cell could be run within a minute or two without the pretrained models.

[17]:
```
results = {}
for num_imgs_per_label in [10, 20, 50, 100, 200, 500]:
```

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```
    sub_train_set = get_smaller_dataset(train_feats_simclr, num_imgs_per_label)
    _, small_set_results = train_logreg(batch_size=64,
                                        train_feats_data=sub_train_set,
                                        test_feats_data=test_feats_simclr,
                                        model_suffix=num_imgs_per_label,
                                        feature_dim=train_feats_simclr.tensors[0].
↪shape[1],
                                        num_classes=10,
                                        lr=1e-3,
                                        weight_decay=1e-3)
    results[num_imgs_per_label] = small_set_results
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:69: UserWarning: Your test_dataloader has `shuffle=True`, it␣
↪is best practice to turn this off for val/test/predict dataloaders.
  warnings.warn(*args, **kwargs)
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:69: UserWarning: The dataloader, test dataloader 0, does not␣
↪have many workers which may be a bottleneck. Consider increasing the value of the `num_
↪workers` argument` (try 16 which is the number of cpus on this machine) in the␣
↪`DataLoader` init to improve performance.
  warnings.warn(*args, **kwargs)
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
Found pretrained model at ../saved_models/tutorial17/LogisticRegression_10.ckpt,␣
↪loading...
Found pretrained model at ../saved_models/tutorial17/LogisticRegression_20.ckpt,␣
↪loading...
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
Found pretrained model at ../saved_models/tutorial17/LogisticRegression_50.ckpt,␣
↪loading...
Found pretrained model at ../saved_models/tutorial17/LogisticRegression_100.ckpt,␣
↪loading...
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

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```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
Found pretrained model at ../saved_models/tutorial17/LogisticRegression_200.ckpt,␣
↪loading...
Found pretrained model at ../saved_models/tutorial17/LogisticRegression_500.ckpt,␣
↪loading...
```

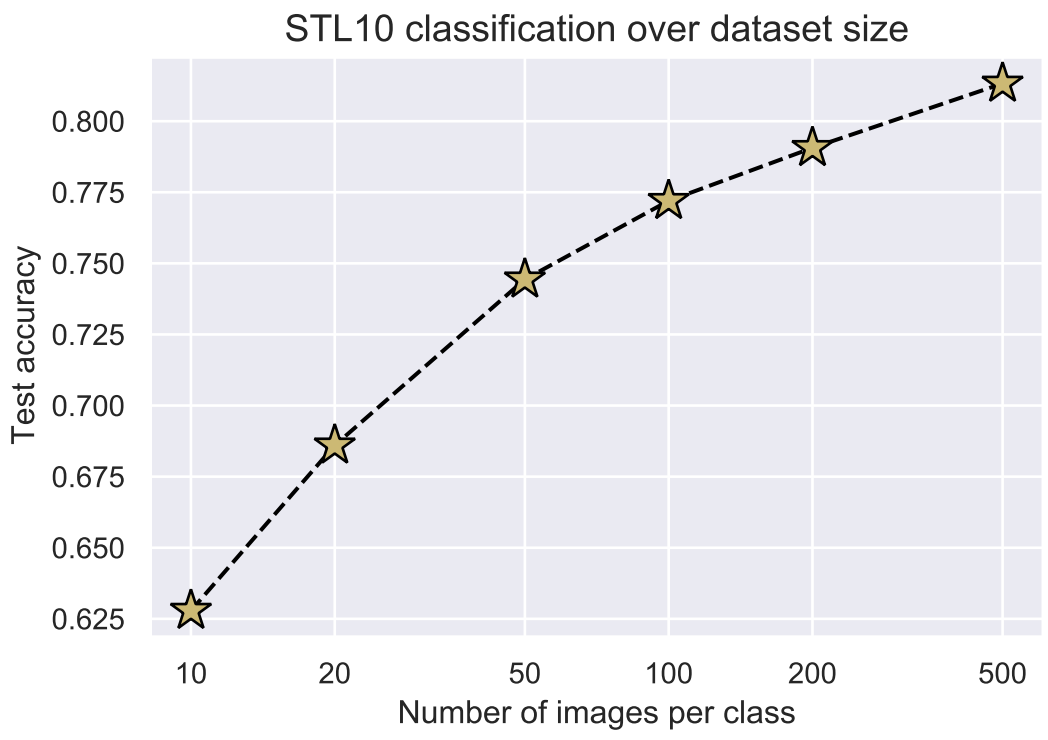
```
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

Finally, let's plot the results.

[18]:
```
dataset_sizes = sorted([k for k in results])
test_scores = [results[k]["test"] for k in dataset_sizes]

fig = plt.figure(figsize=(6,4))
plt.plot(dataset_sizes, test_scores, '--', color="#000", marker="*", markeredgecolor="
↪#000", markerfacecolor="y", markersize=16)
plt.xscale("log")
plt.xticks(dataset_sizes, labels=dataset_sizes)
plt.title("STL10 classification over dataset size", fontsize=14)
plt.xlabel("Number of images per class")
plt.ylabel("Test accuracy")
plt.minorticks_off()
plt.show()

for k, score in zip(dataset_sizes, test_scores):
    print(f'Test accuracy for {k:3d} images per label: {100*score:4.2f}%')
```



```
Test accuracy for  10 images per label: 62.79%
Test accuracy for  20 images per label: 68.60%
Test accuracy for  50 images per label: 74.44%
Test accuracy for 100 images per label: 77.20%
Test accuracy for 200 images per label: 79.06%
Test accuracy for 500 images per label: 81.33%
```

As one would expect, the classification performance improves the more data we have. However, with only 10 images per class, we can already classify more than 60% of the images correctly. This is quite impressive, considering that the images are also higher dimensional than e.g. CIFAR10. With the full dataset, we achieve an accuracy of 81%. The increase between 50 to 500 images per class might suggest a linear increase in performance with an exponentially larger dataset. However, with even more data, we could also finetune $f(\cdot)$ in the training process, allowing for the representations to adapt more to the specific classification task given.

To set the results above into perspective, we will train the base network, a ResNet-18, on the classification task from scratch.

4.29.3 Baseline

As a baseline to our results above, we will train a standard ResNet-18 with random initialization on the labeled training set of STL10. The results will give us an indication of the advantages that contrastive learning on unlabeled data has compared to using only supervised training. The implementation of the model is straightforward since the ResNet architecture is provided in the torchvision library.

[19]:
```
class ResNet(pl.LightningModule):

    def __init__(self, num_classes, lr, weight_decay, max_epochs=100):
        super().__init__()
        self.save_hyperparameters()
        self.model = torchvision.models.resnet18(num_classes=num_classes)

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(),
                                lr=self.hparams.lr,
                                weight_decay=self.hparams.weight_decay)
        lr_scheduler = optim.lr_scheduler.MultiStepLR(optimizer,
                                                      milestones=[int(self.hparams.max_
↪epochs*0.7),
                                                                  int(self.hparams.max_
↪epochs*0.9)],
                                                      gamma=0.1)
        return [optimizer], [lr_scheduler]

    def _calculate_loss(self, batch, mode='train'):
        imgs, labels = batch
        preds = self.model(imgs)
        loss = F.cross_entropy(preds, labels)
        acc = (preds.argmax(dim=-1) == labels).float().mean()

        self.log(mode + '_loss', loss)
        self.log(mode + '_acc', acc)
        return loss
```

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```
    def training_step(self, batch, batch_idx):
        return self._calculate_loss(batch, mode='train')

    def validation_step(self, batch, batch_idx):
        self._calculate_loss(batch, mode='val')

    def test_step(self, batch, batch_idx):
        self._calculate_loss(batch, mode='test')
```

It is clear that the ResNet easily overfits on the training data since its parameter count is more than 1000 times larger than the dataset size. To make the comparison to the contrastive learning models fair, we apply data augmentations similar to the ones we used before: horizontal flip, crop-and-resize, grayscale, and gaussian blur. Color distortions as before are not used because the color distribution of an image showed to be an important feature for the classification. Hence, we observed no noticeable performance gains when adding color distortions to the set of augmentations. Similarly, we restrict the resizing operation before cropping to the max. 125% of its original resolution, instead of 1250% as done in SimCLR. This is because, for classification, the model needs to recognize the full object, while in contrastive learning, we only want to check whether two patches belong to the same image/object. Hence, the chosen augmentations below are overall weaker than in the contrastive learning case.

[20]:
```
train_transforms = transforms.Compose([transforms.RandomHorizontalFlip(),
                                       transforms.RandomResizedCrop(size=96, scale=(0.8,␣
↪1.0)),
                                       transforms.RandomGrayscale(p=0.2),
                                       transforms.GaussianBlur(kernel_size=9, sigma=(0.1,
↪ 0.5)),
                                       transforms.ToTensor(),
                                       transforms.Normalize((0.5,), (0.5,))
                                       ])

train_img_aug_data = STL10(root=DATASET_PATH, split='train', download=True,
                           transform=train_transforms)
```

```
Files already downloaded and verified
```

The training function for the ResNet is almost identical to the Logistic Regression setup. Note that we allow the ResNet to perform validation every 2 epochs to also check whether the model overfits strongly in the first iterations or not.

[21]:
```
def train_resnet(batch_size, max_epochs=100, **kwargs):
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, "ResNet"),
                         accelerator="gpu" if str(device).startswith("cuda") else "cpu",
                         devices=1,
                         max_epochs=max_epochs,
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc"),
                                    LearningRateMonitor("epoch")],
                         check_val_every_n_epoch=2)
    trainer.logger._default_hp_metric = None

    # Data loaders
    train_loader = data.DataLoader(train_img_aug_data, batch_size=batch_size,␣
↪shuffle=True,
                                   drop_last=True, pin_memory=True, num_workers=NUM_
↪WORKERS)
```

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```
    test_loader = data.DataLoader(test_img_data, batch_size=batch_size, shuffle=False,
                                  drop_last=False, pin_memory=True, num_workers=NUM_
↪WORKERS)

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, "ResNet.ckpt")
    if os.path.isfile(pretrained_filename):
        print("Found pretrained model at %s, loading..." % pretrained_filename)
        model = ResNet.load_from_checkpoint(pretrained_filename)
    else:
        pl.seed_everything(42) # To be reproducable
        model = ResNet(**kwargs)
        trainer.fit(model, train_loader, test_loader)
        model = ResNet.load_from_checkpoint(trainer.checkpoint_callback.best_model_path)

    # Test best model on validation set
    train_result = trainer.test(model, train_loader, verbose=False)
    val_result = trainer.test(model, test_loader, verbose=False)
    result = {"train": train_result[0]["test_acc"], "test": val_result[0]["test_acc"]}

    return model, result
```

Finally, let's train the model and check its results:

[22]:
```
resnet_model, resnet_result = train_resnet(batch_size=64,
                                           num_classes=10,
                                           lr=1e-3,
                                           weight_decay=2e-4,
                                           max_epochs=100)
print(f"Accuracy on training set: {100*resnet_result['train']:4.2f}%")
print(f"Accuracy on test set: {100*resnet_result['test']:4.2f}%")
```

```
GPU available: True, used: True
TPU available: False, using: 0 TPU cores
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
Found pretrained model at ../saved_models/tutorial17/ResNet.ckpt, loading...
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/pytorch_lightning/
↪utilities/distributed.py:69: UserWarning: Your test_dataloader has `shuffle=True`, it␣
↪is best practice to turn this off for val/test/predict dataloaders.
  warnings.warn(*args, **kwargs)
```

```
Testing: 0it [00:00, ?it/s]
```

```
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0,1]
```

```
Testing: 0it [00:00, ?it/s]
```

```
Accuracy on training set: 99.76%
Accuracy on test set: 73.31%
```

The ResNet trained from scratch achieves 73.31% on the test set. This is almost 8% less than the contrastive learning model, and even slightly less than SimCLR achieves with 1/10 of the data. This shows that self-supervised, contrastive learning provides considerable performance gains by leveraging large amounts of unlabeled data when little labeled data is available.

4.29.4 Conclusion

In this tutorial, we have discussed self-supervised contrastive learning and implemented SimCLR as an example method. We have applied it to the STL10 dataset and showed that it can learn generalizable representations that we can use to train simple classification models. With 500 images per label, it achieved an 8% higher accuracy than a similar model solely trained from supervision and performs on par with it when only using a tenth of the labeled data. Our experimental results are limited to a single dataset, but recent works such as Ting Chen et al. showed similar trends for larger datasets like ImageNet. Besides the discussed hyperparameters, the size of the model seems to be important in contrastive learning as well. If a lot of unlabeled data is available, larger models can achieve much stronger results and come close to their supervised baselines. Further, there are also approaches for combining contrastive and supervised learning, leading to performance gains beyond supervision (see Khosla et al.). Moreover, contrastive learning is not the only approach to self-supervised learning that has come up in the last two years and showed great results. Other methods include distillation-based methods like BYOL and redundancy reduction techniques like Barlow Twins. There is a lot more to explore in the self-supervised domain, and more, impressive steps ahead are to be expected.

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.30 Tutorial 2 (JAX): Introduction to JAX+Flax

Filled notebook:
Author: Phillip Lippe

Welcome to our JAX tutorial for the Deep Learning course at the University of Amsterdam! The following notebook is meant to give a short introduction to JAX, including writing and training your own neural networks with Flax. But why should you learn JAX, if there are already so many other deep learning frameworks like PyTorch and TensorFlow? The short answer: because it can be extremely fast. For instance, a small GoogleNet on CIFAR10, which we discuss in detail in Tutorial 5, can be trained in JAX 3x faster than in PyTorch with a similar setup. Note that for larger models, larger batch sizes, or smaller GPUs, a considerably smaller speedup is expected, and the code has not been designed for benchmarking. Nonetheless, JAX enables this speedup by compiling functions and numerical programs for accelerators (GPU/TPU) *just in time*, finding the optimal utilization of the hardware. Frameworks with dynamic computation graphs like PyTorch cannot achieve the same efficiency, since they cannot anticipate the next operations before the user calls them. For example, in an Inception block of GoogleNet, we apply multiple convolutional layers in parallel on the same input. JAX can optimize the execution of this layer by compiling the whole forward pass for the available accelerator and fusing operations where possible, reducing memory access and speeding up execution. In contrast, when calling the first convolutional layer in PyTorch, the framework does not know that multiple convolutions on the same feature map will follow. It sends each operation one by one to the GPU, and can only adapt the execution after seeing the next Python calls. Hence, JAX can make more efficient use of the GPU than, for instance, PyTorch.

However, everything comes with a price. In order to efficiently compile programs just-in-time in JAX, the functions need to be written with certain constraints. Firstly, the functions are not allowed to have side-effects, meaning that they are not allowed to affect any variable outside of their namespaces. For instance, in-place operations affect a variable even outside of the function. Moreover, stochastic operations such as `torch.rand(...)` change the global state of pseudo random number generators, which is not allowed in functional JAX (we will see later how JAX handles random number generation). Secondly, JAX compiles the functions based on anticipated shapes of all arrays/tensors in the function. This becomes problematic if the shapes or the program flow within the function depends on the values of the tensor. For instance, in the operation `y = x[x>3]`, the shape of `y` depends on how many values of `x` are greater than 3. We will discuss more of these constraints in this notebook. Still, in most common cases of training neural networks, it is straightforward to write functions within these constraints.

This tutorial is heavily inspired by many great JAX tutorials before, and a (non-exclusive) list of them are:

- JAX 101 with many subtutorials on individual parts of JAX
- JAX - The Sharp Bits discusses the constraints of JAX and how to overcome them
- Jax for the Impatient for a quick intro to JAX with focus on deep learning
- Flax Basics as introduction to the Flax framework

Throughout this tutorial, we will draw comparisons to PyTorch and also use its data loading library (see our PyTorch tutorial for a refresher). JAX is not meant to 'redefine the wheel', so we can combine it framework-agnostic parts from PyTorch (e.g., data loading) and TensorFlow (e.g., logging in TensorBoard). Further, we use Flax as a neural network library in JAX, and Optax to implement common deep learning optimizers. More on them later in the notebook. First, let's get started with some basic JAX operations.

[1]:
```
## Standard libraries
import os
import math
import numpy as np
import time

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgba
import seaborn as sns
sns.set()
```

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```
## Progress bar
from tqdm.auto import tqdm
```

4.30.1 JAX as NumPy on accelerators

Every deep learning framework has its own API for dealing with data arrays. For example, PyTorch uses `torch.Tensor` as data arrays on which it defines several operations like matrix multiplication, taking the mean of the elements, etc. In JAX, this basic API strongly resembles the one of NumPy, and even has the same name in JAX (`jax.numpy`). So, for now, let's think of JAX as NumPy that runs on accelerators. As a first step, let's import JAX and its NumPy API:

[2]:
```
import jax
import jax.numpy as jnp
print("Using jax", jax.__version__)
```

```
Using jax 0.3.13
```

At the current time of writing (June 2022), the newest JAX version is `0.3.13` which supports most of the common NumPy functionalities. The NumPy API of JAX is usually imported as `jnp`, to keep a resemblance to NumPy's import as `np`. In the following subsections, we will discuss the main differences between the classical NumPy API and the one of JAX.

Device Arrays

As a first test, let's create some arbitrary arrays like we would do in NumPy. For instance, let's create an array of zeros with shape `[2,5]`:

[3]:
```
a = jnp.zeros((2, 5), dtype=jnp.float32)
print(a)
```

```
[[0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]]
```

Similarly, we can create an array with values of 0 to 5 by using `arange`:

[4]:
```
b = jnp.arange(6)
print(b)
```

```
[0 1 2 3 4 5]
```

You might now wonder whether the arrays `a` and `b` are simply NumPy arrays. To check that, let's print out the class of `b`:

[5]:
```
b.__class__
```

[5]:
```
jaxlib.xla_extension.DeviceArray
```

Instead of a simple NumPy array, it shows the type `DeviceArray` which is what JAX uses to represent arrays. In contrast to NumPy, JAX can execute the same code on different backends – CPU, GPU and TPU. A `DeviceArray` therefore represents an array which is on one of the backends. Similar to PyTorch, we can check the device of an array by calling `.device()`:

[6]:
```
b.device()
```

[6]:
```
GpuDevice(id=0, process_index=0)
```

As you can see, the array `b` is already natively on a GPU although we did not specify this explicitly as you would do in PyTorch (on Colab, remember to select a GPU in your runtime environment). In order to change the device of an array, we can use `jax.device_get`:

[7]:
```
b_cpu = jax.device_get(b)
print(b_cpu.__class__)
```

```
<class 'numpy.ndarray'>
```

Unsurprisingly, a simple CPU-based array is nothing else than a NumPy array, which allows for a simple conversion between the two frameworks! To explicitly push a NumPy array to the accelerator, you can use `jax.device_put`:

[8]:
```
b_gpu = jax.device_put(b_cpu)
print(f'Device put: {b_gpu.__class__} on {b_gpu.device()}')
```

```
Device put: <class 'jaxlib.xla_extension.DeviceArray'> on gpu:0
```

Nicely enough, JAX will handle any device clash itself when you try to perform operations on a NumPy array and a DeviceArray by modeling the output as DeviceArray again:

[9]:
```
b_cpu + b_gpu
```

[9]:
```
DeviceArray([ 0,  2,  4,  6,  8, 10], dtype=int32)
```

Finally, we can also print all our available devices using `jax.devices()`:

[10]:
```
jax.devices()
```

[10]:
```
[GpuDevice(id=0, process_index=0), GpuDevice(id=1, process_index=0)]
```

A technical detail of running operations on DeviceArrays is that when a JAX function is called, the corresponding operation takes place asynchronously on the accelerator when possible. For instance, if we call `out = jnp.matmul(b, b)`, JAX first returns a placeholder array for `out` which may not be filled with the values as soon as the function calls finishes. This way, Python will not block the execution of follow-up statements, but instead only does it whenever we strictly need the value of `out`, for instance for printing or putting it on CPU. PyTorch uses a very similar principle to allow asynchronous computation. For more details, see JAX - Asynchronous Dispatch.

Immutable tensors

When we would like to change a NumPy array in-place, like replacing the first element of `b` with `1` instead of `0`, we could simply write `b[0]=1`. However, in JAX, this is not possible. A `DeviceArray` object is *immutable*, which means that no in-place operations are possible. The reason for this goes back to our discussion in the introduction: JAX requires programs to be "pure" functions, i.e. no effects on variables outside of the function are allowed. Allowing in-place operations of variables would make the program analysis for JAX's just-in-time compilation difficult. Instead, we can use the expression `b.at[0].set(1)` which, analogous to the in-place operation, returns a new array which is identical to `b`, except that its value at the first position is 1. Let's try that out below:

[11]:
```
b_new = b.at[0].set(1)
print('Original array:', b)
print('Changed array:', b_new)
```

```
Original array: [0 1 2 3 4 5]
Changed array: [1 1 2 3 4 5]
```

However, we said that JAX is very efficient. Isn't creating a new array in this case the opposite? While it is indeed less efficient, it can made much more efficient with JAX's just-in-time compilation. The compiler can recognize unnecessary array duplications, and replace them with in-place operations again. More on the just-in-time compilation later!

Pseudo Random Numbers in JAX

In machine learning, we come across several situations where we need to generate pseudo random numbers: randomly shuffling a dataset, sampling a dropout mask for regularization, training a VAE by sampling from the approximate posterior, etc. In libraries like NumPy and PyTorch, the random number generator are controlled by a seed, which we set initially to obtain the same samples every time we run the code (this is why the numbers are not truly random, hence "pseudo"-random). However, if we call `np.random.normal()` 5 times consecutively, we will get 5 different numbers since every execution changes the state/seed of the pseudo random number generation (PRNG). In JAX, if we would try to generate a random number with this approach, a function creating pseudo-random number would have an effect outside of it. To prevent this, JAX takes a different approach by explicitly passing and iterating the PRNG state. First, let's create a PRNG for the seed 42:

[12]:
```
rng = jax.random.PRNGKey(42)
```

Now, we can use this PRNG state to generate random numbers. Since with this state, the random number generation becomes deterministic, we sample the same number every time. This is not the case in NumPy if we set the seed once before both operations:

[13]:
```
# A non-desirable way of generating pseudo-random numbers...
jax_random_number_1 = jax.random.normal(rng)
jax_random_number_2 = jax.random.normal(rng)
print('JAX - Random number 1:', jax_random_number_1)
print('JAX - Random number 2:', jax_random_number_2)

# Typical random numbers in NumPy
np.random.seed(42)
np_random_number_1 = np.random.normal()
np_random_number_2 = np.random.normal()
print('NumPy - Random number 1:', np_random_number_1)
print('NumPy - Random number 2:', np_random_number_2)
```

```
JAX - Random number 1: -0.18471177
JAX - Random number 2: -0.18471177
NumPy - Random number 1: 0.4967141530112327
NumPy - Random number 2: -0.13826430117118466
```

Usually, we want to have a behavior like NumPy where we get a different random number every time we sample. To achieve this, we can *split* the PRNG state to get usable subkeys every time we need a new pseudo-random number. We can do this with `jax.random.split(...)`:

[14]:
```
rng, subkey1, subkey2 = jax.random.split(rng, num=3)  # We create 3 new keys
jax_random_number_1 = jax.random.normal(subkey1)
jax_random_number_2 = jax.random.normal(subkey2)
print('JAX new - Random number 1:', jax_random_number_1)
print('JAX new - Random number 2:', jax_random_number_2)
```

```
JAX new - Random number 1: 0.107961535
JAX new - Random number 2: -1.2226542
```

Every time you run this cell, you will obtain different random numbers for both operations since we create new PRNG states before sampling. In general, you want to split the PRNG key every time before generating a pseudo-number, to prevent accidentally obtaining the exact same numbers (for instance, sampling the exact same dropout mask every time you run the network makes dropout itself quite useless...). For a deeper dive into the ideas behind the random number generation in JAX, see JAX's tutorial on Pseudo Random Numbers.

4.30.2 Function transformations with Jaxpr

Rosalia Schneider and Vladimir Mikulik summarize the key points of JAX in the JAX 101 tutorial as follows:

> The most important difference, and in some sense the root of all the rest, is that JAX is designed to be functional, as in functional programming. The reason behind this is that the kinds of program transformations that JAX enables are much more feasible in functional-style programs. [...] The important feature of functional programming to grok when working with JAX is very simple: don't write code with side-effects.

Essentially, we want to write our main code of JAX in functions that do not affect anything else besides its outputs. For instance, we do not want to change input arrays in-place, or access global variables. While this might seem limiting at first, you get used to this quite quickly and most JAX functions that need to fulfill these constraints can be written this way without problems. Note that not all possible functions in training a neural network need to fulfill the constraints. For instance, loading or saving of models, the logging, or the data generation can be done in naive functions. Only the network execution, which we want to do very efficiently on our accelerator (GPU or TPU), should strictly follow these constraints.

What does make JAX functions so special, and how can we think about them? A good way of gaining understanding in how JAX handles function is to understand its intermediate representation: jaxpr. Conceptually, you can think of any operation that JAX does on a function, as first trace-specializing the Python function to be transformed into a small and well-behaved intermediate form. This means that we check which operations are performed on which array, and what shapes the arrays are. Based on this representation, JAX then interprets the function with transformation-specific interpretation rules, which includes automatic differentiation or compiling a function in XLA to efficiently use the accelerator.

To illustrate this intermediate representation, let's consider the same simple function we used in the PyTorch tutorial to discuss the concept of dynamic computation graphs:

$$y = \frac{1}{|x|}\sum_i \left[(x_i + 2)^2 + 3\right]$$

Using common NumPy operations in JAX, we can write it as follows:

[15]:
```
def simple_graph(x):
    x = x + 2
    x = x ** 2
    x = x + 3
    y = x.mean()
    return y

inp = jnp.arange(3, dtype=jnp.float32)
print('Input', inp)
print('Output', simple_graph(inp))
```

```
Input [0. 1. 2.]
Output 12.666667
```

To view the jaxpr representation of this function, we can use `jax.make_jaxpr`. Since the tracing depends on the shape of the input, we need to pass an input to the function (here of shape `[3]`):

[16]:
```
jax.make_jaxpr(simple_graph)(inp)
```

[16]:
```
{ lambda ; a:f32[3]. let
    b:f32[3] = add a 2.0
    c:f32[3] = integer_pow[y=2] b
    d:f32[3] = add c 3.0
    e:f32[] = reduce_sum[axes=(0,)] d
    f:f32[] = div e 3.0
  in (f,) }
```

A jaxpr representation follows the structure:

```
jaxpr ::= { lambda Var* ; Var+.
            let Eqn*
            in  [Expr+] }
```

where `Var*` are constants and `Var+` are input arguments. In the cell above, this is `a:f32[3]`, i.e. an array of shape 3 with type `jnp.float32` (`inp`). The list of equations, `Eqn*`, define the intermediate results of the function. You can see that each operation in `simple_graph` is translated to a corresponding equation, like `x = x + 2` is translated to `b:f32[3] = add a 2.0`. Furthermore, you see the specialization of the operations on the input shape, like `x.mean()` being replacing in `e` and `f` with summing and dividing by 3. Finally, `Expr+` in the jaxpr representation are the outputs of the functions. In the example, this is `f`, i.e. the final result of the function. Based on these atomic operations, JAX offers all kind of function transformations, of which we will discuss the most important ones later in this section. Hence, you can consider the jaxpr representation is an intermediate compilation stage of JAX. What happens if we actually try to look at the jaxpr representation of a function with side-effect? Let's consider the following function, which, as an illustrative example, appends the input to a global list:

[17]:
```
global_list = []

# Invalid function with side-effect
def norm(x):
    global_list.append(x)
    x = x ** 2
    n = x.sum()
    n = jnp.sqrt(n)
    return n

jax.make_jaxpr(norm)(inp)
```

[17]:
```
{ lambda ; a:f32[3]. let
    b:f32[3] = integer_pow[y=2] a
    c:f32[] = reduce_sum[axes=(0,)] b
    d:f32[] = sqrt c
  in (d,) }
```

As you can see, the jaxpr representation of the function does not contain any operation for `global_list.append(x)`. This is because jaxpr only understand side-effect-free code, and cannot represent such effects. Thus, we need to stick with pure functions without any side effects, to prevent any unwanted errors in our functions. If you are interested in learning more about the jaxpr representation, check out the JAX documentation on it. But for this tutorial, we just need the basics as discussed above.

Automatic differentiation

The intermediate jaxpr representation defines a computation graph, on which we can perform an essential operation of deep learning framework: automatic differentiation. In frameworks like PyTorch with a dynamic computation graph, we would compute the gradients based on the loss tensor itself, e.g. by calling `loss.backward()`. However, JAX directly works with functions. Instead of backpropagating gradients through tensors, JAX takes as input a function, and outputs another function which directly calculates the gradients for it. While this might seem quite different to what you are used to from other frameworks, it is quite intuitive: your gradient of parameters is really a function of parameters and data.

The transformation that allows us to do this is `jax.grad`, which takes as input the function, and returns another function representing the gradient calculation of the (first) input with respect to the output:

[18]:
```
grad_function = jax.grad(simple_graph)
gradients = grad_function(inp)
print('Gradient', gradients)
```

```
Gradient [1.3333334 2.        2.6666667]
```

The gradient we get here is exactly the one we would obtain when doing the calculation by hand. Moreover, we can also print the jaxpr representation of the gradient function:

[19]:
```
jax.make_jaxpr(grad_function)(inp)
```

[19]:
```
{ lambda ; a:f32[3]. let
    b:f32[3] = add a 2.0
    c:f32[3] = integer_pow[y=2] b
    d:f32[3] = integer_pow[y=1] b
    e:f32[3] = mul 2.0 d
    f:f32[3] = add c 3.0
    g:f32[] = reduce_sum[axes=(0,)] f
    _:f32[] = div g 3.0
    h:f32[] = div 1.0 3.0
    i:f32[3] = broadcast_in_dim[broadcast_dimensions=() shape=(3,)] h
    j:f32[3] = mul i e
  in (j,) }
```

This shows an unique property of JAX: we can print out the exact computation graph for determining the gradients. Compared to the original function, you can see new equations like `d:f32[3] = integer_pow[y=1] b` and `e:f32[3] = mul 2.0 d`, which model the intermediate gradient of $\partial b_i^2 / \partial b_i = 2b_i$. Furthermore, the return value `j` is the multiplication of `e` with $1/3$, which maps to the gradient being:

$$\frac{\partial y}{\partial x_i} = \frac{2}{3}(x_i + 2)$$

Hence, we can not only use JAX to estimate the gradients at a certain input value, but actually return the analytical gradient function which is quite a nice feature and highlights the properties of JAX!

Often, we do not only want the gradients, but also the actual output of the function, for instance for logging the loss. This can be efficiently done using `jax.value_and_grad`:

[20]:
```
val_grad_function = jax.value_and_grad(simple_graph)
val_grad_function(inp)
```

[20]:
```
(DeviceArray(12.666667, dtype=float32),
 DeviceArray([1.3333334, 2.       , 2.6666667], dtype=float32))
```

Further, we can specialize the gradient function to consider multiple input arguments, and add extra outputs that we may not want to differentiate (for instance the accuracy in classification). We will visit the most important ones in the network training later in this section, and refer to other great resources for more details (JAX Quickstart, Autodiff cookbook, Advanced autodiff).

To train neural networks, we need to determine the gradient for every parameter in the network with respect to the loss. Listing all parameters as input arguments quickly gets annoying and infeasible. JAX offers an elegant data structure to summarize all parameters: a pytree (documentation). A pytree is a container-like object which structures its elements as a tree. For instance, a linear neural network might have its parameters organized similar to:

```
params = {
    'linear1': {
        'weights': ...,
        'bias': ...
    },
    ...
}
```

JAX offers functions to process pytrees efficiently, such as obtaining all leafs (i.e. all parameters in a network) or applying a function on each element. We will come back to these structures when training a full network.

Speeding up computation with Just-In-Time compilation

Interestingly, from the previous code cell, you can see in the jaxpr representation of the gradient function that calculating the array `f` and scalar `g` are unnecessary. Intuitively, the gradient of taking the mean is independent of the actual output of the mean, hence we could drop `f` and `g` without any drawback. Finding such cases to improve efficiency and optimizing the code to take full advantage of the available accelerator hardware is one of the big selling points of JAX. It achieves that by *compiling functions just-in-time* with XLA (Accelerated Linear Algebra), using their jaxpr representation. Thereby, XLA fuses operations to reduce execution time of short-lived operations and eliminates intermediate storage buffers where not needed. For more details, see the XLA documentation.

To compile a function, JAX provides the `jax.jit` transformation. We can either apply the transformation directly on a function (as we will do in the next cell), or use the decorator `@jax.jit` before a function.

[21]:
```
jitted_function = jax.jit(simple_graph)
```

The `jitted_function` takes the same input arguments as the original function `simple_graph`. Since the jaxpr representation of a function depends on the input shape, the compilation is started once we put the first input in. However, note that this also means that for every different shape we want to run the function, a new XLA compilation is needed. This is why it is recommended to use padding in cases where your input shape strongly varies (we revisit this topic in the final section of this tutorial). For now, let's create an array with 1000 random values, on which we apply the jitted function:

[22]:
```
# Create a new random subkey for generating new random values
rng, normal_rng = jax.random.split(rng)
large_input = jax.random.normal(normal_rng, (1000,))
# Run the jitted function once to start compilation
_ = jitted_function(large_input)
```

The output is not any different from what you would get from the non-jitted function. However, how is it about the runtime? Let's time both the original and the jitted function. Due to the asynchronous execution on the GPU, we add `.block_until_ready()` on the output, which blocks the Python execution until the accelerator (here GPU) finished computing the result and hence get an accurate time estimate.

[23]:
```
%%timeit
simple_graph(large_input).block_until_ready()
```

```
598 µs ± 104 µs per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[24]:
```
%%timeit
jitted_function(large_input).block_until_ready()
```

```
19.5 µs ± 52.8 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

We see that the compiled function is almost 10-15x faster! This is quite an improvement in performance, and shows the potential of compiling functions with XLA. Furthermore, we can also apply multiple transformations on the same function in JAX, such as applying `jax.jit` on a gradient function:

[25]:
```
jitted_grad_function = jax.jit(grad_function)
_ = jitted_grad_function(large_input)  # Apply once to compile
```

Let's time the functions once more:

[26]:
```
%%timeit
grad_function(large_input).block_until_ready()
```

```
2.55 ms ± 190 µs per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[27]:
```
%%timeit
jitted_grad_function(large_input).block_until_ready()
```

```
17.4 µs ± 60.6 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

Once more, the jitted function is much faster than the original one. Intuitively, this shows the potential speed up we can gain by using `jax.jit` to compile the whole training step of a network. Generally, we want to jit the largest possible chunk of computation to give the compiler maximum freedom.

There are situations in which applying jit to a function is not straight-forward, for instance, if an input argument cannot be traced, or you need to use loops that depend on input arguments. To keep the tutorial simple, and since most neural network training functions do not run into these issues, we do not discuss such special cases here. Instead, we refer to the section on just-in-time compilation in the great tutorials of JAX 101 Tutorial, JAX Quickstart, and Thinking in JAX.

4.30.3 Implementing a Neural Network with Flax

With having reviewed the basics of JAX, we are now ready to implement our own neural network. Technically, we could implement our own neural network from scratch with JAX (see here for an example), but we do not really want to do that every time. Similarly to PyTorch's `torch.nn` package, there exist neural network libraries based on JAX which provide such basic functionality. A (non-exclusive) collection of them are:

- Flax, started by the Google Brain Team, focuses on flexibility and clarity.
- Haiku, from DeepMind, focuses on simplicity and compositionality.
- Trax, maintained by the Google Brain Team, provides solutions for common training tasks
- Equinox, created by Patrick Kidger and Cristian Garcia, implements neural networks as callable PyTrees
- Jraph, from DeepMind, is a graph neural network library (similar to PyTorch Geometric)

For this tutorial series, we will use Flax due to its flexibility, intuitive API, and larger community. However, this should not mean that the other libraries are necessarily worse, and we recommend giving them a try as well to find the best library for yourself!

We will introduce the libraries and all additional parts you might need to train a neural network in Flax, using a simple example classifier on a simple yet well known example: XOR. Given two binary inputs x_1 and x_2, the label to predict is 1 if either x_1 or x_2 is 1 while the other is 0, or the label is 0 in all other cases. The example became famous by the fact that a single neuron, i.e. a linear classifier, cannot learn this simple function. Hence, we will learn how to build a small neural network that can learn this function. To make it a little bit more interesting, we move the XOR into continuous space and introduce some gaussian noise on the binary inputs. Our desired separation of an XOR dataset could look as follows:

The model

The package `flax.linen` defines a series of useful classes like linear networks layers, convolutions, activation functions etc. A full list can be found here. In case you need a certain network layer, check the documentation of the package first before writing the layer yourself as the package likely contains the code for it already. We import it below:

[28]:
```
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax

from flax import linen as nn
```

nn.Module

Similar to PyTorch, a neural network is built up out of modules. Modules can contain other modules, and a neural network is considered to be a module itself as well. The basic template of a module is as follows:

[29]:
```
class MyModule(nn.Module):
    # Some dataclass attributes, like hidden dimension, number of layers, etc. of the␣
↪form:
    # varname : vartype

    def setup(self):
        # Flax uses "lazy" initialization. This function is called once before you
        # call the model, or try to access attributes. In here, define your submodules␣
↪etc.
        pass

    def __call__(self, x):
        # Function for performing the calculation of the module.
        pass
```

The main, obvious difference to PyTorch is that Flax uses lazy initialization. The function `setup` is called once on a module instance before any other methods are called, or when you try to access a attribute of *self* defined in setup. Additional object attributes are defined below the class name. However, in contrast to PyTorch, the parameters are not part of the module. Instead, we can create a set of parameters of the module by calling its `init()` function. This function takes as input a PRNG state for sampling pseudo-random numbers and an example input to the model, and

returns a set of parameters for the module as a pytree. Further, since the init function requires an input to the network, we can infer the input shape for all modules and do not need to explicitly define it during the module creation. This becomes more clear in the example we show in a second.

The `__call__` method represents the `forward` function in PyTorch, and performs the actual computation of the module. It can take additional arguments if needed, like whether we are training or validation.

Simple classifier

To get an intuition behind how we work with modules in Flax, let's define our own small neural network. We will use a minimal network with a input layer, one hidden layer with tanh as activation function, and a output layer. In other words, our networks should look something like this:

The input neurons are shown in blue, which represent the coordinates x_1 and x_2 of a data point. The hidden neurons including a tanh activation are shown in white, and the output neuron in red. In Flax, we can define this as follows:

[30]:
```
class SimpleClassifier(nn.Module):
    num_hidden : int   # Number of hidden neurons
    num_outputs : int  # Number of output neurons

    def setup(self):
        # Create the modules we need to build the network
        # nn.Dense is a linear layer
        self.linear1 = nn.Dense(features=self.num_hidden)
        self.linear2 = nn.Dense(features=self.num_outputs)

    def __call__(self, x):
        # Perform the calculation of the model to determine the prediction
        x = self.linear1(x)
        x = nn.tanh(x)
        x = self.linear2(x)
        return x
```

One thing you may notice is that usually, all layers that we define in `setup` are also used in the `__call__` function. To reduce the code overhead, Flax provides an alternative, more compact network creation with `nn.compact`. With that, we can remove the setup function and instead our model as:

[31]:
```
class SimpleClassifierCompact(nn.Module):
    num_hidden : int   # Number of hidden neurons
    num_outputs : int  # Number of output neurons

    @nn.compact  # Tells Flax to look for defined submodules
    def __call__(self, x):
        # Perform the calculation of the model to determine the prediction
        # while defining necessary layers
        x = nn.Dense(features=self.num_hidden)(x)
        x = nn.tanh(x)
        x = nn.Dense(features=self.num_outputs)(x)
        return x
```

The `nn.compact` annotation of the `__call__` method signals Flax to look for submodules that we define in the forward pass. These are automatically recognized as such, so that we can use them for initialization etc. Which of the two model definition you use is often up to you (see the Flax documentation for some pros and cons for both methods). In the

following tutorials, we will mostly use the compact version, but occasionally come back to the explicit setup function where necessary. For instance, if we define more functions on a module besides `__call__` and want to reuse some modules, it is recommended to use the setup version.

For the examples in this notebook, we will use a tiny neural network with two input neurons and eight hidden neurons. As we perform binary classification, we will use a single output neuron. Note that we do not apply a sigmoid on the output yet. This is because other functions, especially the loss, are more efficient and precise to calculate on the original outputs instead of the sigmoid output. We will discuss the detailed reason later.

Now, let's create an instance of this network:

[32]:
```
model = SimpleClassifier(num_hidden=8, num_outputs=1)
# Printing the model shows its attributes
print(model)
```

```
SimpleClassifier(
    # attributes
    num_hidden = 8
    num_outputs = 1
)
```

At this stage, the model has no parameters initialized. To do this, let's create a random input of our dataset, and apply the init function:

[33]:
```
rng, inp_rng, init_rng = jax.random.split(rng, 3)
inp = jax.random.normal(inp_rng, (8, 2))  # Batch size 8, input size 2
# Initialize the model
params = model.init(init_rng, inp)
print(params)
```

```
FrozenDict({
    params: {
        linear1: {
            kernel: DeviceArray([[ 0.31476864, -0.4647768 , -0.7862042 , -0.48842615,
                          -0.65373844,  0.3892545 ,  0.3038056 ,  0.04179859],
                         [-0.3298236 ,  1.1110363 ,  0.54909396, -0.8168818 ,
                           0.40057245, -0.8665987 ,  1.2087964 ,  1.0364622 ]],
↪   dtype=float32),
            bias: DeviceArray([0., 0., 0., 0., 0., 0., 0., 0.], dtype=float32),
        },
        linear2: {
            kernel: DeviceArray([[-0.27971813],
                         [-0.7466775 ],
                         [ 0.29791608],
                         [-0.26267236],
                         [-0.5084385 ],
                         [ 0.04573093],
                         [-0.47257012],
                         [ 0.50458497]], dtype=float32),
            bias: DeviceArray([0.], dtype=float32),
        },
    },
})
```

Now, we have parameters with which we can apply the network. We see that the parameters follow the same structure as defined in our module, and each linear layer contains one `kernel`, i.e. the weights, and a bias parameter. With this, we could apply the model on an input using the `apply` function:

[34]:
```
model.apply(params, inp)
```

[34]:
```
DeviceArray([[-0.48368204],
             [ 0.04365474],
             [ 0.06668529],
             [-0.34203646],
             [ 0.4835147 ],
             [ 0.37424874],
             [ 0.14232653],
             [-0.5916512 ]], dtype=float32)
```

The model returns an output array of shape `[8,1]`, which corresponds to the one output neuron in the model for all 8 batch elements. With that, we now know how to initialize a model, and run a model. Next, let's look at the data.

The data

As mentioned before, JAX is not meant to 'reinvent the wheel' for every part of the deep learning pipeline. Hence, JAX and Flax do not natively provide a data loading functionality, but instead refer to other available libraries like Tensorflow and PyTorch. Here, let's use again the package `torch.utils.data` library.

[35]:
```
import torch.utils.data as data
```

The data package defines two classes which are the standard interface for handling data in PyTorch: `data.Dataset`, and `data.DataLoader`. The dataset class provides an uniform interface to access the training/test data, while the data loader makes sure to efficiently load and stack the data points from the dataset into batches during training.

The dataset class

The dataset class summarizes the basic functionality of a dataset in a natural way. To define a dataset in PyTorch, we simply specify two functions: `__getitem__`, and `__len__`. The get-item function has to return the i-th data point in the dataset, while the len function returns the size of the dataset. For the XOR dataset, we can define the dataset class as follows:

[36]:
```
class XORDataset(data.Dataset):

    def __init__(self, size, seed, std=0.1):
        """
        Inputs:
            size - Number of data points we want to generate
            seed - The seed to use to create the PRNG state with which we want to␣
↪generate the data points
            std - Standard deviation of the noise (see generate_continuous_xor function)
        """
        super().__init__()
        self.size = size
        self.np_rng = np.random.RandomState(seed=seed)
        self.std = std
        self.generate_continuous_xor()

    def generate_continuous_xor(self):
        # Each data point in the XOR dataset has two variables, x and y, that can be␣
↪either 0 or 1
```

(continues on next page)

(continued from previous page)

```
        # The label is their XOR combination, i.e. 1 if only x or only y is 1 while the␣
↪other is 0.
        # If x=y, the label is 0.
        data = self.np_rng.randint(low=0, high=2, size=(self.size, 2)).astype(np.float32)
        label = (data.sum(axis=1) == 1).astype(np.int32)
        # To make it slightly more challenging, we add a bit of gaussian noise to the␣
↪data points.
        data += self.np_rng.normal(loc=0.0, scale=self.std, size=data.shape)

        self.data = data
        self.label = label

    def __len__(self):
        # Number of data point we have. Alternatively self.data.shape[0], or self.label.
↪shape[0]
        return self.size

    def __getitem__(self, idx):
        # Return the idx-th data point of the dataset
        # If we have multiple things to return (data point and label), we can return␣
↪them as tuple
        data_point = self.data[idx]
        data_label = self.label[idx]
        return data_point, data_label
```

Note that in contrast to our PyTorch tutorial, we use NumPy to generate the random data. Similar to JAX, NumPy also allows the pseudo-number generation based on a PRNG state. Hence, for better reproducibility, we are doing the same here. Let's try to create such a dataset and inspect it:

[37]:
```
dataset = XORDataset(size=200, seed=42)
print("Size of dataset:", len(dataset))
print("Data point 0:", dataset[0])
```

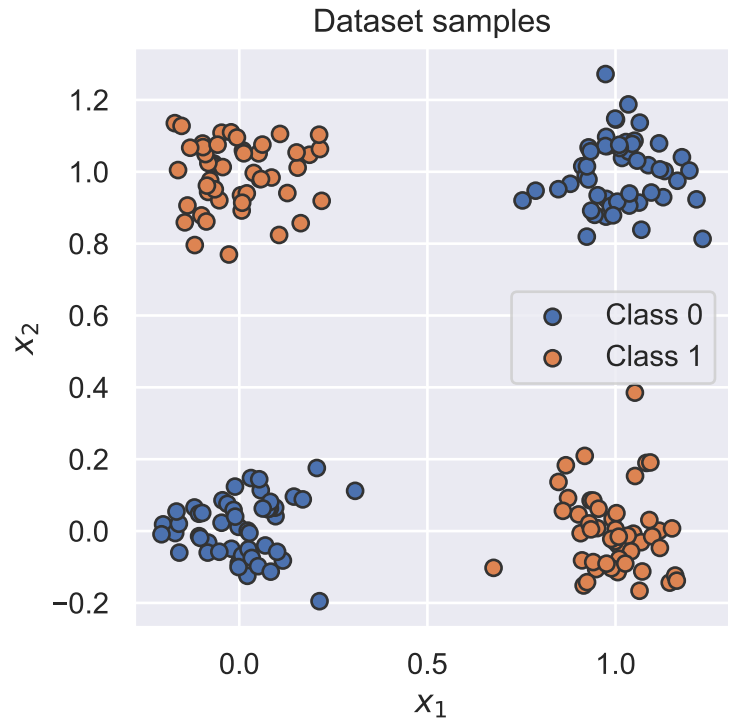
```
Size of dataset: 200
Data point 0: (array([-0.06800247,  1.0232254 ], dtype=float32), 1)
```

To better relate to the dataset, we visualize the samples below.

[38]:
```
def visualize_samples(data, label):
    data_0 = data[label == 0]
    data_1 = data[label == 1]

    plt.figure(figsize=(4,4))
    plt.scatter(data_0[:,0], data_0[:,1], edgecolor="#333", label="Class 0")
    plt.scatter(data_1[:,0], data_1[:,1], edgecolor="#333", label="Class 1")
    plt.title("Dataset samples")
    plt.ylabel(r"$x_2$")
    plt.xlabel(r"$x_1$")
    plt.legend()
```

[39]:
```
visualize_samples(dataset.data, dataset.label)
plt.show()
```



The data loader class

The class `torch.utils.data.DataLoader` represents a Python iterable over a dataset with support for automatic batching, multi-process data loading and many more features. The data loader communicates with the dataset using the function `__getitem__`, and stacks its outputs as tensors over the first dimension to form a batch. In contrast to the dataset class, we usually don't have to define our own data loader class, but can just create an object of it with the dataset as input. Additionally, we can configure our data loader with the following input arguments (only a selection, see full list here):

- `batch_size`: Number of samples to stack per batch
- `shuffle`: If True, the data is returned in a random order. This is important during training for introducing stochasticity.
- `num_workers`: Number of subprocesses to use for data loading. The default, 0, means that the data will be loaded in the main process which can slow down training for datasets where loading a data point takes a considerable amount of time (e.g. large images). More workers are recommended for those, but can cause issues on Windows computers. For tiny datasets as ours, 0 workers are usually faster.
- `persistent_workers`: If True, workers will not be shutdown after an iteration over the dataset has finished. This can be useful if the time per epoch is small, or if you face issues with workers being killed during training.
- `drop_last`: If True, the last batch is dropped in case it is smaller than the specified batch size. This occurs when the dataset size is not a multiple of the batch size. Only potentially helpful during training to keep a consistent batch size.
- `collate_fn`: A function that defines how the elements per batch are combined. By default, PyTorch stacks them as PyTorch tensors. For JAX, we will change it to NumPy arrays.

Let's create a simple data loader below with a function that stacks batch elements as NumPy array instead of PyTorch Tensors:

[40]:
```
# This collate function is taken from the JAX tutorial with PyTorch Data Loading
# https://jax.readthedocs.io/en/latest/notebooks/Neural_Network_and_Data_Loading.html
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

data_loader = data.DataLoader(dataset, batch_size=8, shuffle=True, collate_fn=numpy_
↪collate)
```

[41]:
```
# next(iter(...)) catches the first batch of the data loader
# If shuffle is True, this will return a different batch every time we run this cell
# For iterating over the whole dataset, we can simple use "for batch in data_loader: ..."
data_inputs, data_labels = next(iter(data_loader))

# The shape of the outputs are [batch_size, d_1,...,d_N] where d_1,...,d_N are the
# dimensions of the data point returned from the dataset class
print("Data inputs", data_inputs.shape, "\n", data_inputs)
print("Data labels", data_labels.shape, "\n", data_labels)
```

```
Data inputs (8, 2)
 [[ 1.0504987   1.0865755 ]
 [ 0.02809919 -0.06226995]
 [ 0.06141667  1.0757508 ]
 [ 0.08356921 -0.11297069]
 [ 1.0324166  -0.01301431]
 [ 1.0024511   0.04979983]
 [ 0.3078881   0.11195749]
 [ 1.0371146   0.9396015 ]]
Data labels (8,)
 [0 0 1 0 1 1 0 0]
```

Optimization

After defining the model and the dataset, it is time to prepare the optimization of the model. During training, we will perform the following steps:

1. Get a batch from the data loader
2. Obtain the predictions from the model for the batch
3. Calculate the loss based on the difference between predictions and labels
4. Backpropagation: calculate the gradients for every parameter with respect to the loss
5. Update the parameters of the model in the direction of the gradients

We have seen how we can do step 1, 2 and 4 in JAX and Flax. Now, we will look at step 3 and 5.

Stochastic Gradient Descent

For updating the parameters, Flax does not directly provide support for optimizers, but instead refers to another package called `optax` (documentation). Optax is an optimization library for JAX, which offers most common deep learning optimizers (SGD, Adam, Adagrad, RMSProp, etc.) and utilities (gradient clipping, weight decay, etc.).

[42]:
```
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax
```

For now, we will use the simplest optimizer, namely `optax.sgd`. Stochastic Gradient Descent updates parameters by multiplying the gradients with a small constant, called learning rate, and subtracting those from the parameters (hence minimizing the loss). Therefore, we slowly move towards the direction of minimizing the loss. A good default value of the learning rate for a small network as ours is 0.1. Remember that we again aim to write functional code. Hence, the optimizer does not take as input the parameters, but only the optimizer hyperparameters.

[43]:
```
# Input to the optimizer are optimizer settings like learning rate
optimizer = optax.sgd(learning_rate=0.1)
```

Since JAX calculates gradients via function transformations, we do not have functions like `backward()`, `optimizer.step()` or `optimizer.backward()` as in PyTorch. Instead, a optimizer is a function on the parameters and gradients. To simplify this step and bundle important parts of the training procedure, Flax offers the `flax.training` package. As a first step, we can create a `TrainState` which bundles the parameters, the optimizer, and the forward step of the model:

[44]:
```
from flax.training import train_state

model_state = train_state.TrainState.create(apply_fn=model.apply,
                                            params=params,
                                            tx=optimizer)
```

With this state object, it is easier to handle the training.

Loss function

For performing gradient updates, we need a function that can calculate the loss for a batch. Afterwards, we can apply JAX's gradient transformation to obtain a gradient function of it. In our setting, which is binary classification, we can use Binary Cross Entropy (BCE) which is defined as follows:

$$\mathcal{L}_{BCE} = -\sum_i \left[y_i \log x_i + (1 - y_i) \log(1 - x_i) \right]$$

where y are our labels, and x our predictions, both in the range of $[0, 1]$. Similar to PyTorch, Optax already provides a function for this: `optax.sigmoid_binary_cross_entropy(logits, labels)`. We calculate the loss on the logits instead of the sigmoid outputs for numerical stability. Let's write a function that takes as input a state (for the forward function), parameters, and a batch, and return the binary cross entropy loss and accuracy:

[45]:
```
def calculate_loss_acc(state, params, batch):
    data_input, labels = batch
    # Obtain the logits and predictions of the model for the input data
    logits = state.apply_fn(params, data_input).squeeze(axis=-1)
```

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```
    pred_labels = (logits > 0).astype(jnp.float32)
    # Calculate the loss and accuracy
    loss = optax.sigmoid_binary_cross_entropy(logits, labels).mean()
    acc = (pred_labels == labels).mean()
    return loss, acc
```

Note that we explicitly add the parameters here as an input argument since we want to calculate the gradients with respect to them later. An example execution of the function would look like:

[46]:
```
batch = next(iter(data_loader))
calculate_loss_acc(model_state, model_state.params, batch)
```

[46]:
```
(DeviceArray(0.6830494, dtype=float32), DeviceArray(0.625, dtype=float32))
```

Creating an efficient training and validation step

With this loss function and the optimizer, we are now ready to create an efficient training and validation/test step. First, let's consider the training. As input to each training step, we have a training state and a batch. We then want to calculate the loss for the input and take the gradients of it. Finally, we update the parameters with our optimizer and return the new state. All this can be summarized in the following function:

[47]:
```
@jax.jit  # Jit the function for efficiency
def train_step(state, batch):
    # Gradient function
    grad_fn = jax.value_and_grad(calculate_loss_acc,  # Function to calculate the loss
                                 argnums=1,  # Parameters are second argument of the␣
↪function
                                 has_aux=True  # Function has additional outputs, here␣
↪accuracy
                                )
    # Determine gradients for current model, parameters and batch
    (loss, acc), grads = grad_fn(state, state.params, batch)
    # Perform parameter update with gradients and optimizer
    state = state.apply_gradients(grads=grads)
    # Return state and any other value we might want
    return state, loss, acc
```

By using the transformation `jax.jit`, the whole gradient calculation and application is optimized in XLA, providing an efficient function for updating the model.

Next, let's look at the evaluation function. Here, we do not need to calculate gradients, but only want to get the accuracy of the model for the batch. This becomes a simpler version of the training step:

[48]:
```
@jax.jit  # Jit the function for efficiency
def eval_step(state, batch):
    # Determine the accuracy
    _, acc = calculate_loss_acc(state, state.params, batch)
    return acc
```

These two functions provide us now efficient utilities to train our model.

Training

Finally, we are ready to train our model. As a first step, we create a slightly larger dataset and specify a data loader with a larger batch size.

[49]:
```
train_dataset = XORDataset(size=2500, seed=42)
train_data_loader = data.DataLoader(train_dataset, batch_size=128, shuffle=True, collate_
↪fn=numpy_collate)
```

Now, we can write a small training function. In contrast to PyTorch, we do not need to explicitly push our model to GPU, since the parameters are already automatically created on GPU. Further, since the model itself is stateless, we do not have a `train()` or `eval()` function to switch between modes of e.g. dropout. When necessary, we can add an argument `train : bool` to the model forward pass. For this simple network here, however, this is not necessary.

Following the PyTorch tutorial, let's write a function here that trains a model for several epochs:

[50]:
```
def train_model(state, data_loader, num_epochs=100):
    # Training loop
    for epoch in tqdm(range(num_epochs)):
        for batch in data_loader:
            state, loss, acc = train_step(state, batch)
            # We could use the loss and accuracy for logging here, e.g. in TensorBoard
            # For simplicity, we skip this part here
    return state
```

[51]:
```
trained_model_state = train_model(model_state, train_data_loader, num_epochs=100)
```

```
  0%|          | 0/100 [00:00<?, ?it/s]
```

Training this model for 100 epochs does take barely a second... This shows the impressive speed JAX can reach, especially for small models!

Saving a model

After we finished training a model, we save the model to disk so that we can load the same weights at a later time. In JAX, this means we want to save the `state.params` dictionary. Luckily, the `flax.training` package again provides us with nice utilities for that, which uses TensorFlow as underlying framework.

[52]:
```
from flax.training import checkpoints
```

To save the whole model state, we can write:

[53]:
```
checkpoints.save_checkpoint(ckpt_dir='my_checkpoints/',  # Folder to save checkpoint in
                            target=trained_model_state,  # What to save. To only save␣
↪parameters, use model_state.params
                            step=100,  # Training step or other metric to save best␣
↪model on
                            prefix='my_model',  # Checkpoint file name prefix
                            overwrite=True   # Overwrite existing checkpoint files
                           )
```

[53]:
```
'my_checkpoints/my_model100'
```

To load this state dict again, we can use `checkpoints.restore_checkpoint`:

[54]:
```
loaded_model_state = checkpoints.restore_checkpoint(
                                                    ckpt_dir='my_checkpoints/',   # Folder with␣
↪the checkpoints
                                                    target=model_state,   # (optional) matching␣
↪object to rebuild state in
                                                    prefix='my_model'  # Checkpoint file name␣
↪prefix
                                                   )
```

The states `loaded_model_state` and `trained_model_state` have the identical parameter values.

Evaluation

Once we have trained a model, it is time to evaluate it on a held-out test set. As our dataset consist of randomly generated data points, we need to first create a test set with a corresponding data loader.

[55]:
```
test_dataset = XORDataset(size=500, seed=123)
# drop_last -> Don't drop the last batch although it is smaller than 128
test_data_loader = data.DataLoader(test_dataset,
                                   batch_size=128,
                                   shuffle=False,
                                   drop_last=False,
                                   collate_fn=numpy_collate)
```

We can use our `eval_step` function to efficiently evaluate our model:

[56]:
```
def eval_model(state, data_loader):
    all_accs, batch_sizes = [], []
    for batch in data_loader:
        batch_acc = eval_step(state, batch)
        all_accs.append(batch_acc)
        batch_sizes.append(batch[0].shape[0])
    # Weighted average since some batches might be smaller
    acc = sum([a*b for a,b in zip(all_accs, batch_sizes)]) / sum(batch_sizes)
    print(f"Accuracy of the model: {100.0*acc:4.2f}%")
```

[57]:
```
eval_model(trained_model_state, test_data_loader)
```

```
Accuracy of the model: 100.00%
```

If we trained our model correctly, we should see a score close to 100% accuracy. However, this is only possible because of our simple task, and unfortunately, we usually don't get such high scores on test sets of more complex tasks.

Binding model parameters

Once we have trained the model, we might want to do multiple application of the same model and parameters. It can get a bit annoying to always write `model.apply(params, ...)` and keep track of the model and parameters separately. To prevent this, Flax's module can be bound to specific parameters to simplify our application. Specifically, we can bind the instance `model` of our `SimpleClassifier` class to our trained parameter as follows:

[58]:
```
trained_model = model.bind(trained_model_state.params)
```

With the model being binded to the parameters, we can use it as we would any PyTorch module. For instance, to apply it to an input array, we can simply run:

[59]:
```
data_input, labels = next(iter(data_loader))
out = trained_model(data_input)  # No explicit parameter passing necessary anymore
out.shape
```

[59]:
```
(8, 1)
```

This can simplify the analysis of models, and provide a more familiar interface to PyTorch users.

Visualizing classification boundaries

To visualize what our model has learned, we can perform a prediction for every data point in a range of $[-0.5, 1.5]$, and visualize the predicted class as in the sample figure at the beginning of this section. This shows where the model has created decision boundaries, and which points would be classified as 0, and which as 1. We therefore get a background image out of blue (class 0) and orange (class 1). The spots where the model is uncertain we will see a blurry overlap. The specific code is less relevant compared to the output figure which should hopefully show us a clear separation of classes:

[60]:
```
def visualize_classification(model, data, label):
    data_0 = data[label == 0]
    data_1 = data[label == 1]

    fig = plt.figure(figsize=(4,4), dpi=500)
    plt.scatter(data_0[:,0], data_0[:,1], edgecolor="#333", label="Class 0")
    plt.scatter(data_1[:,0], data_1[:,1], edgecolor="#333", label="Class 1")
    plt.title("Dataset samples")
    plt.ylabel(r"$x_2$")
    plt.xlabel(r"$x_1$")
    plt.legend()

    # Let's make use of a lot of operations we have learned above
    c0 = np.array(to_rgba("C0"))
    c1 = np.array(to_rgba("C1"))
    x1 = jnp.arange(-0.5, 1.5, step=0.01)
    x2 = jnp.arange(-0.5, 1.5, step=0.01)
    xx1, xx2 = jnp.meshgrid(x1, x2, indexing='ij')  # Meshgrid function as in numpy
    model_inputs = np.stack([xx1, xx2], axis=-1)
    logits = model(model_inputs)
    preds = nn.sigmoid(logits)
    output_image = (1 - preds) * c0[None,None] + preds * c1[None,None]  # Specifying
↪"None" in a dimension creates a new one
    output_image = jax.device_get(output_image)  # Convert to numpy array. This only␣
↪works for tensors on CPU, hence first push to CPU
```

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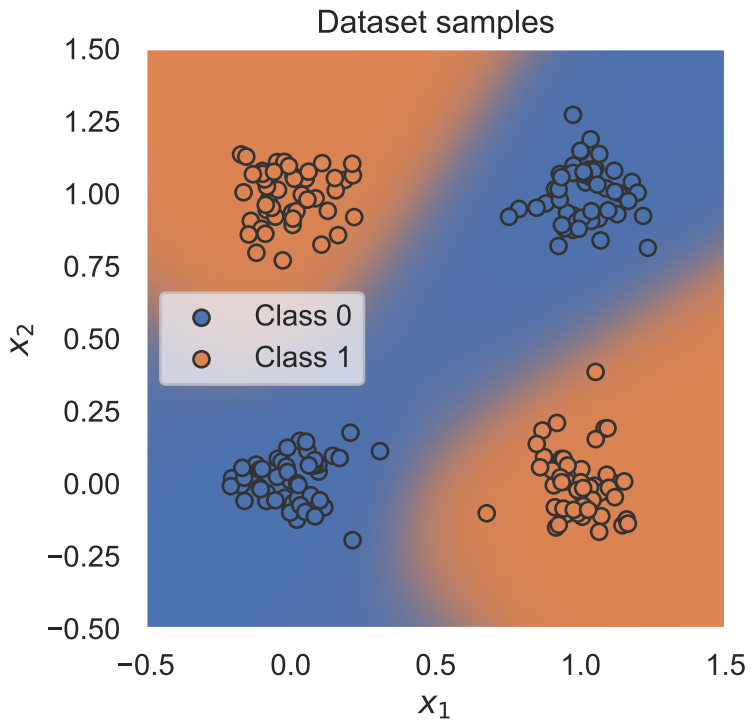
```
    plt.imshow(output_image, origin='lower', extent=(-0.5, 1.5, -0.5, 1.5))
    plt.grid(False)
    return fig

_ = visualize_classification(trained_model, dataset.data, dataset.label)
plt.show()
```



The decision boundaries might not look exactly as in the figure in the preamble of this section, since this has been created with the PyTorch version of the tutorial. Nevertheless, the result on the accuracy metric should be the approximately the same.

Conclusion

This concludes our tutorial on training a neural network with JAX. While the functional programming perspective of JAX may seem very different to PyTorch at first, it enables a considerable speedup in training, not only for tiny models like here. If you are interested in seeing more practical use cases of JAX, we recommend checking out our other JAX Tutorials, such as:

- Tutorial 5 (JAX): Inception, ResNet and DenseNet gives an intro to training convolutional classifiers on CIFAR10;
- Tutorial 6 (JAX): Transformers and Multi-Head Attention builds a Transformer from scratch with Flax;
- Tutorial 7 (JAX): Graph Neural Networks implements basic Graph Neural Network layers;
- Tutorial 9 (JAX): Deep Autoencoders shows how to train autoencoders on CIFAR10;
- Tutorial 11 (JAX): Normalizing Flows for image modeling discusses Normalizing Flows as generative model on images;
- Tutorial 15 (JAX): Vision Transformers trains a Transformer on image classification for CIFAR10.

4.30.4 The Fancy Bits

After reading this tutorial, you might wonder why we left out some key advertisement points of JAX: automatic vectorization, easy parallelization on multiple accelerators, etc. The reason why we did not include them in our previous discuss is that for building simple networks, and actual most models in our tutorials, you do not really need these methods. However, since they can be handy at some times, for instance, if you have access to a large cluster or are faced with functions that are annoying to vectorize, we review them here in a separate section: the Fancy Bits of JAX (the title is inspired by JAX's tutorial JAX - The Sharp Bits).

Automatic Vectorization with vmap

In machine learning, we often vectorize methods to efficiently process multiple inputs or batch elements at the same time. Usually, we have to write the code ourselves to support additional dimensions to vectorize over. However, since JAX can already transform functions to run efficiently on accelerators or calculate gradients, it can also automatically vectorize a function. For instance, let's consider a simple linear layer where we write a function for a single input `x` of shape `[c_in]`, a weight matrix `[c_in, c_out]`, and a bias vector `[c_out]`:

[61]:
```
def simple_linear(x, w, b):
    # We could already vectorize this function with matmul, but as an example,
    # let us use a non-vectorized function with same output
    return (x[:,None] * w).sum(axis=0) + b
```

[62]:
```
# Example inputs
rng, x_rng, w_rng, b_rng = jax.random.split(rng, 4)
x_in = jax.random.normal(x_rng, (4,))
w_in = jax.random.normal(w_rng, (4, 3))
b_in = jax.random.normal(b_rng, (3,))

simple_linear(x_in, w_in, b_in)
```

[62]:
```
DeviceArray([-0.5393317,  1.4906642,  0.7108946], dtype=float32)
```

Now, we would like the function to support a batch dimension on `x`, i.e. `[batch, c_in]`. Our naive implementation above does not support this, since we specialized the axis we sum over. So, let's make JAX do the work for us and vectorize the function by using `jax.vmap`:

[63]:
```
vectorized_linear = jax.vmap(simple_linear,
                             in_axes=(0, None, None),  # Which axes to vectorize for␣
↪each input
                             out_axes=0  # Which axes to map to in the output
                            )
```

Specifying `None` for the in-axes of the input arguments `w` and `b` means that we do not want to vectorize any of their input dimensions. With this vmap specification, the function `vectorized_linear` now supports an extra batch dimension in `x`! Let's try it out:

[64]:
```
x_vec_in = jnp.stack([x_in]*5, axis=0)

vectorized_linear(x_vec_in, w_in, b_in)
```

[64]:
```
DeviceArray([[-0.5393317,  1.4906642,  0.7108946],
             [-0.5393317,  1.4906642,  0.7108946],
             [-0.5393317,  1.4906642,  0.7108946],
```

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```
             [-0.5393317,  1.4906642,  0.7108946],
             [-0.5393317,  1.4906642,  0.7108946]], dtype=float32)
```

The new function indeed vectorized our code, calculating N applications of the weights and bias to the input. We can also vectorize the code to run multiple inputs `x` on multiple weights `w` and biases `b` by changing the input argument `in_axes` to `(0, 0, 0)`, or simply `0`. Morever, we can again stack multiple function transformations, such as jitting a vectorized function. Further details on `jax.vmap` can be found in this tutorial and its documentation.

Parallel evaluation with pmap

`jax.vmap` vectorizes a function on a single accelerator. But what if we have multiple GPUs or TPUs available? In PyTorch, we can parallelize a model over multiple GPUs using `nn.DistributedDataParallel`. In JAX, this is yet another function transformation: `jax.pmap`. Similar to `jax.vmap`, we can specify over which axes each input should be parallelized. In a network training, we usually want to parallelize over an extra batch dimension in the data, while the parameters are identical for all devices. For more details on `jax.pmap`, see Parallel Evaluation in JAX.

Working with PyTrees

Network parameters in Flax are stored in a PyTree. We have visited them before, but what we haven't discuss yet is JAX's utilities to operate on pytrees! One common application is to obtain a list of all parameters in the network. This corresponds to extracting all leafs from a PyTree, for which JAX provides the function `jax.tree_leaves`:

[65]:
```
parameters = jax.tree_leaves(model_state.params)
print('We have parameters with the following shapes:', ', '.join([str(p.shape) for p in␣
↪parameters]))
print('Overall parameter count:', sum([np.prod(p.shape) for p in parameters]))
```

```
We have parameters with the following shapes: (8,), (2, 8), (1,), (8, 1)
Overall parameter count: 33
```

We can also create new PyTrees that are the result of applying a function on all elements in the tree using `jax.tree_map`. For instance, let's obtain a PyTree with all parameter shapes:

[66]:
```
jax.tree_map(lambda p: p.shape, model_state.params)
```

[66]:
```
FrozenDict({
    params: {
        linear1: {
            bias: (8,),
            kernel: (2, 8),
        },
        linear2: {
            bias: (1,),
            kernel: (8, 1),
        },
    },
})
```

The nodes of PyTrees do not necessarily need to be NumPy or JAX arrays, but can be arbitrary objects. Overall, PyTrees provide a simple, structured representation of data useful in many applications. More details can be found in JAX's Tutorial Working with PyTrees.

4.30.5 The Sharp Bits

Since JAX functions need to be written with certain constraints, there are situations where this can get annoying or difficult. A great overview of those, why they are needed, and most importantly, what to do about them, can be found in the original JAX tutorial JAX - The Sharp Bits . In this final section of the tutorial, we want to visit a few of those points we have not explicitly discussed yet. Furthermore, we also focus on the combination with Flax, and what can be annoying when training models.

Dynamic shapes

JAX has the great advantage of providing just-in-time compilation of functions to speed up the computation. For this, it uses its intermediate representation jaxpr, which is specialized to the shapes of the input arguments. However, this also means that a jitted function is specialized to a certain shape, and running the jitted function with a different input shape requires recompiling the function. For instance, consider the following simple function:

[67]:
```
def my_function(x):
    print('Running the function with shape', x.shape)
    return x.mean()

jitted_function = jax.jit(my_function)
```

The print statement is only executed once when the function is compiled, and for all consecutive function calls, this print statement will be ignored since it is not part of the jaxpr representation. Let's run the function now with multiple different input shapes:

[68]:
```
for i in range(10):
    jitted_function(jnp.zeros(i+1,))
```

```
Running the function with shape (1,)
Running the function with shape (2,)
Running the function with shape (3,)
Running the function with shape (4,)
Running the function with shape (5,)
Running the function with shape (6,)
Running the function with shape (7,)
Running the function with shape (8,)
Running the function with shape (9,)
Running the function with shape (10,)
```

As we can see, the function is compiled for every different input we give it. This can become inefficient if we actually work with many different shapes. However, running the function again with one of the previous input shapes will not require another compilation:

[69]:
```
# Running the functions a second time will not print out anything since
# the functions are already jitted for the respective input shapes.
for i in range(10):
    jitted_function(jnp.zeros(i+1,))
```

If we have a very limited set of different shapes, we do not see a big performance difference. For instance, in our evaluation, the last batch size is smaller than the previous since we have a limited size of the evaluation dataset. However, for other applications, we might encounter this problem much more often: NLP and time series, and graphs. In these cases, it is recommend to pad the batches to prevent many re-compilations (see Flax's padding guide for details). We briefly review the two scenarios below.

NLP and time series

In Natural Language Processing, our data consist of sentences which greatly vary in size. Already for batching the elements, we need to apply padding, such that the shape of the batch is determined by the largest sentence in the batch. However, this largest length can vary between batches, especially when we shuffle the dataset before each epoch. In PyTorch, this is not a problem, since the dynamic computation graph allows us to stop the computation whenever we need to. In contrast, JAX would need to recompile the forward pass for every single largest sentence length, which can quickly become very expensive. Padding is needed to reduce the number of compilations, but at the same time introduces unnecessary computation. Hence, we have a tradeoff between number of compilations and extra compute per batch. In the extreme case, PyTorch may even become faster than JAX here.

Graphs

Similar to NLP, graphs can vary in their size. Often, graphs differ in their number of nodes, but especially in the number of edges. Furthermore, when we start batching the graphs, the variation of node sizes and edge count considerably increases. Again, padding is needed to reduce the number of compilations, and we will revisit this topic in Tutorial 7 (TBD).

Debugging in jitted functions

During coding, we likely want to debug our model and sometimes print out intermediate values. In JAX, when jitting functions, this is not as straightforward. As we could see from the previous cells, a print statement is only executed once during compilation, and afterwards removed since it is not part of the jaxpr representation. Furthermore, there can be issues when tracking NaNs in your code (see the sharp bits tutorial), and errors like out-of-bounds indexing are silently handled on accelerators by returning -1 instead of an error (see the corresponding section in the sharp bits tutorial). However, if necessary, one can either run the unjitted version of the forward pass first, and even introduce print statements to the jitted version where needed (see here for a great explanation). Still, it is not as straight-forward as in PyTorch, for example.

Modules with different train and evaluation functions

Certain deep learning layers have different behaviors under evaluation than during training. For instance, dropout randomly masks out a number of neurons during training, but leaves the graph untouched during evaluation. In PyTorch, we can easily switch between the two states via `model.train()` and `model.eval()` without having to manually specify it in the dropout module instance. However, in JAX, we do not have global states in the model, and thus need to pass this information to every module in the forward pass that may need it. In our example above, this was not needed, since the forward pass of the simple classifier is identical during training and evaluation. Alternatively, since the parameters are not bound to a specific model during training, one can also create two models: one training model, and one evaluation model. Nonetheless, one still needs to add the information to every module with changing behaviors, which adds a certain overhead compared to PyTorch. We will discuss two common modules with such behaviors below: dropout and BatchNorm.

Dropout

In Flax, Dropout has an argument `deterministic` which turns off dropout when True, and otherwise applies the random masking as intended during training. This deterministic switch can either be defined in the constructor, or in every forward call. Furthermore, dropout has the special case that it is a random operation during training, meaning that it also needs a PRNG state. Fortunately, we do not have to pass this state in every PRNG state, but instead, can simply pass `rngs={'dropout': dropout_rng}` with `dropout_rng` being the PRNG state. For an example, see our Tutorial 6 on Transformers in which we use dropout in several occasions.

BatchNorm

Batch Normalization transforms the input in two different ways. During training, we determine the mean and standard deviation of the input, and normalize the data with it to a zero mean and standard deviation of one. During evaluation, on the other hand, we take a running statistic over the previous several batches, and use those to estimate the mean and standard deviation. This is necessary to keep the evaluation stable and invariant to the specific batches we choose. Still, in the Flax module (documentation), we need to give the argument `use_running_average` (bool) to either the constructor or each forward pass. Furthermore, BatchNorm has a specific property we haven't discussed yet and is a bit tricky in JAX: keeping track of the running average. During every forward pass, we want to record the mean and standard deviation of the current batch, and update our current average over the past batches. However, this requires changing an input tensor, and returning this changed tensor again. In Flax, we can do this by defining the batch statistics as a mutable tensor. Check out our Tutorial 5 to see BatchNorm being used in practice with Flax.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.31 Tutorial 3 (JAX): Activation Functions

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code. We do not provide speed comparisons for this notebook since they tend to be uninformative for such small networks and potentially bottlenecked by other factors.

In this tutorial, we will take a closer look at (popular) activation functions and investigate their effect on optimization properties in neural networks. Activation functions are a crucial part of deep learning models as they add the non-linearity to neural networks. There is a great variety of activation functions in the literature, and some are more beneficial than others. The goal of this tutorial is to show the importance of choosing a good activation function (and how to do so), and what problems might occur if we don't.

Before we start, we import our standard libraries and set up basic functions:

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
from typing import Any, Sequence
import pickle
from copy import deepcopy

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import seaborn as sns
sns.set()

## Progress bar
from tqdm.auto import tqdm

## JAX
import jax
import jax.numpy as jnp
from jax import random

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/chex/_src/pytypes.py:37:␣
↪FutureWarning: jax.tree_structure is deprecated, and will be removed in a future␣
↪release. Use jax.tree_util.tree_structure instead.
  PyTreeDef = type(jax.tree_structure(None))
WARNING:absl:GlobalAsyncCheckpointManager is not imported correctly. Checkpointing of␣
↪GlobalDeviceArrays will not be available.To use the feature, install tensorstore.
```

In contrast to PyTorch, we do not have to set the seed as a global variable since we do not allow for functions with side effects. Instead, we explicitly define a PRNG key whenever needed for random operations like network initializations.

Additionally, the following cell defines two paths: `DATASET_PATH` and `CHECKPOINT_PATH`. The dataset path is the directory where we will download datasets used in the notebooks. It is recommended to store all datasets from PyTorch in one joined directory to prevent duplicate downloads. The checkpoint path is the directory where we will store trained model weights and additional files. The needed files will be automatically downloaded. In case you are on Google Colab, it is recommended to change the directories to start from the current directory (i.e. remove `../../` for both dataset and checkpoint path).

[2]:
```
# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial3_jax"

# Verifying the device that will be used throughout this notebook
print("Device:", jax.devices()[0])
```

```
Device: gpu:0
```

The following cell downloads all pretrained models we will use in this notebook. The files are stored on a separate repository to reduce the size of the notebook repository, especially for building the documentation on ReadTheDocs.

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial3/"
# Files to download
pretrained_files = ["FashionMNIST_elu.config", "FashionMNIST_elu.tar",
                    "FashionMNIST_leakyrelu.config", "FashionMNIST_leakyrelu.tar",
                    "FashionMNIST_relu.config", "FashionMNIST_relu.tar",
                    "FashionMNIST_sigmoid.config", "FashionMNIST_sigmoid.tar",
                    "FashionMNIST_swish.config", "FashionMNIST_swish.tar",
                    "FashionMNIST_tanh.config", "FashionMNIST_tanh.tar"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please contact the author with the full output␣
↪including the following error:\n", e)
```

4.31.1 Common activation functions

As a first step, we will implement some common activation functions by ourselves. Of course, most of them can also be found in the `flax.linen` or `jax.nn` package (see the documentation for an overview). However, we'll write our own functions here for a better understanding and insights.

Every activation function will be an `nn.Module` so that we can integrate them nicely in a network. We start with implementing two of the "oldest" activation functions that are still commonly used for various tasks: sigmoid and tanh. Both the sigmoid and tanh activation can be also found as JAX functions (`nn.sigmoid`, `nn.tanh`). Note that since all modules are essentially functions, you can directly use functions in `nn.Sequential` (e.g. `nn.Sequential([nn.Dense(8), nn.sigmoid, nn.Dense(1)])`. Still, for a better understanding, we implement them by hand:

[4]:
```
##############################

class Sigmoid(nn.Module):

    def __call__(self, x):
        return 1 / (1 + jnp.exp(-x))

##############################

class Tanh(nn.Module):

    def __call__(self, x):
        x_exp, neg_x_exp = jnp.exp(x), jnp.exp(-x)
        return (x_exp - neg_x_exp) / (x_exp + neg_x_exp)

##############################
```

Another popular activation function that has allowed the training of deeper networks, is the Rectified Linear Unit (ReLU). Despite its simplicity of being a piecewise linear function, ReLU has one major benefit compared to sigmoid and tanh: a strong, stable gradient for a large range of values. Based on this idea, a lot of variations of ReLU have been proposed, of which we will implement the following three: LeakyReLU, ELU, and Swish. LeakyReLU replaces the zero settings in the negative part with a smaller slope to allow gradients to flow also in this part of the input. Similarly, ELU replaces the negative part with an exponential decay. The third, most recently proposed activation function is Swish, which is actually the result of a large experiment with the purpose of finding the "optimal" activation function. Compared to the other activation functions, Swish is both smooth and non-monotonic (i.e. contains a change of sign in the gradient). This has been shown to prevent dead neurons as in standard ReLU activation, especially for deep networks. If interested, a more detailed discussion of the benefits of Swish can be found in this paper [1].

Let's implement the four activation functions below:

[5]:
```
##############################

class ReLU(nn.Module):

    def __call__(self, x):
        return jnp.maximum(x, 0)

##############################

class LeakyReLU(nn.Module):
    alpha : float = 0.1

    def __call__(self, x):
```

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```
        return jnp.where(x > 0, x, self.alpha * x)

##############################

class ELU(nn.Module):

    def __call__(self, x):
        return jnp.where(x > 0, x, jnp.exp(x)-1)

##############################

class Swish(nn.Module):

    def __call__(self, x):
        return x * nn.sigmoid(x)

##############################
```

For later usage, we summarize all our activation functions in a dictionary mapping the name to the class object. In case you implement a new activation function by yourself, add it here to include it in future comparisons as well:

[6]:
```
act_fn_by_name = {
    "sigmoid": Sigmoid,
    "tanh": Tanh,
    "relu": ReLU,
    "leakyrelu": LeakyReLU,
    "elu": ELU,
    "swish": Swish
}
```

Visualizing activation functions

To get an idea of what each activation function actually does, we will visualize them in the following. Since modules are functions in disguise, we can do this by applying JAX's gradient transformation `jax.grad`. However, note that we want to take the gradients for multiple inputs independently and the gradient transformation requires the output of the forward pass to be a single scalar. We can implement this by simply summing the outputs of the activation function, since a sum distributes the gradients equally to all its inputs.

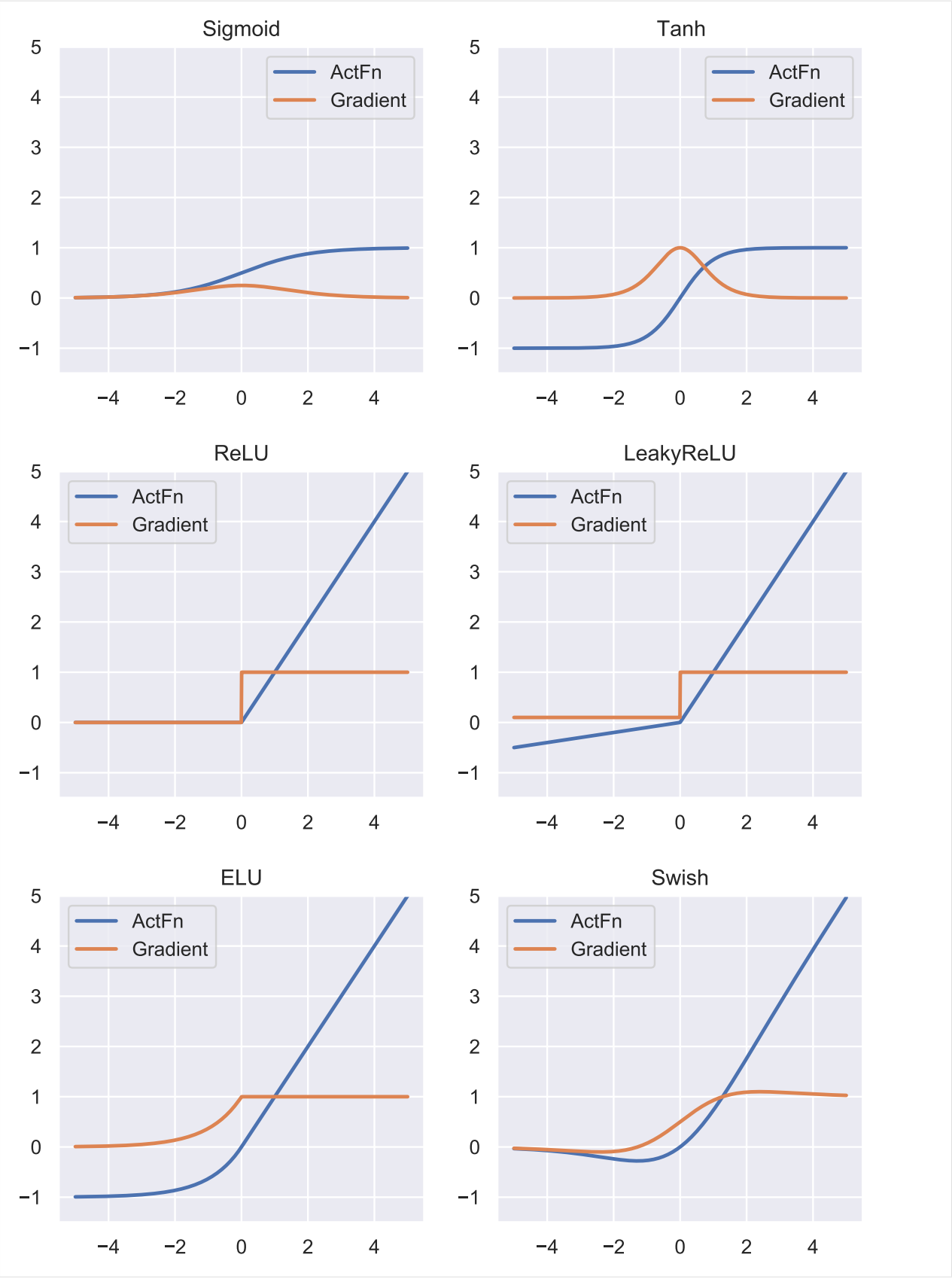
[7]:
```
def get_grads(act_fn, x):
    """
    Computes the gradients of an activation function at specified positions.

    Inputs:
        act_fn - An module or function of the forward pass of the activation function.
        x - 1D input array.
    Output:
        An array with the same size of x containing the gradients of act_fn at x.
    """
    return jax.vmap(jax.grad(act_fn))(x)
```

Now we can visualize all our activation functions including their gradients:

[8]:
```
def vis_act_fn(act_fn, ax, x):
    # Run activation function
    y = act_fn(x)
    y_grads = get_grads(act_fn, x)
    # Push x, y and gradients back to cpu for plotting
    # x, y, y_grads = x.cpu().numpy(), y.cpu().numpy(), y_grads.cpu().numpy()
    ## Plotting
    ax.plot(x, y, linewidth=2, label="ActFn")
    ax.plot(x, y_grads, linewidth=2, label="Gradient")
    ax.set_title(act_fn.__class__.__name__)
    ax.legend()
    ax.set_ylim(-1.5, x.max())

# Add activation functions if wanted
act_fns = [act_fn() for act_fn in act_fn_by_name.values()]
x = np.linspace(-5, 5, 1000) # Range on which we want to visualize the activation␣
↪functions
## Plotting
rows = math.ceil(len(act_fns)/2.0)
fig, ax = plt.subplots(rows, 2, figsize=(8, rows*4))
for i, act_fn in enumerate(act_fns):
    vis_act_fn(act_fn, ax[divmod(i,2)], x)
fig.subplots_adjust(hspace=0.3)
plt.show()
```


Sigmoid
Tanh
ReLU
LeakyReLU
ELU
Swish
ActFn
Gradient
5
4
3
2
1
0
−1
−4
−2
0
2
4

4.31.2 Analysing the effect of activation functions

After implementing and visualizing the activation functions, we are aiming to gain insights into their effect. We do this by using a simple neural network trained on FashionMNIST and examine various aspects of the model, including the performance and gradient flow.

Setup

Firstly, let's set up a neural network. The chosen network views the images as 1D tensors and pushes them through a sequence of linear layers and a specified activation function. Feel free to experiment with other network architectures. We explicitly set the initialization for the weights and biases to stay close to the PyTorch implementation of the Tutorial. As we will see in Tutorial 4, the initialization has a considerable influence on which networks may be trainable with which activation functions.

[9]:
```
# To keep the results close to the PyTorch tutorial, we use the same init function as␣
↪PyTorch
# which is uniform(-1/sqrt(in_features), 1/sqrt(in_features)) - similar to He et al./
↪kaiming
# The default for Flax is lecun_normal (i.e., half the variance of He) and zeros for␣
↪bias.
init_func = lambda x: (lambda rng, shape, dtype: random.uniform(rng,
                                                                shape=shape,
                                                                minval=-1/np.sqrt(x.
↪shape[1]),
                                                                maxval=1/np.sqrt(x.
↪shape[1]),
                                                                dtype=dtype))

# Network
class BaseNetwork(nn.Module):
    act_fn : nn.Module
    num_classes : int = 10
    hidden_sizes : Sequence = (512, 256, 256, 128)

    @nn.compact
    def __call__(self, x, return_activations=False):
        x = x.reshape(x.shape[0], -1) # Reshape images to a flat vector
        # We collect all activations throughout the network for later visualizations
        # Remember that in jitted functions, unused tensors will anyways be removed.
        activations = []
        for hd in self.hidden_sizes:
            x = nn.Dense(hd,
                         kernel_init=init_func(x),
                         bias_init=init_func(x))(x)
            activations.append(x)
            x = self.act_fn(x)
            activations.append(x)
        x = nn.Dense(self.num_classes,
                     kernel_init=init_func(x),
                     bias_init=init_func(x))(x)
        return x if not return_activations else (x, activations)
```

We also add functions for loading and saving the model. The hyperparameters are stored in a configuration file (simple

json file):

[10]:
```
def _get_config_file(model_path, model_name):
    # Name of the file for storing hyperparameter details
    return os.path.join(model_path, model_name + ".config")

def _get_model_file(model_path, model_name):
    # Name of the file for storing network parameters
    return os.path.join(model_path, model_name + ".tar")

def load_model(model_path, model_name, state=None):
    """
    Loads a saved model from disk.

    Inputs:
        model_path - Path of the checkpoint directory
        model_name - Name of the model (str)
        state - (Optional) If given, the parameters are loaded into this training state. Otherwise,
                a new one is created alongside a network architecture.
    """
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_file(model_path, model_name)
    assert os.path.isfile(config_file), f"Could not find the config file \"{config_file}\". Are you sure this is the correct path and you have your model config stored here?"
    assert os.path.isfile(model_file), f"Could not find the model file \"{model_file}\". Are you sure this is the correct path and you have your model stored here?"
    with open(config_file, "r") as f:
        config_dict = json.load(f)
    if state is None:
        act_fn_name = config_dict["act_fn"].pop("name").lower()
        act_fn = act_fn_by_name[act_fn_name](**config_dict.pop("act_fn"))
        net = BaseNetwork(act_fn=act_fn, **config_dict)
        state = train_state.TrainState(step=0,
                                       params=None,
                                       apply_fn=net.apply,
                                       tx=None,
                                       opt_state=None)
    else:
        net = None
    # You can also use flax's checkpoint package. To show an alternative,
    # you can instead load the parameters simply from a pickle file.
    with open(model_file, 'rb') as f:
        params = pickle.load(f)
    state = state.replace(params=params)
    return state, net

def save_model(model, params, model_path, model_name):
    """
    Given a model, we save the parameters and hyperparameters.

    Inputs:
        model - Network object without parameters
```

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```
        params - Parameters to save of the model
        model_path - Path of the checkpoint directory
        model_name - Name of the model (str)
    """
    config_dict = {
        'num_classes': model.num_classes,
        'hidden_sizes': model.hidden_sizes,
        'act_fn': {'name': model.act_fn.__class__.__name__.lower()}
    }
    if hasattr(model.act_fn, 'alpha'):
        config_dict['act_fn']['alpha'] = model.act_fn.alpha
    os.makedirs(model_path, exist_ok=True)
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_
↪file(model_path, model_name)
    with open(config_file, "w") as f:
        json.dump(config_dict, f)
    # You can also use flax's checkpoint package. To show an alternative,
    # you can instead save the parameters simply in a pickle file.
    with open(model_file, 'wb') as f:
        pickle.dump(params, f)
```

We also set up the dataset we want to train it on, namely FashionMNIST. FashionMNIST is a more complex version of MNIST and contains black-and-white images of clothes instead of digits. The 10 classes include trousers, coats, shoes, bags and more. To load this dataset, we will make use of yet another PyTorch package, namely `torchvision` (documentation). The `torchvision` package consists of popular datasets, model architectures, and common image transformations for computer vision. We will use the package for many of the notebooks in this course to simplify our dataset handling.

Let's load the dataset below, and visualize a few images to get an impression of the data.

[11]:
```
import torch
import torch.utils.data as data
import torchvision
from torchvision.datasets import FashionMNIST
from torchvision import transforms

# Transformations applied on each image => bring them into a numpy array and normalize␣
↪between -1 and 1
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    img = (img / 255. - 0.5) / 0.5
    return img

# We need to stack the batch elements as numpy arrays
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)
```

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```
# Loading the training dataset. We need to split it into a training and validation part
train_dataset = FashionMNIST(root=DATASET_PATH,
                             train=True,
                             transform=image_to_numpy,
                             download=True)
train_set, val_set = torch.utils.data.random_split(train_dataset,
                                                   [50000, 10000],
                                                   generator=torch.Generator().manual_
↪seed(42))

# Loading the test set
test_set = FashionMNIST(root=DATASET_PATH,
                        train=False,
                        transform=image_to_numpy,
                        download=True)

# We define a set of data loaders that we can use for various purposes later.
# Note that for actually training a model, we will use different data loaders
# with a lower batch size.
train_loader = data.DataLoader(train_set,
                               batch_size=1024,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate)
val_loader   = data.DataLoader(val_set,
                               batch_size=1024,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate)
test_loader  = data.DataLoader(test_set,
                               batch_size=1024,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate)
```

[12]:
```
exmp_imgs = [train_set[i][0] for i in range(16)]
# Organize the images into a grid for nicer visualization
img_grid = torchvision.utils.make_grid(torch.from_numpy(np.stack(exmp_imgs, axis=0))[:,
↪None],
                                       nrow=4,
                                       normalize=True,
                                       pad_value=0.5)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("FashionMNIST examples")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

Visualizing the gradient flow after initialization

As mentioned previously, one important aspect of activation functions is how they propagate gradients through the network. Imagine we have a very deep neural network with more than 50 layers. The gradients for the input layer, i.e. the very first layer, have passed >50 times the activation function, but we still want them to be of a reasonable size. If the gradient through the activation function is (in expectation) considerably smaller than 1, our gradients will vanish until they reach the input layer. If the gradient through the activation function is larger than 1, the gradients exponentially increase and might explode.

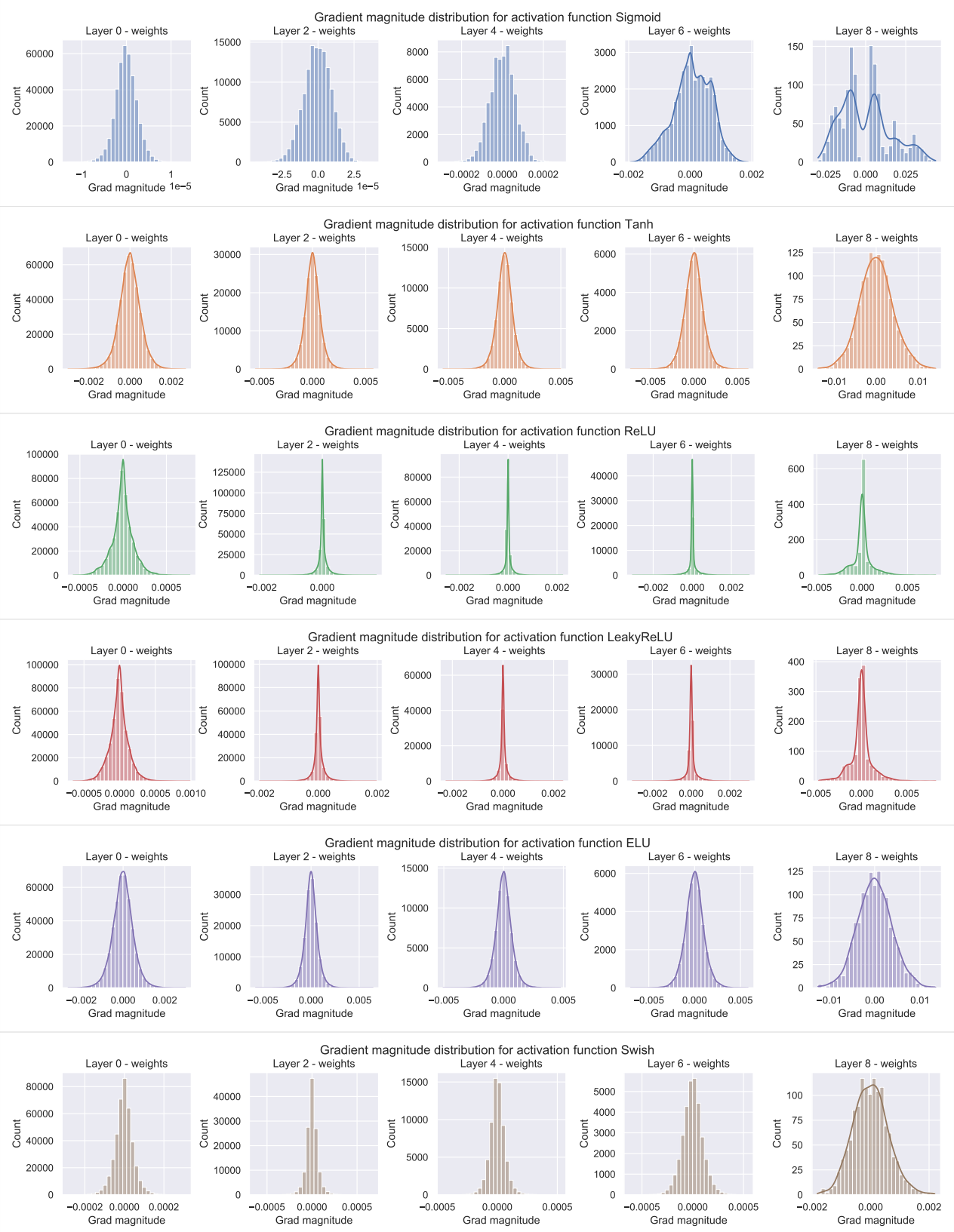
To get a feeling of how every activation function influences the gradients, we can look at a freshly initialized network and measure the gradients for each parameter for a batch of 256 images:

[13]:
```
small_loader = data.DataLoader(train_set, batch_size=256, shuffle=False, collate_
↪fn=numpy_collate)
exmp_batch = next(iter(small_loader))
```

[14]:
```
def visualize_gradients(net, params, color="C0"):
    """
    Inputs:
        net - Object of class BaseNetwork
        color - Color in which we want to visualize the histogram (for easier separation␣
↪of activation functions)
    """
    # Pass one batch through the network, and calculate the gradients for the weights
    def loss_func(p):
        imgs, labels = exmp_batch
        logits = net.apply(p, imgs)
        loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
        return loss
    grads = jax.grad(loss_func)(params)
    grads = jax.device_get(grads)
    # We limit our visualization to the weight parameters and exclude the bias to reduce␣
↪the number of plots
    grads = jax.tree_util.tree_leaves(grads)
    grads = [g.reshape(-1) for g in grads if len(g.shape) > 1]

    ## Plotting
    columns = len(grads)
    fig, ax = plt.subplots(1, columns, figsize=(columns*3.5, 2.5))
    fig_index = 0
    for g_idx, g in enumerate(grads):
        key = f'Layer {g_idx * 2} - weights'
        key_ax = ax[g_idx%columns]
        sns.histplot(data=g, bins=30, ax=key_ax, color=color, kde=True)
        key_ax.set_title(str(key))
        key_ax.set_xlabel("Grad magnitude")
    fig.suptitle(f"Gradient magnitude distribution for activation function {net.act_fn.__
↪class__.__name__}", fontsize=14, y=1.05)
    fig.subplots_adjust(wspace=0.45)
    plt.show()
    plt.close()
```

[15]:
```
# Seaborn prints warnings if histogram has small values. We can ignore them for now
import warnings
warnings.filterwarnings('ignore')
## Create a plot for every activation function
for i, act_fn_name in enumerate(act_fn_by_name):
    act_fn = act_fn_by_name[act_fn_name]()
    net_actfn = BaseNetwork(act_fn=act_fn)
    params = net_actfn.init(random.PRNGKey(0), exmp_batch[0])
    visualize_gradients(net_actfn, params, color=f"C{i}")
```



The sigmoid activation function shows a clearly undesirable behavior. While the gradients for the output layer are very

large with up to 0.1, the input layer has the lowest gradient norm across all activation functions with only 1e-5. This is due to its small maximum gradient of 1/4, and finding a suitable learning rate across all layers is not possible in this setup. All the other activation functions show to have similar gradient norms across all layers. Interestingly, the ReLU activation has a spike around 0 which is caused by its zero-part on the left, and dead neurons (we will take a closer look at this later on).

Note that additionally to the activation, the initialization of the weight parameters can be crucial. By default, PyTorch uses the Kaiming initialization for linear layers optimized for ReLU activations. In Tutorial 4, we will take a closer look at initialization, but assume for now that the Kaiming initialization works for all activation functions reasonably well.

Training a model

Next, we want to train our model with different activation functions on FashionMNIST and compare the gained performance. All in all, our final goal is to achieve the best possible performance on a dataset of our choice. First, let's write the training and evaluation step that we can compile just-in-time (`jax.jit`) for efficiency:

[16]:
```
def calculate_loss(params, apply_fn, batch):
    imgs, labels = batch
    logits = apply_fn(params, imgs)
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
    acc = (labels == logits.argmax(axis=-1)).mean()
    return loss, acc

@jax.jit
def train_step(state, batch):
    grad_fn = jax.value_and_grad(calculate_loss,
                                 has_aux=True)
    (_, acc), grads = grad_fn(state.params, state.apply_fn, batch)
    state = state.apply_gradients(grads=grads)
    return state, acc

@jax.jit
def eval_step(state, batch):
    _, acc = calculate_loss(state.params, state.apply_fn, batch)
    return acc
```

Using these functions, we write a training loop in the next cell including a validation after every epoch and a final test on the best model:

[17]:
```
def train_model(net, model_name, max_epochs=50, patience=7, batch_size=256,␣
↪overwrite=False):
    """
    Train a model on the training set of FashionMNIST

    Inputs:
        net - Object of BaseNetwork
        model_name - (str) Name of the model, used for creating the checkpoint names
        max_epochs - Number of epochs we want to (maximally) train for
        patience - If the performance on the validation set has not improved for
↪#patience epochs, we stop training early
        batch_size - Size of batches used in training
        overwrite - Determines how to handle the case when there already exists a␣
↪checkpoint. If True, it will be overwritten. Otherwise, we skip training.
```

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```
    """
    file_exists = os.path.isfile(_get_model_file(CHECKPOINT_PATH, model_name))
    if file_exists and not overwrite:
        print("Model file already exists. Skipping training...")
        state = None
    else:
        if file_exists:
            print("Model file exists, but will be overwritten...")

        # Initializing parameters and training state
        params = net.init(random.PRNGKey(42), exmp_batch[0])
        state = train_state.TrainState.create(apply_fn=net.apply,
                                              params=params,
                                              tx=optax.sgd(learning_rate=1e-2,
                                                           momentum=0.9))

        # Defining data loader
        train_loader_local = data.DataLoader(train_set,
                                             batch_size=batch_size,
                                             shuffle=True,
                                             drop_last=True,
                                             collate_fn=numpy_collate,
                                             generator=torch.Generator().manual_seed(42))

        val_scores = []
        best_val_epoch = -1
        for epoch in range(max_epochs):
            ############
            # Training #
            ############
            train_acc = 0.
            for batch in tqdm(train_loader_local, desc=f"Epoch {epoch+1}", leave=False):
                state, acc = train_step(state, batch)
                train_acc += acc
            train_acc /= len(train_loader_local)

            ##############
            # Validation #
            ##############
            val_acc = test_model(state, val_loader)
            val_scores.append(val_acc)
            print(f"[Epoch {epoch+1:2d}] Training accuracy: {train_acc:05.2%},␣
↪Validation accuracy: {val_acc:4.2%}")

            if len(val_scores) == 1 or val_acc > val_scores[best_val_epoch]:
                print("\t   (New best performance, saving model...)")
                save_model(net, state.params, CHECKPOINT_PATH, model_name)
                best_val_epoch = epoch
            elif best_val_epoch <= epoch - patience:
                print(f"Early stopping due to no improvement over the last {patience}␣
↪epochs")
                break
```

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```
        # Plot a curve of the validation accuracy
        plt.plot([i for i in range(1,len(val_scores)+1)], val_scores)
        plt.xlabel("Epochs")
        plt.ylabel("Validation accuracy")
        plt.title(f"Validation performance of {model_name}")
        plt.show()
        plt.close()

    state, _ = load_model(CHECKPOINT_PATH, model_name, state=state)
    test_acc = test_model(state, test_loader)
    print((f" Test accuracy: {test_acc:4.2%} ").center(50, "=")+"\n")
    return state, test_acc


def test_model(state, data_loader):
    """
    Test a model on a specified dataset.

    Inputs:
        state - Training state including parameters and model apply function.
        data_loader - DataLoader object of the dataset to test on (validation or test)
    """
    true_preds, count = 0., 0
    for batch in data_loader:
        acc = eval_step(state, batch)
        batch_size = batch[0].shape[0]
        true_preds += acc * batch_size
        count += batch_size
    test_acc = true_preds / count
    return test_acc
```

We train one model for each activation function. We recommend using the pretrained models to save time if you are running this notebook on CPU.

[18]:
```
for act_fn_name in act_fn_by_name:
    print(f"Training BaseNetwork with {act_fn_name} activation...")
    act_fn = act_fn_by_name[act_fn_name]()
    net_actfn = BaseNetwork(act_fn=act_fn)
    train_model(net_actfn, f"FashionMNIST_{act_fn_name}", overwrite=False)
```

```
Training BaseNetwork with sigmoid activation...
Model file already exists. Skipping training...
============= Test accuracy: 78.46% ==============

Training BaseNetwork with tanh activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.57% ==============

Training BaseNetwork with relu activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.65% ==============
```

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```
Training BaseNetwork with leakyrelu activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.33% ==============

Training BaseNetwork with elu activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.32% ==============

Training BaseNetwork with swish activation...
Model file already exists. Skipping training...
============= Test accuracy: 88.33% ==============
```

Surprisingly, in contrast to the PyTorch implementation, the model using the sigmoid activation function actually trains. However, when looking at the validation curve, one can see that the model stays at random performance for many epochs, before it slowly starts learning. The different learning behavior can therefore be explained by small differences in, e.g., initialization or sampled batches.

All the other activation functions gain similar performance to each other and the PyTorch implementation. To have a more accurate conclusion, we would have to train the models for multiple seeds and look at the averages. However, the "optimal" activation function also depends on many other factors (hidden sizes, number of layers, type of layers, task, dataset, optimizer, learning rate, initialization, etc.) so that a thorough grid search would not be useful in our case. In the literature, activation functions that have shown to work well with deep networks are all types of ReLU functions we experiment with here, with small gains for specific activation functions in specific networks.

Visualizing the activation distribution

After we have trained the models, we can look at the actual activation values that find inside the model. For instance, how many neurons are set to zero in ReLU? Where do we find most values in Tanh? To answer these questions, we can write a simple function which takes a trained model, applies it to a batch of images, and plots the histogram of the activations inside the network:

[19]:
```
def visualize_activations(net, color="C0"):
    activations = {}

    imgs, labels = exmp_batch
    _, activations = net(imgs, return_activations=True)

    ## Plotting
    columns = 4
    rows = math.ceil(len(activations)/columns)
    fig, ax = plt.subplots(rows, columns, figsize=(columns*2.7, rows*2.5))
    act_fn_name = net.act_fn.__class__.__name__
    for idx, activ in enumerate(activations):
        key_ax = ax[idx//columns][idx%columns]
        sns.histplot(data=activ.reshape(-1), bins=50, ax=key_ax, color=color, kde=True,␣
↪stat="density")
        key_ax.set_title(f"Layer {idx} - {'Dense' if idx%2==0 else act_fn_name}")
    fig.suptitle(f"Activation distribution for activation function {act_fn_name}",␣
↪fontsize=14)
    fig.subplots_adjust(hspace=0.4, wspace=0.4)
```

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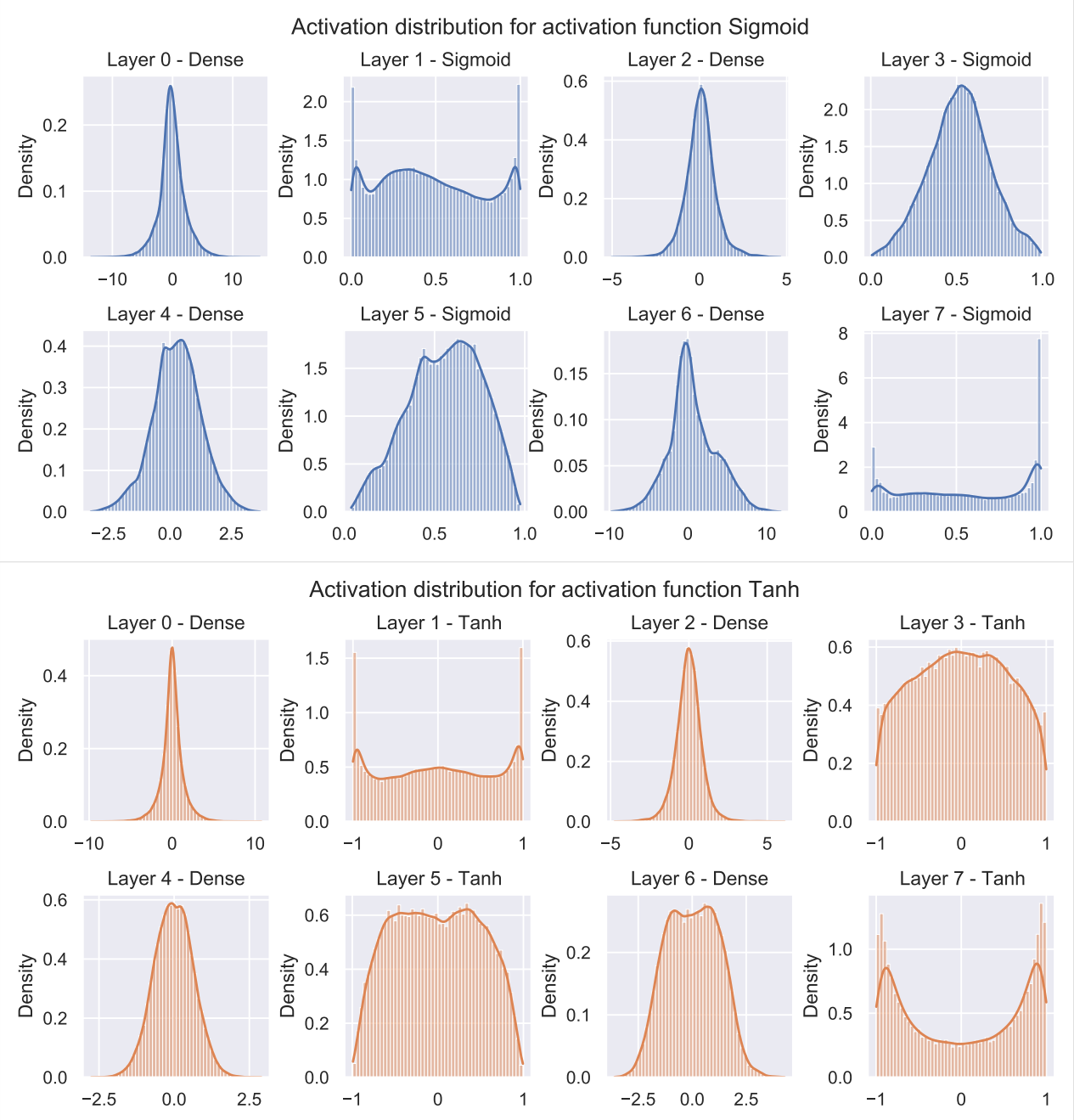
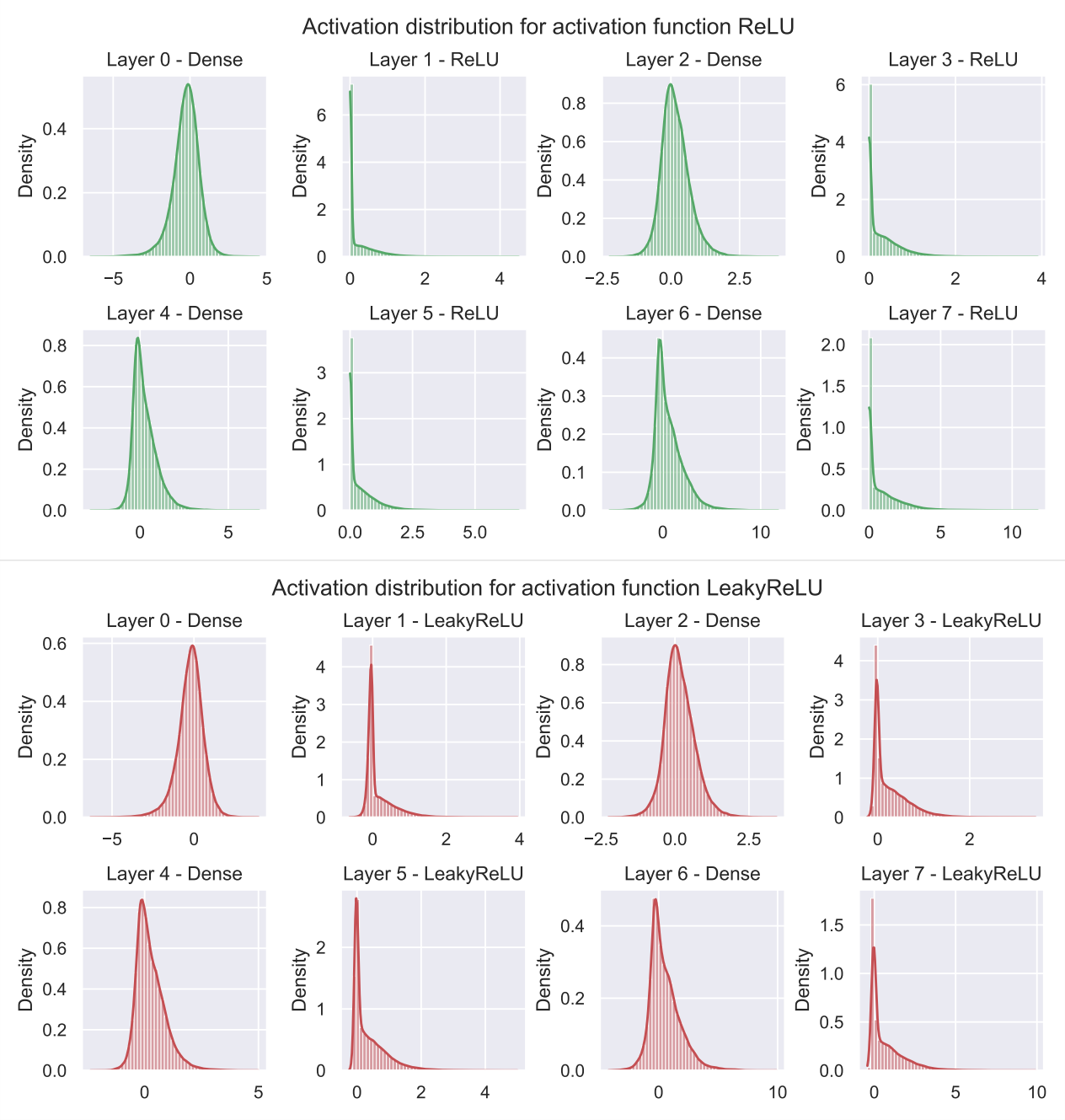
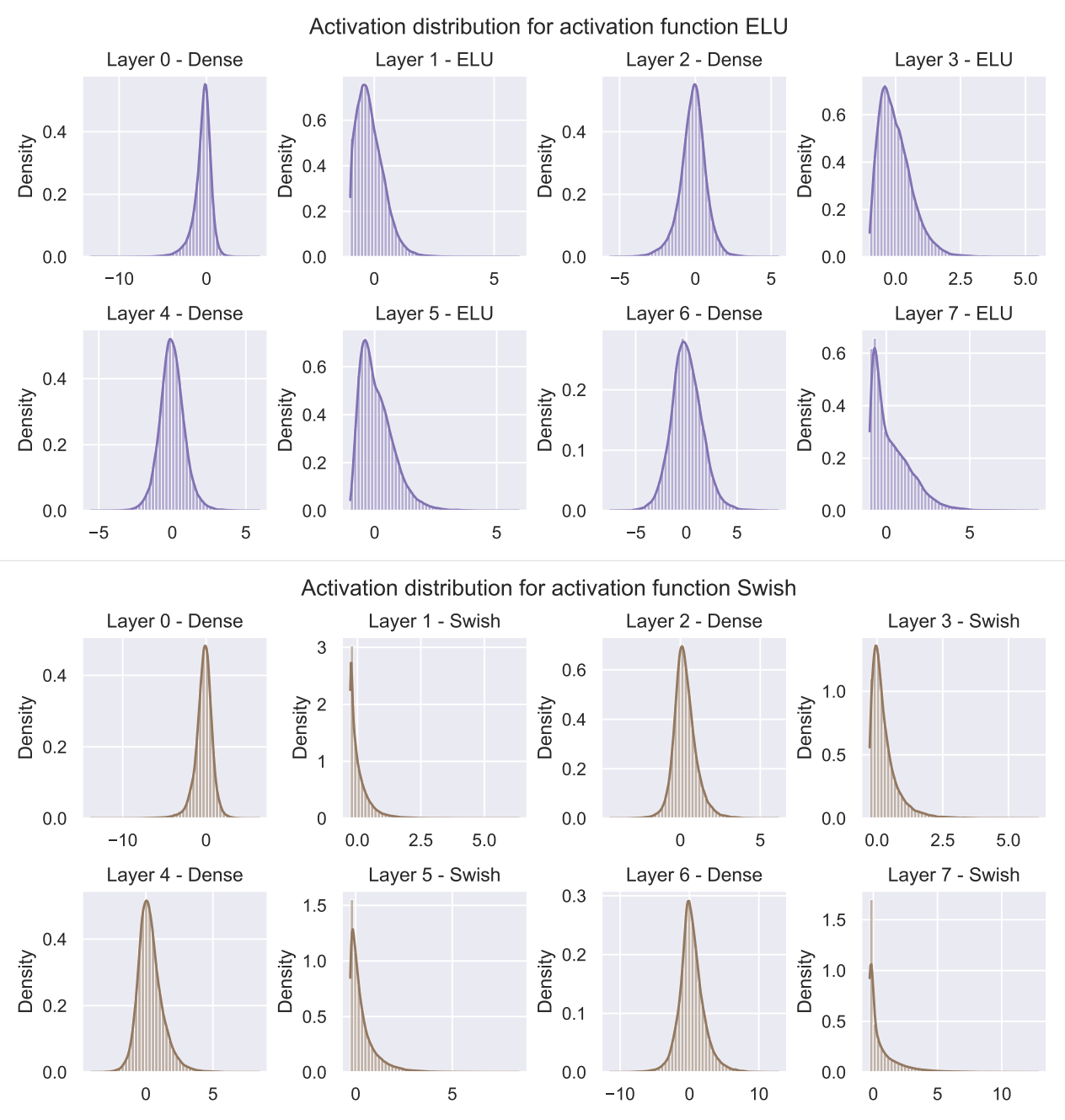
```
    plt.show()
    plt.close()
```

[20]:
```
for i, act_fn_name in enumerate(act_fn_by_name):
    state, net_actfn = load_model(model_path=CHECKPOINT_PATH, model_name=f"FashionMNIST_
↪{act_fn_name}")
    net_actfn = net_actfn.bind(state.params)
    visualize_activations(net_actfn, color=f"C{i}")
```




Activation distribution for activation function ReLU
Layer 0 - Dense
Layer 1 - ReLU
Layer 2 - Dense
Layer 3 - ReLU
Layer 4 - Dense
Layer 5 - ReLU
Layer 6 - Dense
Layer 7 - ReLU
Density
Activation distribution for activation function LeakyReLU
Layer 0 - Dense
Layer 1 - LeakyReLU
Layer 2 - Dense
Layer 3 - LeakyReLU
Layer 4 - Dense
Layer 5 - LeakyReLU
Layer 6 - Dense
Layer 7 - LeakyReLU
Density



For the model with sigmoid activation, we see a very high peak for the values 0 and 1 in the last layer. This suggests that the model is close to the saturation bounds, in which gradients do not properly flow back. Further, this is also the effect of the inconsistent gradient magnitudes we have seen before: since the layer closest to the output had the highest gradients, we see it is much stronger converged than, e.g., the second layer.

The tanh shows a more diverse behavior overall. While for the input layer we experience a larger amount of neurons to be close to -1 and 1, where the gradients are close to zero, the activations in the two consecutive layers are closer to zero. This is probably because the input layers look for specific features in the input image, and the consecutive layers combine those together. The activations for the last layer are again more biased to the extreme points because the classification layer can be seen as a weighted average of those values (the gradients push the activations to those extremes).

The ReLU has a strong peak at 0, as we initially expected. The effect of having no gradients for negative values is that the network does not have a Gaussian-like distribution after the linear layers, but a longer tail towards the positive values. The LeakyReLU shows a very similar behavior while ELU follows again a more Gaussian-like distribution. The Swish activation seems to lie in between, although it is worth noting that Swish uses significantly higher values than other activation functions (up to 15).

As all activation functions show slightly different behavior although obtaining similar performance for our simple network, it becomes apparent that the selection of the "optimal" activation function really depends on many factors, and is not the same for all possible networks.

Finding dead neurons in ReLU networks

One known drawback of the ReLU activation is the occurrence of "dead neurons", i.e. neurons with no gradient for any training input. The issue of dead neurons is that as no gradient is provided for the layer, we cannot train the parameters of this neuron in the previous layer to obtain output values besides zero. For dead neurons to happen, the output value of a specific neuron of the linear layer before the ReLU has to be negative for all input images. Considering the large number of neurons we have in a neural network, it is not unlikely for this to happen.

To get a better understanding of how much of a problem this is, and when we need to be careful, we will measure how many dead neurons different networks have. For this, we implement a function which runs the network on the whole training set and records whether a neuron is exactly 0 for all data points or not:

[21]:
```
def measure_number_dead_neurons(net, params):
    # For each neuron, we create a boolean variable initially set to 1. If it has an␣
↪activation unequals 0 at any time,
    # we set this variable to 0. After running through the whole training set, only dead␣
↪neurons will have a 1.
    neurons_dead = [
        jnp.ones(hd, dtype=jnp.dtype('bool')) for hd in net.hidden_sizes
    ] # Same shapes as hidden size in BaseNetwork

    get_activations = jax.jit(lambda inp: net.apply(params, inp, return_
↪activations=True)[1])
    for imgs, _ in tqdm(train_loader, leave=False): # Run through whole training set
        activations = get_activations(imgs)
        for layer_index, activ in enumerate(activations[1::2]):
            # Are all activations == 0 in the batch, and we did not record the opposite␣
↪in the last batches?
            neurons_dead[layer_index] = jnp.logical_and(neurons_dead[layer_index],␣
↪(activ == 0).all(axis=0))
    number_neurons_dead = [t.sum().item() for t in neurons_dead]
    print("Number of dead neurons:", number_neurons_dead)
    print("In percentage:", ", ".join([f"{num_dead / tens.shape[0]:4.2%}" for tens, num_
↪dead in zip(neurons_dead, number_neurons_dead)]))
```

First, we can measure the number of dead neurons for an untrained network:

[22]:
```
net_relu = BaseNetwork(act_fn=ReLU())
params = net_relu.init(random.PRNGKey(42), exmp_batch[0])
measure_number_dead_neurons(net_relu, params)
```

```
  0%|          | 0/49 [00:00<?, ?it/s]
```

```
Number of dead neurons: [0, 0, 3, 7]
In percentage: 0.00%, 0.00%, 1.17%, 5.47%
```

We see that only a minor amount of neurons are dead, but that they increase with the depth of the layer. However, this is not a problem for the small number of dead neurons we have as the input to later layers is changed due to updates to the weights of previous layers. Therefore, dead neurons in later layers can potentially become "alive"/active again.

How does this look like for a trained network (with the same initialization)?

[23]:
```
state, net_relu = load_model(model_path=CHECKPOINT_PATH, model_name="FashionMNIST_relu")
measure_number_dead_neurons(net_relu, state.params)
```

```
  0%|          | 0/49 [00:00<?, ?it/s]
```

```
Number of dead neurons: [0, 0, 3, 3]
In percentage: 0.00%, 0.00%, 1.17%, 2.34%
```

The number of dead neurons indeed decreased in the later layers. However, it should be noted that dead neurons are especially problematic in the input layer. As the input does not change over epochs (the training set is kept as it is), training the network cannot turn those neurons back active. Still, the input data has usually a sufficiently high standard deviation to reduce the risk of dead neurons.

Finally, we check how the number of dead neurons behaves with increasing layer depth. For instance, let's take the following 10-layer neural network:

[24]:
```
net_relu = BaseNetwork(act_fn=ReLU(), hidden_sizes=[256, 256, 256, 256, 256, 128, 128,␣
↪128, 128, 128])
params = net_relu.init(random.PRNGKey(42), exmp_batch[0])
measure_number_dead_neurons(net_relu, params)
```

```
  0%|          | 0/49 [00:00<?, ?it/s]
```

```
Number of dead neurons: [0, 1, 1, 19, 75, 53, 71, 57, 64, 69]
In percentage: 0.00%, 0.39%, 0.39%, 7.42%, 29.30%, 41.41%, 55.47%, 44.53%, 50.00%, 53.91%
```

The number of dead neurons is significantly higher than before which harms the gradient flow especially in the first iterations. For instance, more than 50% of the neurons in the last layers are dead which creates a considerable bottleneck. Hence, it is advisible to use other nonlinearities like Swish for very deep networks.

4.31.3 Conclusion

In this notebook, we have reviewed a set of six activation functions (sigmoid, tanh, ReLU, LeakyReLU, ELU, and Swish) in neural networks, and discussed how they influence the gradient distribution across layers. Sigmoid tends to fail in deep neural networks as the highest gradient it provides is 0.25 leading to vanishing gradients in early layers. All ReLU-based activation functions have shown to perform well, and besides the original ReLU, do not have the issue of dead neurons. When implementing your own neural network, it is recommended to start with a ReLU-based network and select the specific activation function based on the properties of the network.

4.31.4 References

[1] Ramachandran, Prajit, Barret Zoph, and Quoc V. Le. "Searching for activation functions." arXiv preprint arXiv:1710.05941 (2017). Paper link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.32 Tutorial 4 (JAX): Optimization and Initialization

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code. We do not provide speed comparisons for this notebook since they tend to be uninformative for such small networks and potentially bottlenecked by other factors.

In this tutorial, we will review techniques for optimization and initialization of neural networks. When increasing the depth of neural networks, there are various challenges we face. Most importantly, we need to have a stable gradient flow through the network, as otherwise, we might encounter vanishing or exploding gradients. This is why we will take a closer look at the following concepts: initialization and optimization.

In the first half of the notebook, we will review different initialization techniques, and go step by step from the simplest initialization to methods that are nowadays used in very deep networks. In the second half, we focus on optimization comparing the optimizers SGD, SGD with Momentum, and Adam.

Let's start with importing our standard libraries:

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
import copy
from typing import Any, Sequence, Callable, NamedTuple, Optional, Tuple
PyTree = Any  # Type definition for PyTree, for readability
from copy import deepcopy
import pickle

## Imports for plotting
import matplotlib.pyplot as plt
from matplotlib import cm
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import seaborn as sns
sns.set()
```

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```
## Progress bar
from tqdm.auto import tqdm

## JAX
import jax
import jax.numpy as jnp
from jax import random
from jax.tree_util import tree_map
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/chex/_src/pytypes.py:37:␣
↪FutureWarning: jax.tree_structure is deprecated, and will be removed in a future␣
↪release. Use jax.tree_util.tree_structure instead.
  PyTreeDef = type(jax.tree_structure(None))
WARNING:absl:GlobalAsyncCheckpointManager is not imported correctly. Checkpointing of␣
↪GlobalDeviceArrays will not be available.To use the feature, install tensorstore.
```

We will use the same path variables `DATASET_PATH` and `CHECKPOINT_PATH` as in Tutorial 3. Adjust the paths if necessary.

[2]:
```
# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial4_jax"

# Verifying the device that will be used throughout this notebook
print("Device:", jax.devices()[0])
```

```
Device: gpu:0
```

In the last part of the notebook, we will train models using three different optimizers. The pretrained models for those are downloaded below.

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
```

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```
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial4/"
# Files to download
pretrained_files = ["FashionMNIST_SGD.config",    "FashionMNIST_SGD_results.json",
↪"FashionMNIST_SGD.tar",
                    "FashionMNIST_SGDMom.config", "FashionMNIST_SGDMom_results.json",
↪"FashionMNIST_SGDMom.tar",
                    "FashionMNIST_Adam.config",   "FashionMNIST_Adam_results.json",
↪"FashionMNIST_Adam.tar"   ]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.32.1 Preparation

Throughout this notebook, we will use a deep fully connected network, similar to our previous tutorial. We will also again apply the network to FashionMNIST, so you can relate to the results of Tutorial 3. We start by loading the FashionMNIST dataset:

[4]:
```
import torch
import torch.utils.data as data
from torchvision.datasets import FashionMNIST
from torchvision import transforms


# Transformations applied on each image => bring them into a numpy array and normalize␣
↪to mean 0 and std 1
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    img = (img / 255. - 0.2861) / 0.3530
    return img

# We need to stack the batch elements as numpy arrays
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
```

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```
        return np.array(batch)

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = FashionMNIST(root=DATASET_PATH,
                             train=True,
                             transform=image_to_numpy,
                             download=True)
train_set, val_set = torch.utils.data.random_split(train_dataset,
                                                   [50000, 10000],
                                                   generator=torch.Generator().manual_
↪seed(42))

# Loading the test set
test_set = FashionMNIST(root=DATASET_PATH,
                        train=False,
                        transform=image_to_numpy,
                        download=True)

# We define a set of data loaders that we can use for various purposes later.
# Note that for actually training a model, we will use different data loaders
# with a lower batch size.
train_loader = data.DataLoader(train_set,
                               batch_size=1024,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate)
val_loader   = data.DataLoader(val_set,
                               batch_size=1024,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate)
test_loader  = data.DataLoader(test_set,
                               batch_size=1024,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate)
```

In comparison to the previous tutorial, we have changed the parameters of the normalization transformation in `image_to_numpy`. The normalization is now designed to give us an expected mean of 0 and a standard deviation of 1 across pixels. This will be particularly relevant for the discussion about initialization we will look at below, and hence we change it here. It should be noted that in most classification tasks, both normalization techniques (between -1 and 1 or mean 0 and stddev 1) have shown to work well. We can calculate the normalization parameters by determining the mean and standard deviation on the original images:

[5]:
```
print("Mean", (train_dataset.data.float() / 255.0).mean().item())
print("Std", (train_dataset.data.float() / 255.0).std().item())
```

```
Mean 0.28604060411453247
Std 0.3530242443084717
```

We can verify the transformation by looking at the statistics of a single batch:

[6]:
```
imgs, _ = next(iter(train_loader))
```

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```
print(f"Mean: {imgs.mean().item():5.3f}")
print(f"Standard deviation: {imgs.std().item():5.3f}")
print(f"Maximum: {imgs.max().item():5.3f}")
print(f"Minimum: {imgs.min().item():5.3f}")
```

```
Mean: 0.008
Standard deviation: 1.009
Maximum: 2.022
Minimum: -0.810
```

Note that the maximum and minimum are not 1 and -1 anymore, but shifted towards the positive values. This is because FashionMNIST contains a lot of black pixels, similar to MNIST.

Next, we create a linear neural network. We use the same setup as in the previous tutorial.

[7]:
```
# Network
class BaseNetwork(nn.Module):
    act_fn : Callable
    num_classes : int = 10
    hidden_sizes : Sequence = (512, 256, 256, 128)
    kernel_init : Callable = nn.linear.default_kernel_init

    @nn.compact
    def __call__(self, x, return_activations=False):
        x = x.reshape(x.shape[0], -1) # Reshape images to a flat vector
        # We collect all activations throughout the network for later visualizations
        # Remember that in jitted functions, unused tensors will anyways be removed.
        activations = []
        for hd in self.hidden_sizes:
            x = nn.Dense(hd,
                         kernel_init=self.kernel_init)(x)
            activations.append(x)
            x = self.act_fn(x)
            activations.append(x)
        x = nn.Dense(self.num_classes,
                     kernel_init=self.kernel_init)(x)
        activations.append(x)
        return x if not return_activations else (x, activations)
```

For the activation functions, we make use of JAX's and Flax's library instead of implementing ourselves. However, we also define an `Identity` activation function. Although this activation function would significantly limit the network's modeling capabilities, we will use it in the first steps of our discussion about initialization (for simplicity).

[8]:
```
act_fn_by_name = {
    "tanh": nn.tanh,
    "relu": nn.relu,
    "identity": lambda x: x
}
```

Finally, we define a few plotting functions that we will use for our discussions. These functions help us to (1) visualize the weight/parameter distribution inside a network, (2) visualize the gradients that the parameters at different layers receive, and (3) the activations, i.e. the output of the linear layers. The detailed code is not important, but feel free to take a closer look if interested.

[9]:
```
##############################################################

def plot_dists(val_dict, color="C0", xlabel=None, stat="count", use_kde=True):
    columns = len(val_dict)
    fig, ax = plt.subplots(1, columns, figsize=(columns*3, 2.5))
    fig_index = 0
    for key in sorted(val_dict.keys()):
        key_ax = ax[fig_index%columns]
        sns.histplot(val_dict[key], ax=key_ax, color=color, bins=50, stat=stat,
                     kde=use_kde and ((val_dict[key].max()-val_dict[key].min())>1e-8)) #␣
↪Only plot kde if there is variance
        key_ax.set_title(f"{key} " + (r"(%i $\to$ %i)" % (val_dict[key].shape[1], val_
↪dict[key].shape[0]) if len(val_dict[key].shape)>1 else ""))
        if xlabel is not None:
            key_ax.set_xlabel(xlabel)
        fig_index += 1
    fig.subplots_adjust(wspace=0.4)
    return fig

##################################################################

def visualize_weight_distribution(params, color="C0"):
    params, _ = jax.tree_util.tree_flatten(params)
    params = [p.reshape(-1) for p in params if len(p.shape) > 1]  # Remove biases
    params = jax.device_get(params)
    weights = {f'Layer {layer_idx*2}': p for layer_idx, p in enumerate(params)}

    ## Plotting
    fig = plot_dists(weights, color=color, xlabel="Weight vals")
    fig.suptitle("Weight distribution", fontsize=14, y=1.05)
    plt.show()
    plt.close()

##################################################################

small_loader = data.DataLoader(train_set, batch_size=1024, shuffle=False, collate_
↪fn=numpy_collate)
exmp_imgs, exmp_labels = next(iter(small_loader))

def visualize_gradients(model, params, color="C0", print_variance=False):
    """
    Inputs:
        net - Object of class BaseNetwork
        color - Color in which we want to visualize the histogram (for easier separation␣
↪of activation functions)
    """
    # Pass one batch through the network, and calculate the gradients for the weights
    def loss_func(p):
        logits = model.apply(p, exmp_imgs)
        loss = optax.softmax_cross_entropy_with_integer_labels(logits, exmp_labels).
↪mean()
        return loss
    grads = jax.grad(loss_func)(params)
```

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```
    grads = jax.device_get(grads)
    # We limit our visualization to the weight parameters and exclude the bias to reduce␣
↪the number of plots
    grads = jax.tree_util.tree_leaves(grads)
    grads = [g.reshape(-1) for g in grads if len(g.shape) > 1]
    grads = {f'Layer {layer_idx*2}': g for layer_idx, g in enumerate(grads)}

    ## Plotting
    fig = plot_dists(grads, color=color, xlabel="Grad magnitude")
    fig.suptitle("Gradient distribution", fontsize=14, y=1.05)
    plt.show()
    plt.close()

    if print_variance:
        for key in sorted(grads.keys()):
            print(f"{key} - Variance: {np.var(grads[key])}")

##################################################################

def visualize_activations(model, params, color="C0", print_variance=False):
    # Pass one batch through the network, and calculate the activations
    _, activations = model.apply(params, exmp_imgs, return_activations=True)
    activations = {f'Layer {layer_idx*2}': act.reshape(-1) for layer_idx, act in␣
↪enumerate(activations[::2])}

    ## Plotting
    fig = plot_dists(activations, color=color, stat="density", xlabel="Activation vals")
    fig.suptitle("Activation distribution", fontsize=14, y=1.05)
    plt.show()
    plt.close()

    if print_variance:
        for key in sorted(activations.keys()):
            print(f"{key} - Variance: {np.var(activations[key])}")


##################################################################
```

4.32.2 Initialization

Before starting our discussion about initialization, it should be noted that there exist many very good blog posts about the topic of neural network initialization (for example deeplearning.ai, or a more math-focused blog post). In case something remains unclear after this tutorial, we recommend skimming through these blog posts as well.

When initializing a neural network, there are a few properties we would like to have. First, the variance of the input should be propagated through the model to the last layer, so that we have a similar standard deviation for the output neurons. If the variance would vanish the deeper we go in our model, it becomes much harder to optimize the model as the input to the next layer is basically a single constant value. Similarly, if the variance increases, it is likely to explode (i.e. head to infinity) the deeper we design our model. The second property we look out for in initialization techniques is a gradient distribution with equal variance across layers. If the first layer receives much smaller gradients than the last layer, we will have difficulties in choosing an appropriate learning rate.

As a starting point for finding a good method, we will analyze different initialization based on our linear neural network with no activation function (i.e. an identity). We do this because initializations depend on the specific activation function used in the network, and we can adjust the initialization schemes later on for our specific choice.

[10]:
```
def init_simple_model(kernel_init, act_fn=act_fn_by_name['identity']):
    model = BaseNetwork(act_fn=act_fn,
                        kernel_init=kernel_init)
    params = model.init(random.PRNGKey(42), exmp_imgs)
    return model, params
```

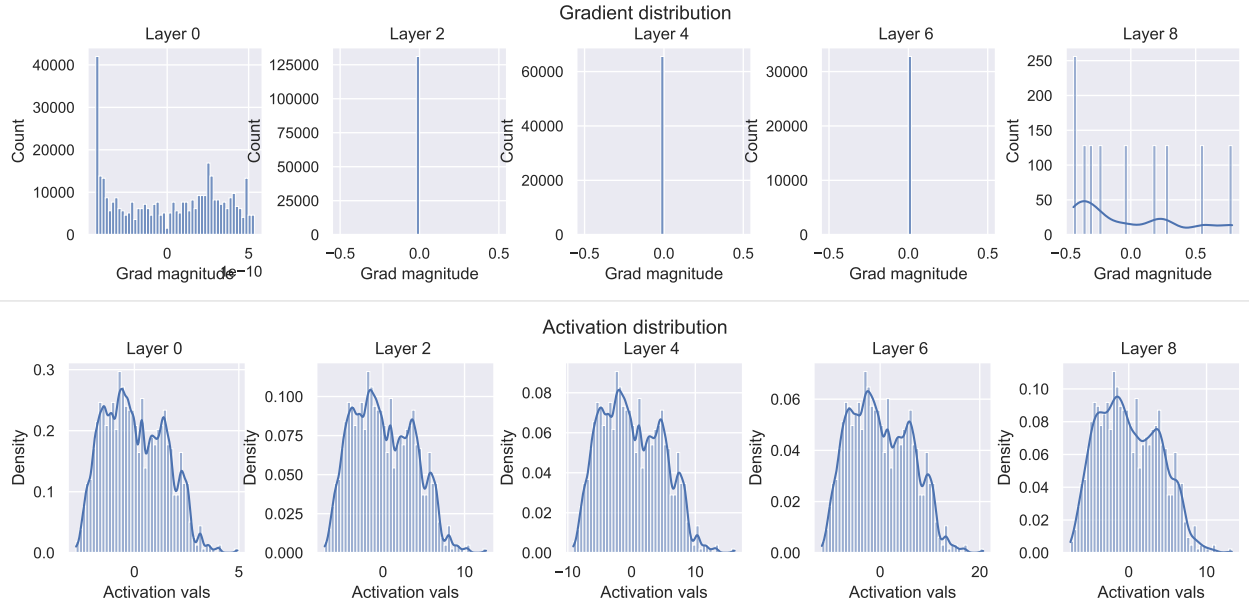
Note that in contrast to the PyTorch version of this tutorial, we keep the bias initialization fixed. As the default, JAX uses a zero initialization. In practice, the initialization of the bias is less relevant as long as it is reasonably close to zero, since it is only a (learnable) constant added to the features.

Constant initialization

The first initialization we can consider is to initialize all weights with the same constant value. Intuitively, setting all weights to zero is not a good idea as the propagated gradient will be zero. However, what happens if we set all weights to a value slightly larger or smaller than 0? To find out, we can implement a function for setting all parameters below and visualize the gradients.

[11]:
```
# An initialization function in JAX takes as input a PRNG key,
# the shape of the parameter to create, and the data type
# (usually jnp.float32). We create this function based on the
# input parameter 'c' here, indicating the constant value
def get_const_init_func(c=0.0):
    return lambda key, shape, dtype: c*jnp.ones(shape, dtype=dtype)

model, params = init_simple_model(get_const_init_func(c=0.005))
visualize_gradients(model, params)
visualize_activations(model, params, print_variance=True)
```




```
Layer 0 - Variance: 2.0582759380340576
Layer 2 - Variance: 13.489117622375488
```

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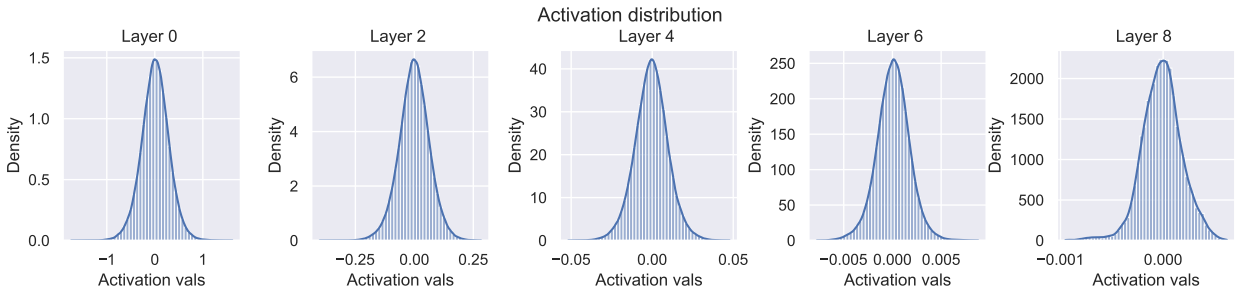
```
Layer 4 - Variance: 22.100563049316406
Layer 6 - Variance: 36.20956039428711
Layer 8 - Variance: 14.831436157226562
```

As we can see, only the first and the last layer have diverse gradient distributions while the other three layers have the same gradient for all weights (note that this value is unequal 0, but often very close to it). Having the same gradient for parameters that have been initialized with the same values means that we will always have the same value for those parameters. This would make our layer useless and reduce our effective number of parameters to 1. Thus, we cannot use a constant initialization to train our networks.

Constant variance

From the experiment above, we have seen that a constant value is not working. So instead, how about we initialize the parameters by randomly sampling from a distribution like a Gaussian? The most intuitive way would be to choose one variance that is used for all layers in the network. Let's implement it below, and visualize the activation distribution across layers.

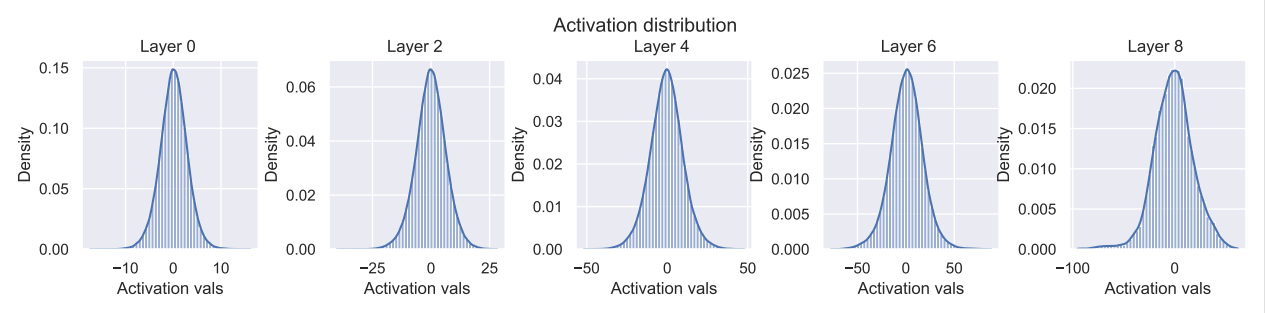
[12]:
```
def get_var_init_func(std=0.01):
    return lambda key, shape, dtype: std*random.normal(key, shape, dtype=dtype)

model, params = init_simple_model(get_var_init_func(std=0.01))
visualize_activations(model, params, print_variance=True)
```




```
Layer 0 - Variance: 0.08219309151172638
Layer 2 - Variance: 0.00415463000535965
Layer 4 - Variance: 0.00010465682862559333
Layer 6 - Variance: 2.8326080609986093e-06
Layer 8 - Variance: 3.75452451351066e-08
```

The variance of the activation becomes smaller and smaller across layers, and almost vanishes in the last layer. Alternatively, we could use a higher standard deviation:

[13]:
```
model, params = init_simple_model(get_var_init_func(std=0.1))
visualize_activations(model, params, print_variance=True)
```




```
Layer 0 - Variance: 8.21930980682373
Layer 2 - Variance: 41.54630661010742
Layer 4 - Variance: 104.6568603515625
Layer 6 - Variance: 283.26092529296875
Layer 8 - Variance: 375.4525451660156
```

With a higher standard deviation, the activations are likely to explode. You can play around with the specific standard deviation values, but it will be hard to find one that gives us a good activation distribution across layers and is very specific to our model. If we would change the hidden sizes or number of layers, you would have to search all over again, which is neither efficient nor recommended.

How to find appropriate initialization values

From our experiments above, we have seen that we need to sample the weights from a distribution, but are not sure which one exactly. As a next step, we will try to find the optimal initialization from the perspective of the activation distribution. For this, we state two requirements:

1. The mean of the activations should be zero
2. The variance of the activations should stay the same across every layer

Suppose we want to design an initialization for the following layer: $y = Wx + b$ with $y \in \mathbb{R}^{d_y}$, $x \in \mathbb{R}^{d_x}$. Our goal is that the variance of each element of y is the same as the input, i.e. $\text{Var}(y_i) = \text{Var}(x_i) = \sigma_x^2$, and that the mean is zero. We assume x to also have a mean of zero, because, in deep neural networks, y would be the input of another layer. This requires the bias and weight to have an expectation of 0. Actually, as b is a single element per output neuron and is constant across different inputs, we set it to 0 overall.

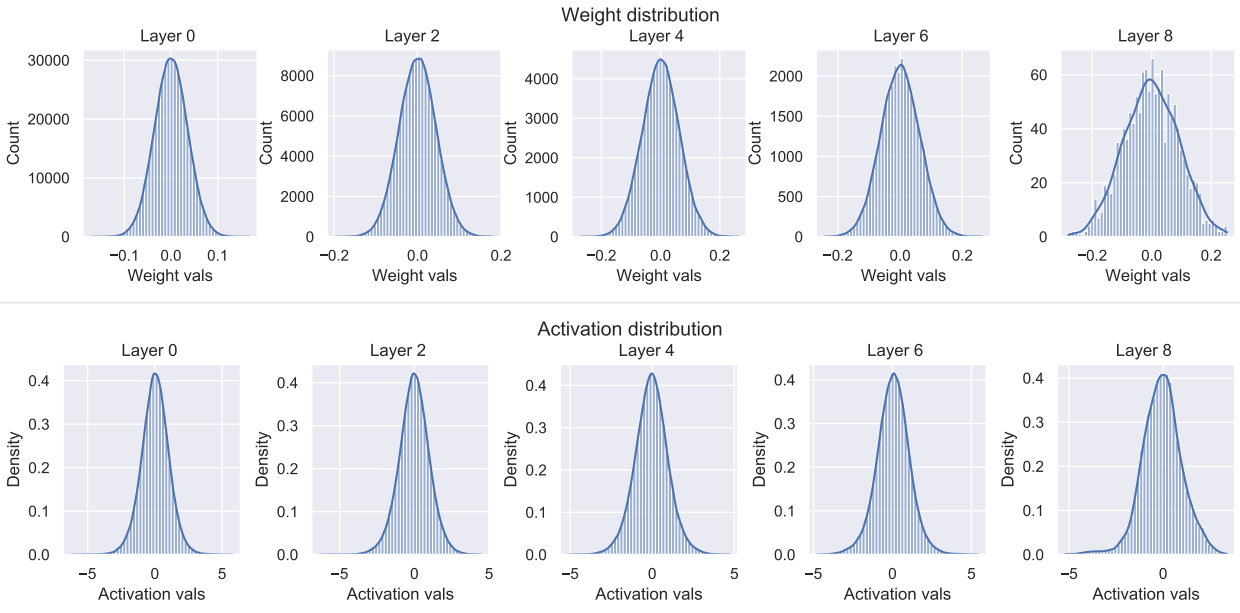
Next, we need to calculate the variance with which we need to initialize the weight parameters. Along the calculation, we will need the following variance rule: given two independent variables, the variance of their product is $\text{Var}(X \cdot Y) = \mathbb{E}(Y)^2\text{Var}(X) + \mathbb{E}(X)^2\text{Var}(Y) + \text{Var}(X)\text{Var}(Y) = \mathbb{E}(Y^2)\mathbb{E}(X^2) - \mathbb{E}(Y)^2\mathbb{E}(X)^2$ (X and Y are not refering to x and y, but any random variable).

The needed variance of the weights, $\text{Var}(w_{ij})$, is calculated as follows:

$$
\begin{aligned}
y_i &= \sum_j w_{ij} x_j && \text{Calculation of a single output neuron without bias} \\
\text{Var}(y_i) = \sigma_x^2 &= \text{Var}\left(\sum_j w_{ij} x_j\right) \\
&= \sum_j \text{Var}(w_{ij} x_j) && \text{Inputs and weights are independent of each other} \\
&= \sum_j \text{Var}(w_{ij}) \cdot \text{Var}(x_j) && \text{Variance rule (see above) with expectations being zero} \\
&= d_x \cdot \text{Var}(w_{ij}) \cdot \text{Var}(x_j) && \text{Variance equal for all } d_x \text{ elements} \\
&= \sigma_x^2 \cdot d_x \cdot \text{Var}(w_{ij}) \\
\Rightarrow \text{Var}(w_{ij}) = \sigma_W^2 &= \frac{1}{d_x}
\end{aligned}
$$

Thus, we should initialize the weight distribution with a variance of the inverse of the input dimension d_x. Let's implement it below and check whether this holds:

[14]:
```
equal_var_init = lambda key, shape, dtype: 1.0/np.sqrt(shape[0]) * random.normal(key,␣
↪shape, dtype=dtype)

model, params = init_simple_model(equal_var_init)
visualize_weight_distribution(params)
visualize_activations(model, params, print_variance=True)
```




```
Layer 0 - Variance: 1.0483813285827637
Layer 2 - Variance: 1.0350143909454346
Layer 4 - Variance: 1.018454670906067
Layer 6 - Variance: 1.0767643451690674
Layer 8 - Variance: 1.1150107383728027
```

As we expected, the variance stays indeed constant across layers. Note that our initialization does not restrict us to a normal distribution, but allows any other distribution with a mean of 0 and variance of $1/d_x$. You often see that a

uniform distribution is used for initialization. A small benefit of using a uniform instead of a normal distribution is that we can exclude the chance of initializing very large or small weights.

Besides the variance of the activations, another variance we would like to stabilize is the one of the gradients. This ensures a stable optimization for deep networks. It turns out that we can do the same calculation as above starting from $\Delta x = W\Delta y$, and come to the conclusion that we should initialize our layers with $1/d_y$ where d_y is the number of output neurons. You can do the calculation as a practice, or check a thorough explanation in this blog post. As a compromise between both constraints, Glorot and Bengio (2010) proposed to use the harmonic mean of both values. This leads us to the well-known Xavier initialization:

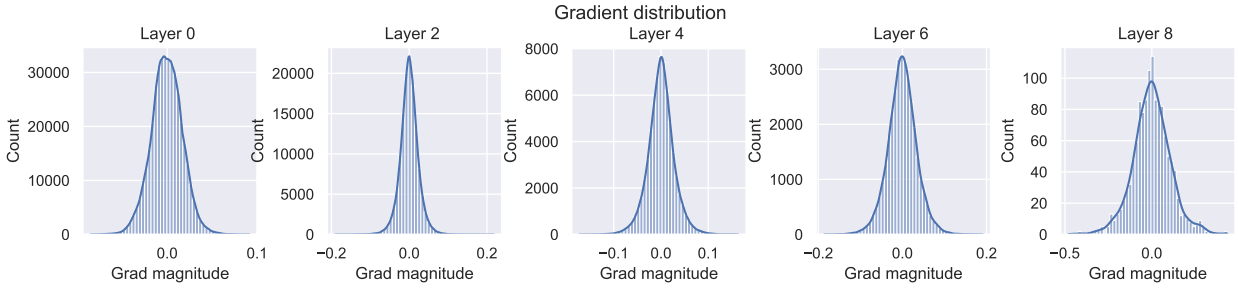
$$W \sim \mathcal{N}\left(0, \frac{2}{d_x + d_y}\right)$$

If we use a uniform distribution, we would initialize the weights with:

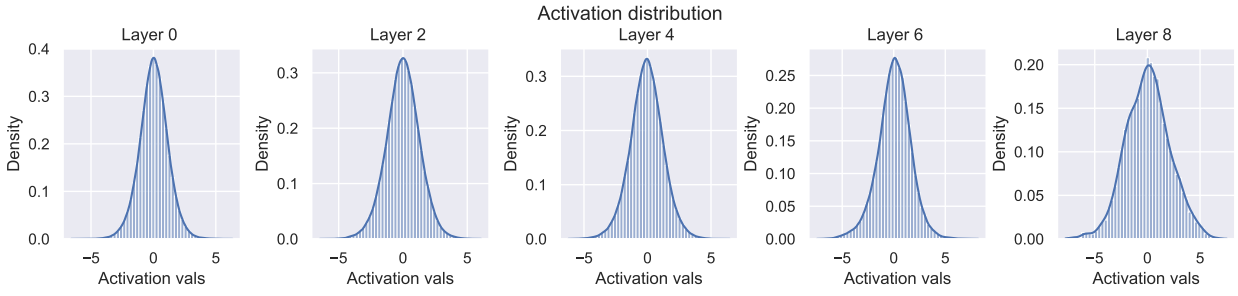
$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{d_x + d_y}}, \frac{\sqrt{6}}{\sqrt{d_x + d_y}}\right]$$

Let's shortly implement it and validate its effectiveness:

[15]:
```
def xavier_init(key, shape, dtype):
    bound = math.sqrt(6)/math.sqrt(shape[0]+shape[1])
    return random.uniform(key, shape, dtype,
                          minval=-bound, maxval=bound)

model, params = init_simple_model(xavier_init)
visualize_gradients(model, params, print_variance=True)
visualize_activations(model, params, print_variance=True)
```



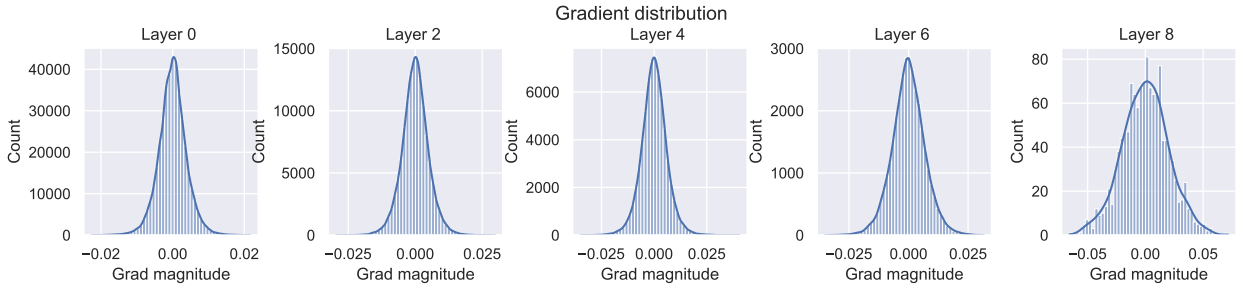

```
Layer 0 - Variance: 0.00029831365100108087
Layer 2 - Variance: 0.0005463268025778234
Layer 4 - Variance: 0.0007796576828695834
Layer 6 - Variance: 0.0011752902064472437
Layer 8 - Variance: 0.011736484244465828
```



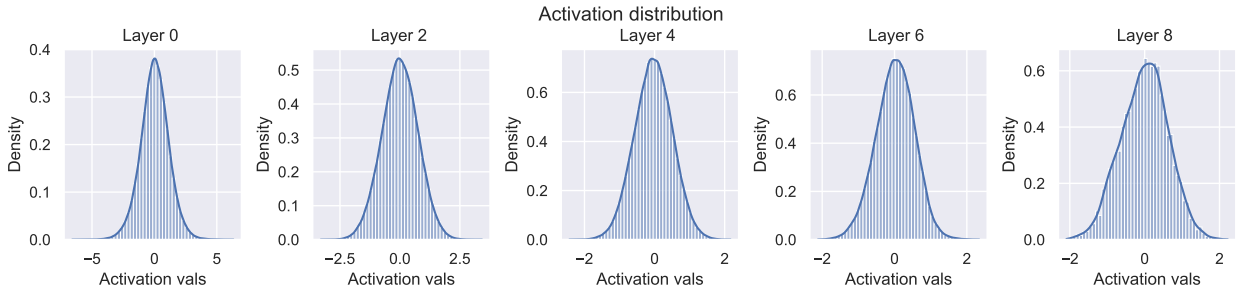
```
Layer 0 - Variance: 1.2806072235107422
Layer 2 - Variance: 1.6784099340438843
Layer 4 - Variance: 1.6767947673797607
Layer 6 - Variance: 2.5439999103546143
Layer 8 - Variance: 4.41333532333374
```

We see that the Xavier initialization balances the variance of gradients and activations. Note that the significantly higher variance for the output layer is due to the large difference of input and output dimension (128 vs 10). However, we currently assumed the activation function to be linear. So what happens if we add a non-linearity? In a tanh-based network, a common assumption is that for small values during the initial steps in training, the $\tanh$ works as a linear function such that we don't have to adjust our calculation. We can check if that is the case for us as well:

[16]:
```
model, params = init_simple_model(xavier_init, act_fn=nn.tanh)
visualize_gradients(model, params, print_variance=True)
visualize_activations(model, params, print_variance=True)
```




```
Layer 0 - Variance: 1.520933165011229e-05
Layer 2 - Variance: 2.4512757590855472e-05
Layer 4 - Variance: 3.6233024729881436e-05
Layer 6 - Variance: 4.8036039515864104e-05
Layer 8 - Variance: 0.00040259156958200004
```




```
Layer 0 - Variance: 1.2806072235107422
Layer 2 - Variance: 0.5610313415527344
Layer 4 - Variance: 0.29278191924095154
Layer 6 - Variance: 0.2838047742843628
Layer 8 - Variance: 0.39267846941947937
```

Although the variance decreases over depth, it is apparent that the activation distribution becomes more focused on the low values. Therefore, our variance will stabilize around 0.25 if we would go even deeper. Hence, we can conclude that the Xavier initialization works well for Tanh networks. But what about ReLU networks? Here, we cannot take the previous assumption of the non-linearity becoming linear for small values. The ReLU activation function sets (in expectation) half of the inputs to 0 so that also the expectation of the input is not zero. However, as long as the expectation of W is zero and $b = 0$, the expectation of the output is zero. The part where the calculation of the ReLU

initialization differs from the identity is when determining $\text{Var}(w_{ij}x_j)$:

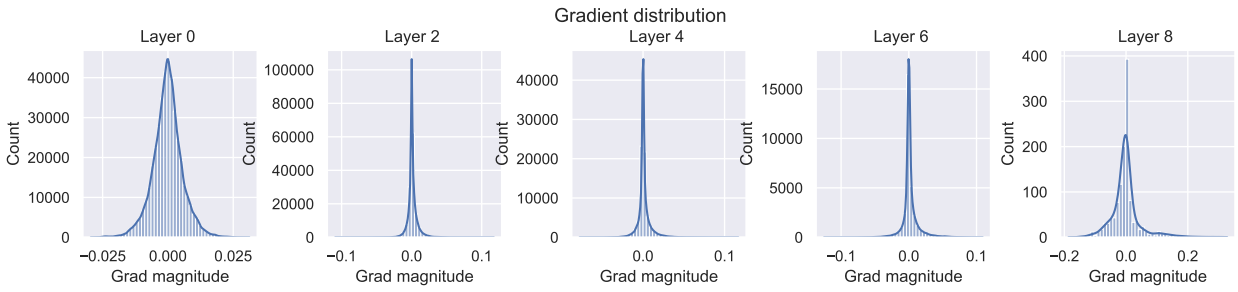
$$\text{Var}(w_{ij}x_j) = \underbrace{\mathbb{E}[w_{ij}^2]}_{=\text{Var}(w_{ij})}\ \mathbb{E}[x_j^2] - \underbrace{\mathbb{E}[w_{ij}]^2}_{=0}\mathbb{E}[x_j]^2 = \text{Var}(w_{ij})\mathbb{E}[x_j^2]$$

If we assume now that x is the output of a ReLU activation (from a previous layer, $x = max(0, \tilde{y})$), we can calculate the expectation as follows:

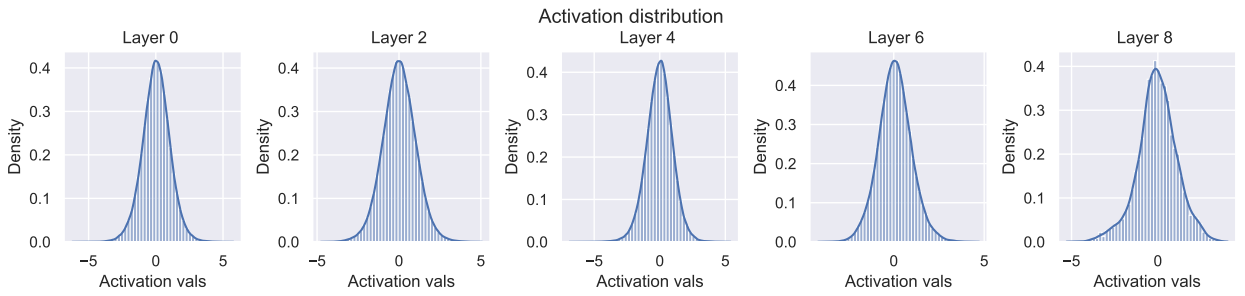
$$\begin{aligned}\mathbb{E}[x^2] &= \mathbb{E}[\max(0,\tilde{y})^2] \\ &= \frac{1}{2}\mathbb{E}[\tilde{y}^2] && \tilde{y} \text{ is zero-centered and symmetric} \\ &= \frac{1}{2}\text{Var}(\tilde{y})\end{aligned}$$

Thus, we see that we have an additional factor of 1/2 in the equation, so that our desired weight variance becomes $2/d_x$. This gives us the Kaiming initialization (see He, K. et al. (2015)). Note that the Kaiming initialization does not use the harmonic mean between input and output size. In their paper (Section 2.2, Backward Propagation, last paragraph), they argue that using d_x or d_y both lead to stable gradients throughout the network, and only depend on the overall input and output size of the network. Hence, we can use here only the input d_x:

[17]:
```
num_input_feats = np.prod(exmp_imgs.shape[1:])
def kaiming_init(key, shape, dtype):
    # The first layer does not have ReLU applied on its input
    # Note that this detection only works if we do not use 784
    # feature size anywhere - better to explicitly handle
    # layer numbers
    if shape[0] == num_input_feats:
        std = 1/np.sqrt(shape[0])
    else:
        std = np.sqrt(2/shape[0])
    return std * random.normal(key, shape, dtype)

model, params = init_simple_model(kaiming_init, act_fn=nn.relu)
visualize_gradients(model, params, print_variance=True)
visualize_activations(model, params, print_variance=True)
```




```
Layer 0 - Variance: 3.25944201904349e-05
Layer 2 - Variance: 4.664550942834467e-05
Layer 4 - Variance: 6.605686212424189e-05
Layer 6 - Variance: 0.00015451121726073325
Layer 8 - Variance: 0.002561226487159729
```




```
Layer 0 - Variance: 1.0483813285827637
Layer 2 - Variance: 1.0137324333190918
Layer 4 - Variance: 0.9987665414810181
Layer 6 - Variance: 0.8383973836898804
Layer 8 - Variance: 1.316560983657837
```

The variance stays stable across layers. We can conclude that the Kaiming initialization indeed works well for ReLU-based networks. Note that for Leaky-ReLU etc., we have to slightly adjust the factor of 2 in the variance as half of the values are not set to zero anymore.

4.32.3 Optimization

Besides initialization, selecting a suitable optimization algorithm can be an important choice for deep neural networks. Before taking a closer look at them, we should define code for training the models. Most of the following code is copied from the previous tutorial, and only slightly altered to fit our needs.

[18]:
```
def _get_config_file(model_path, model_name):
    # Name of the file for storing hyperparameter details
    return os.path.join(model_path, model_name + ".config")

def _get_model_file(model_path, model_name):
    # Name of the file for storing network parameters
    return os.path.join(model_path, model_name + ".tar")

def _get_result_file(model_path, model_name):
    return os.path.join(model_path, model_name + "_results.json")

def load_model(model_path, model_name, state=None):
    """
    Loads a saved model from disk.

    Inputs:
        model_path - Path of the checkpoint directory
        model_name - Name of the model (str)
        state - (Optional) If given, the parameters are loaded into this training state. Otherwise,
                a new one is created alongside a network architecture.
    """
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_file(model_path, model_name)
    assert os.path.isfile(config_file), f"Could not find the config file \"{config_file}\". Are you sure this is the correct path and you have your model config stored here?"
```

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```
    assert os.path.isfile(model_file), f"Could not find the model file \"{model_file}\". Are you sure this is the correct path and you have your model stored here?"
    with open(config_file, "r") as f:
        config_dict = json.load(f)
    if state is None:
        net = BaseNetwork(act_fn=nn.relu, **config_dict)
        state = train_state.TrainState(step=0,
                                       params=None,
                                       apply_fn=net.apply,
                                       tx=None,
                                       opt_state=None)
    else:
        net = None
    # You can also use flax's checkpoint package. To show an alternative,
    # you can instead load the parameters simply from a pickle file.
    with open(model_file, 'rb') as f:
        params = pickle.load(f)
    state = state.replace(params=params)
    return state, net

def save_model(model, params, model_path, model_name):
    """
    Given a model, we save the parameters and hyperparameters.

    Inputs:
        model - Network object without parameters
        params - Parameters to save of the model
        model_path - Path of the checkpoint directory
        model_name - Name of the model (str)
    """
    config_dict = {'hidden_sizes': model.hidden_sizes,
                   'num_classes': model.num_classes}
    os.makedirs(model_path, exist_ok=True)
    config_file, model_file = _get_config_file(model_path, model_name), _get_model_file(model_path, model_name)
    with open(config_file, "w") as f:
        json.dump(config_dict, f)
    # You can also use flax's checkpoint package. To show an alternative,
    # you can instead save the parameters simply in a pickle file.
    with open(model_file, 'wb') as f:
        pickle.dump(params, f)

def calculate_loss(params, apply_fn, batch):
    imgs, labels = batch
    logits = apply_fn(params, imgs)
    loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
    acc = (labels == logits.argmax(axis=-1)).mean()
    return loss, acc

@jax.jit
def train_step(state, batch):
    grad_fn = jax.value_and_grad(calculate_loss,
```

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```
                                    has_aux=True)
    (_, acc), grads = grad_fn(state.params, state.apply_fn, batch)
    state = state.apply_gradients(grads=grads)
    return state, acc

@jax.jit
def eval_step(state, batch):
    _, acc = calculate_loss(state.params, state.apply_fn, batch)
    return acc

def train_model(net, params, optimizer, model_name, max_epochs=50, batch_size=256,␣
↪overwrite=False):
    """
    Train a model on the training set of FashionMNIST

    Inputs:
        net - Object of BaseNetwork
        params - The parameters to use as initialization
        optimizer - Optimizer to use
        model_name - (str) Name of the model, used for creating the checkpoint names
        max_epochs - Number of epochs we want to (maximally) train for
        batch_size - Size of batches used in training
        overwrite - Determines how to handle the case when there already exists a␣
↪checkpoint. If True, it will be overwritten. Otherwise, we skip training.
    """
    file_exists = os.path.isfile(_get_model_file(CHECKPOINT_PATH, model_name))
    if file_exists and not overwrite:
        print("Model file already exists. Skipping training...")
        state = None
        with open(_get_result_file(CHECKPOINT_PATH, model_name), "r") as f:
            results = json.load(f)
    else:
        if file_exists:
            print("Model file exists, but will be overwritten...")

        # Initializing training state
        results = None
        state = train_state.TrainState.create(apply_fn=net.apply,
                                              params=params,
                                              tx=optimizer)

        # Defining data loader
        train_loader_local = data.DataLoader(train_set,
                                             batch_size=batch_size,
                                             shuffle=True,
                                             drop_last=True,
                                             collate_fn=numpy_collate,
                                             generator=torch.Generator().manual_seed(42))

        train_scores = []
        val_scores = []
        best_val_epoch = -1
```

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```
        for epoch in range(max_epochs):
            ############
            # Training #
            ############
            train_acc = 0.
            for batch in tqdm(train_loader_local, desc=f"Epoch {epoch+1}", leave=False):
                state, acc = train_step(state, batch)
                train_acc += acc
            train_acc /= len(train_loader_local)
            train_scores.append(train_acc.item())

            ##############
            # Validation #
            ##############
            val_acc = test_model(state, val_loader)
            val_scores.append(val_acc)
            print(f"[Epoch {epoch+1:2d}] Training accuracy: {train_acc:05.2%}, Validation accuracy: {val_acc:4.2%}")

            if len(val_scores) == 1 or val_acc > val_scores[best_val_epoch]:
                print("\t   (New best performance, saving model...)")
                save_model(net, state.params, CHECKPOINT_PATH, model_name)
                best_val_epoch = epoch

    state, _ = load_model(CHECKPOINT_PATH, model_name, state=state)
    if results is None:
        test_acc = test_model(state, test_loader)
        results = {"test_acc": test_acc, "val_scores": val_scores,
                   "train_scores": train_scores}
        with open(_get_result_file(CHECKPOINT_PATH, model_name), "w") as f:
            json.dump(results, f)

    # Plot a curve of the validation accuracy
    sns.set()
    plt.plot([i for i in range(1,len(results["train_scores"])+1)], results["train_scores"], label="Train")
    plt.plot([i for i in range(1,len(results["val_scores"])+1)], results["val_scores"], label="Val")
    plt.xlabel("Epochs")
    plt.ylabel("Validation accuracy")
    plt.ylim(min(results["val_scores"]), max(results["train_scores"])*1.01)
    plt.title(f"Validation performance of {model_name}")
    plt.legend()
    plt.show()
    plt.close()

    print((f" Test accuracy: {results['test_acc']:4.2%} ").center(50, "=")+"\n")
    return state


def test_model(state, data_loader):
    """
```

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```
    Test a model on a specified dataset.

    Inputs:
        state - Training state including parameters and model apply function.
        data_loader - DataLoader object of the dataset to test on (validation or test)
    """
    true_preds, count = 0., 0
    for batch in data_loader:
        acc = eval_step(state, batch)
        batch_size = batch[0].shape[0]
        true_preds += acc * batch_size
        count += batch_size
    test_acc = true_preds / count
    return test_acc.item()
```

First, we need to understand what an optimizer actually does. The optimizer is responsible to update the network's parameters given the gradients. Hence, we effectively implement a function $w^t = f(w^{t-1}, g^t, ...)$ with w being the parameters, and $g^t = \nabla_{w^{(t-1)}} \mathcal{L}^{(t)}$ the gradients at time step t. A common, additional parameter to this function is the learning rate, here denoted by η. Usually, the learning rate can be seen as the "step size" of the update. A higher learning rate means that we change the weights more in the direction of the gradients, a smaller means we take shorter steps.

As most optimizers only differ in the implementation of f, we can define a template for an optimizer in JAX below. Note that in comparison to PyTorch, the optimizers must be functional and have no effects outside the function. Hence, we follow the basic implementation principles of optax and define an optimizer to be a tuple of two main functions:

- `init`: Given a set of parameters, initialize any state variables that the optimizer may need. While is might not be necessary for the simplest optimizers, more sophisticated like Adam need to keep track of gradient statistics, which can be initialized here.
- `update`: Given the gradients, the optimizer state, and the parameters, return the updates that should be applied to the parameters, and an updated optimizer state.

The updates can be applied to the parameters using `optax.apply_updates(params, updates)` which adds each update value to its respective parameter. In simplified form, it applies `tree_map(lambda p, u: p + u, params, updates)`. As a reminder, `jax.tree_util.tree_map` is a function that runs over PyTrees and applies a function to all leafs, returning a new PyTree with the results. If we input multiple PyTrees, it runs over them synchronously and applies the functions on tuples of leafs, one of each PyTree. In the function above, this means that a new PyTree is created for which each leaf has the sum of the respective leaf in `params` and `updates`.

In contrast to PyTorch, there is no `zero_grad` function since the gradients are the output of a separate gradient function, not an object-based backpropagation through a dynamic computation graph. The template is setup below:

[19]:
```
class Optimizer(NamedTuple):
    # Given the parameters, initialize any optimizer state as tuple
    init : Callable[[PyTree], tuple]
    # Given the gradients, optimizer state, and evt. parameters, return
    # the parameter updates and new optimizer state
    update : Callable[[PyTree, tuple, Optional[PyTree]], Tuple[PyTree, tuple]]
```

The first optimizer we are going to implement is the standard Stochastic Gradient Descent (SGD). SGD updates the parameters using the following equation:

$$w^{(t)} = w^{(t-1)} - \eta \cdot g^{(t)}$$

As simple as the equation is also our implementation of SGD:

[20]:
```
def sgd(lr):
    def init(params):
        return tuple()

    def update(updates, state, params=None):
        updates = tree_map(lambda u: -lr * u, updates)
        return updates, state

    return Optimizer(init, update)
```

Note that we define SGD as a function that returns a tuple of the init and update function, which depends on the input parameter `lr`, i.e., the learning rate. SGD does not have any state it needs to keep track of. Hence, the init function returns an empty tuple. The update function simply multiplies all gradients with the learning rate. The negative sign is needed since the `apply_updates` function *adds* the updates to the parameters, not subtracts.

In the lecture, we also have discussed the concept of momentum which replaces the gradient in the update by an exponential average of all past gradients including the current one:

$$m^{(t)} = \beta_1 m^{(t-1)} + (1 - \beta_1) \cdot g^{(t)}$$
$$w^{(t)} = w^{(t-1)} - \eta \cdot m^{(t)}$$

Let's also implement it below:

[21]:
```
def sgd_momentum(lr, momentum=0.0):
    def init(params):
        param_momentum = tree_map(jnp.zeros_like, params)
        return param_momentum

    def update(updates, state, params=None):
        state = tree_map(lambda m, g: (1 - momentum) * g + momentum * m,
                         state,
                         updates)
        updates = tree_map(lambda m: - lr * m,
                           state)
        return updates, state

    return Optimizer(init, update)
```

We track the momentum parameters $m^{(t)}$ in a PyTree, which is initialized with all zeros, but with the same shape and structure as the parameters. At each update iteration, we update our momentum parameters with above's equation, and use it to calculate the new updates.

As a third and final optimizer, we arrive at Adam. Adam combines the idea of momentum with an adaptive learning rate, which is based on an exponential average of the squared gradients, i.e. the gradients norm. Furthermore, we add a bias correction for the momentum and adaptive learning rate for the first iterations:

$$m^{(t)} = \beta_1 m^{(t-1)} + (1 - \beta_1) \cdot g^{(t)}$$
$$v^{(t)} = \beta_2 v^{(t-1)} + (1 - \beta_2) \cdot \left(g^{(t)}\right)^2$$
$$\hat{m}^{(t)} = \frac{m^{(t)}}{1 - \beta_1^t}, \hat{v}^{(t)} = \frac{v^{(t)}}{1 - \beta_2^t}$$
$$w^{(t)} = w^{(t-1)} - \frac{\eta}{\sqrt{\hat{v}^{(t)}} + \epsilon} \circ \hat{m}^{(t)}$$

Epsilon is a small constant used to improve numerical stability for very small gradient norms. Remember that the

adaptive learning rate does not replace the learning rate hyperparameter η, but rather acts as an extra factor and ensures that the gradients of various parameters have a similar norm.

[22]:
```
def adam(lr, beta1=0.9, beta2=0.999, eps=1e-8):
    def init(params):
        step = 0.
        param_momentum = tree_map(jnp.zeros_like, params)
        param_2nd_momentum = tree_map(jnp.zeros_like, params)
        return (step, param_momentum, param_2nd_momentum)

    def update(updates, state, params=None):
        # Update momentum and adapt. lr
        step, param_momentum, param_2nd_momentum = state
        step += 1
        param_momentum = tree_map(lambda m, g: (1 - beta1) * g + beta1 * m,
                                  param_momentum,
                                  updates)
        param_2nd_momentum = tree_map(lambda m2, g: (1 - beta2) * g**2 + beta2 * m2,
                                      param_2nd_momentum,
                                      updates)
        # Calculate update for single parameter
        def update_param(m, m2):
            # Bias correction
            m /= 1 - beta1 ** step
            m2 /= 1 - beta2 ** step
            return - m * lr / (jnp.sqrt(m2) + eps)
        # Update for all parameters
        updates = tree_map(update_param,
                           param_momentum,
                           param_2nd_momentum)
        return updates, (step, param_momentum, param_2nd_momentum)

    return Optimizer(init, update)
```

Our state consists of a counter `step` that keeps track of the time step t, the momentums $m^{(t)}$ and the second momentum/adaptive learning rate parameters $v^{(t)}$. At each update step, we update $m^{(t)}$ and $v^{(t)}$, and afterwards calculate the updates for each parameters based on $m^{(t)}$ and $v^{(t)}$.

Comparing optimizers on model training

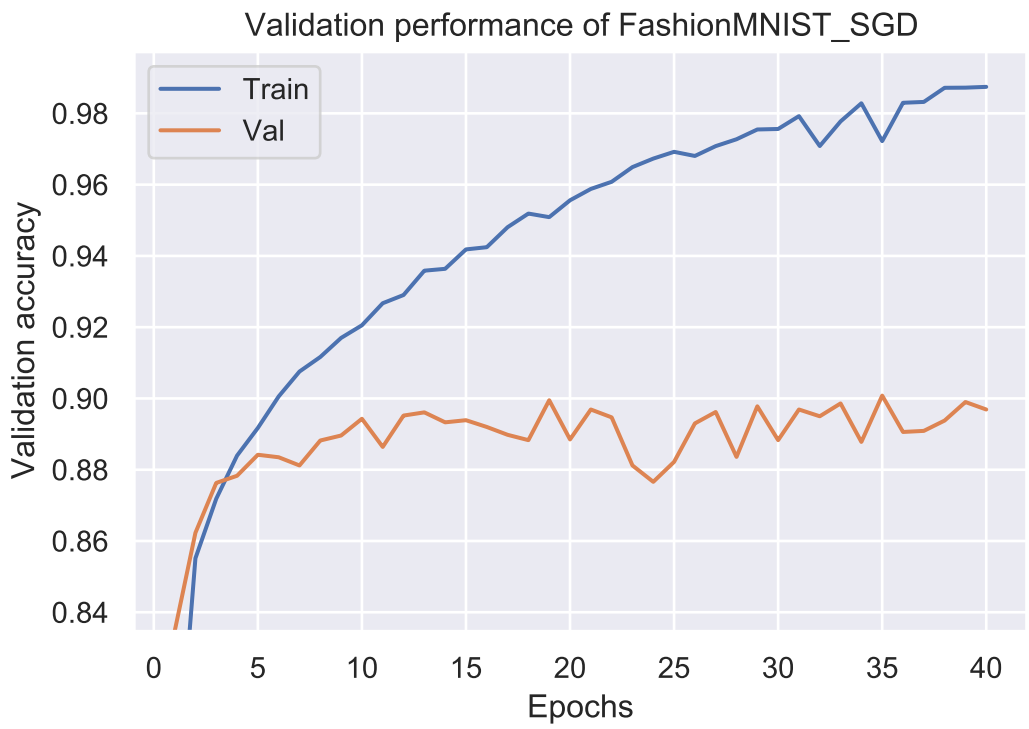
After we have implemented three optimizers (SGD, SGD with momentum, and Adam), we can start to analyze and compare them. First, we test them on how well they can optimize a neural network on the FashionMNIST dataset. We use again our linear network, this time with a ReLU activation and the kaiming initialization, which we have found before to work well for ReLU-based networks. Note that the model is over-parameterized for this task, and we can achieve similar performance with a much smaller network (for example `100,100,100`). However, our main interest is in how well the optimizer can train *deep* neural networks, hence the over-parameterization.

[23]:
```
model, params = init_simple_model(kaiming_init, act_fn=nn.relu)
```

For a fair comparison, we train the exact same model with the same seed with the three optimizers below. Feel free to change the hyperparameters if you want, the models are relatively fast to train.

[24]:
```
_ = train_model(model, params, sgd(lr=1e-1),
                "FashionMNIST_SGD",
                max_epochs=40, batch_size=256)
```

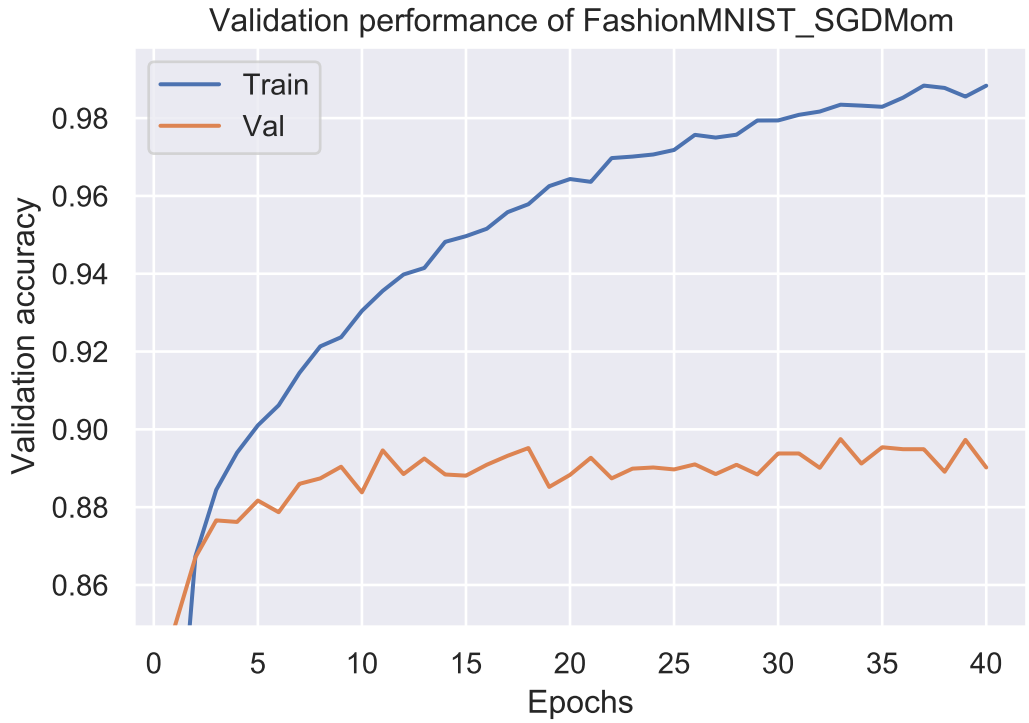
```
Model file already exists. Skipping training...
```




```
============== Test accuracy: 89.61% ==============
```

[25]:
```
_ = train_model(model, params, sgd_momentum(lr=1e-1, momentum=0.9),
                "FashionMNIST_SGDMom",
                max_epochs=40, batch_size=256)
```

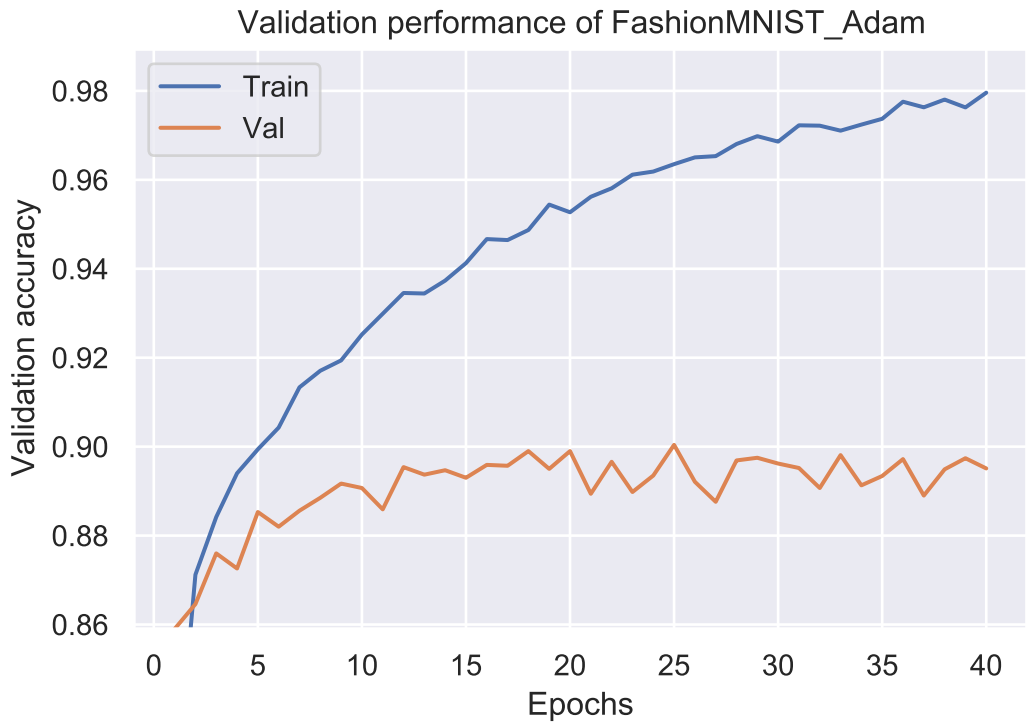
```
Model file already exists. Skipping training...
```




```
============= Test accuracy: 89.30% ==============
```

[26]:
```
_ = train_model(model, params, adam(lr=1e-3),
                "FashionMNIST_Adam",
                max_epochs=40, batch_size=256)
```

```
Model file already exists. Skipping training...
```




```
============= Test accuracy: 89.06% ==============
```

The result is that all optimizers perform similarly well with the given model. The differences are too small to find any significant conclusion. However, keep in mind that this can also be attributed to the initialization we chose. When changing the initialization to worse (e.g. constant variance), Adam usually shows to be more robust because of its adaptive learning rate. To show the specific benefits of the optimizers, we will continue to look at some possible loss surfaces in which momentum and adaptive learning rate are crucial.

Pathological curvatures

A pathological curvature is a type of surface that is similar to ravines and is particularly tricky for plain SGD optimization. In words, pathological curvatures typically have a steep gradient in one direction with an optimum at the center, while in a second direction we have a slower gradient towards a (global) optimum. Let's first create an example surface of this and visualize it:

[27]:
```
def pathological_curve_loss(w1, w2):
    # Example of a pathological curvature. There are many more possible, feel free to␣
↪experiment here!
    x1_loss = nn.tanh(w1)**2 + 0.01 * jnp.abs(w1)
    x2_loss = nn.sigmoid(w2)
    return x1_loss + x2_loss
```

[28]:
```
def plot_curve(curve_fn, x_range=(-5,5), y_range=(-5,5), plot_3d=False, cmap=cm.viridis,␣
↪title="Pathological curvature"):
    fig = plt.figure()
    ax = plt.axes(projection='3d') if plot_3d else plt.axes()
```

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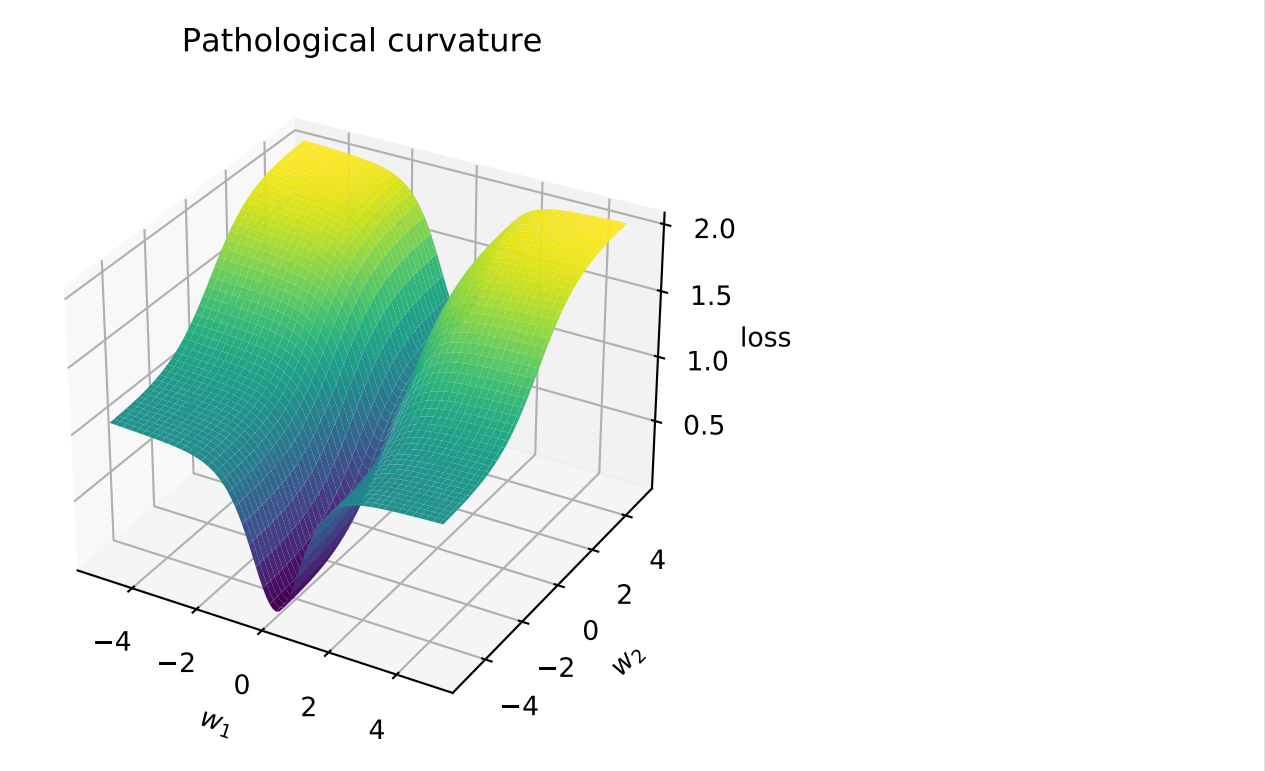
```
    x = np.arange(x_range[0], x_range[1], (x_range[1]-x_range[0])/100.)
    y = np.arange(y_range[0], y_range[1], (y_range[1]-y_range[0])/100.)
    x, y = np.meshgrid(x, y)
    z = curve_fn(x, y)
    z = jax.device_get(z)

    if plot_3d:
        ax.plot_surface(x, y, z, cmap=cmap, linewidth=1, color="#000", antialiased=False)
        ax.set_zlabel("loss")
    else:
        ax.imshow(z[::-1], cmap=cmap, extent=(x_range[0], x_range[1], y_range[0], y_
↪range[1]))
    plt.title(title)
    ax.set_xlabel(r"$w_1$")
    ax.set_ylabel(r"$w_2$")
    plt.tight_layout()
    return ax

sns.reset_orig()
_ = plot_curve(pathological_curve_loss, plot_3d=True)
plt.show()
```



In terms of optimization, you can image that w_1 and w_2 are weight parameters, and the curvature represents the loss surface over the space of w_1 and w_2. Note that in typical networks, we have many, many more parameters than two, and such curvatures can occur in multi-dimensional spaces as well.

Ideally, our optimization algorithm would find the center of the ravine and focuses on optimizing the parameters towards the direction of w_2. However, if we encounter a point along the ridges, the gradient is much greater in w_1 than w_2, and we might end up jumping from one side to the other. Due to the large gradients, we would have to reduce our learning

rate slowing down learning significantly.

To test our algorithms, we can implement a simple function to train two parameters on such a surface:

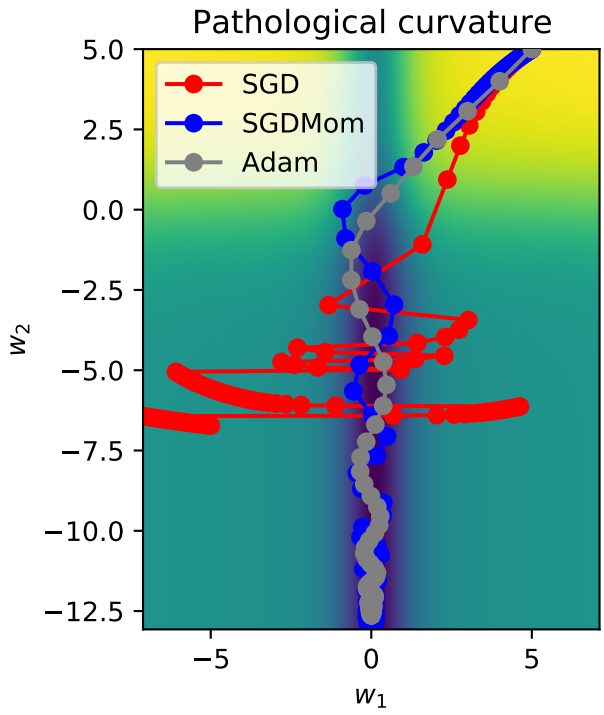
[29]:
```
def train_curve(optimizer, curve_func=pathological_curve_loss, num_updates=100, init=[5,
↪5]):
    """
    Inputs:
        optimizer - Optimizer to use
        curve_func - Loss function (e.g. pathological curvature)
        num_updates - Number of updates/steps to take when optimizing
        init - Initial values of parameters. Must be a list/tuple with two elements␣
↪representing w_1 and w_2
    Outputs:
        Numpy array of shape [num_updates, 3] with [t,:2] being the parameter values at␣
↪step t, and [t,2] the loss at t.
    """
    weights = jnp.array(init, dtype=jnp.float32)
    grad_fn = jax.jit(jax.value_and_grad(lambda w: curve_func(w[0], w[1])))
    opt_state = optimizer.init(weights)

    list_points = []
    for _ in range(num_updates):
        loss, grads = grad_fn(weights)
        list_points.append(jnp.concatenate([weights, loss[None]], axis=0))
        updates, opt_state = optimizer.update(grads, opt_state)
        weights = optax.apply_updates(weights, updates)
    points = jnp.stack(list_points, axis=0)
    points = jax.device_get(points)
    return points
```

Next, let's apply the different optimizers on our curvature. Note that we set a much higher learning rate for the optimization algorithms as you would in a standard neural network. This is because we only have 2 parameters instead of tens of thousands or even millions.

[30]:
```
SGD_points = train_curve(sgd(lr=10))
SGDMom_points = train_curve(sgd_momentum(lr=10, momentum=0.9))
Adam_points = train_curve(adam(lr=1))
```

To understand best how the different algorithms worked, we visualize the update step as a line plot through the loss surface. We will stick with a 2D representation for readability.

[31]:
```
all_points = np.concatenate([SGD_points, SGDMom_points, Adam_points], axis=0)
ax = plot_curve(pathological_curve_loss,
                x_range=(-np.absolute(all_points[:,0]).max(), np.absolute(all_points[:,
↪0]).max()),
                y_range=(all_points[:,1].min(), all_points[:,1].max()),
                plot_3d=False)
ax.plot(SGD_points[:,0], SGD_points[:,1], color="red", marker="o", zorder=1, label="SGD")
ax.plot(SGDMom_points[:,0], SGDMom_points[:,1], color="blue", marker="o", zorder=2,␣
↪label="SGDMom")
ax.plot(Adam_points[:,0], Adam_points[:,1], color="grey", marker="o", zorder=3, label=
↪"Adam")
plt.legend()
plt.show()
```

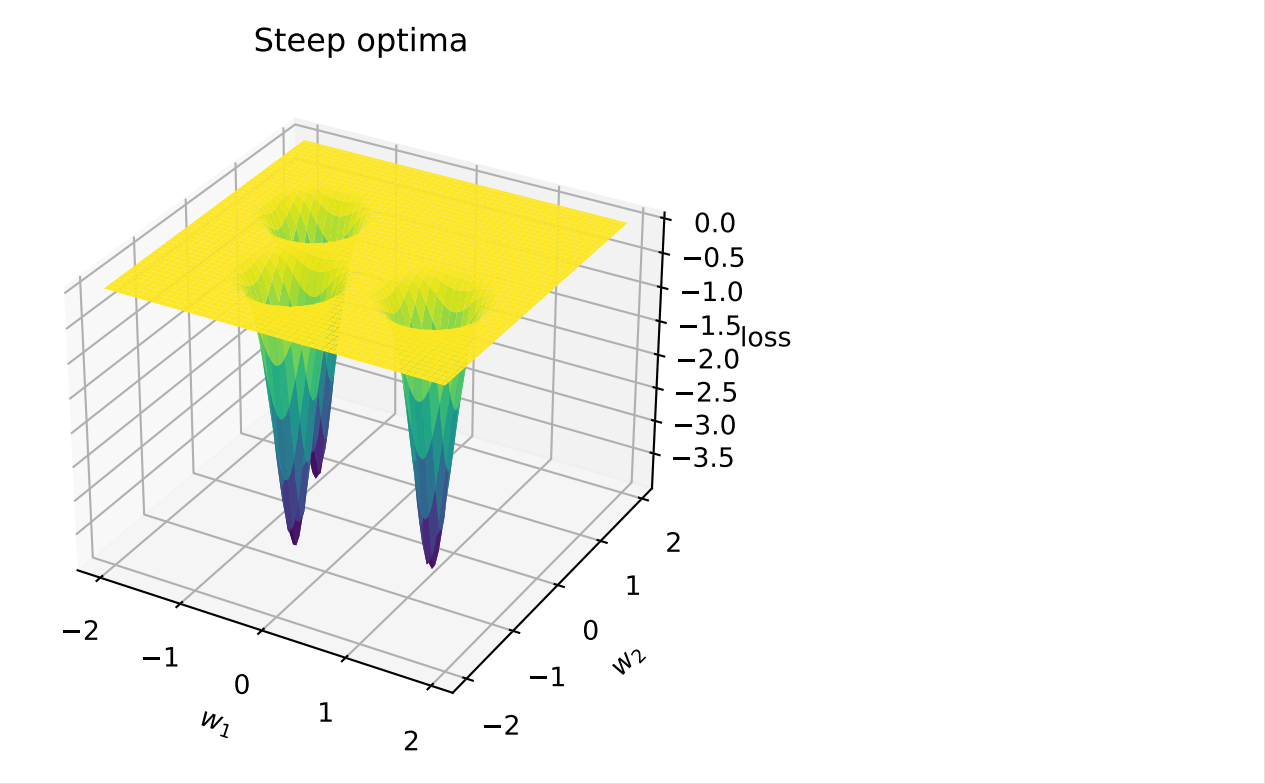


We can clearly see that SGD is not able to find the center of the optimization curve and has a problem converging due to the steep gradients in w_1. In contrast, Adam and SGD with momentum nicely converge as the changing direction of w_1 is canceling itself out. On such surfaces, it is crucial to use momentum.

Steep optima

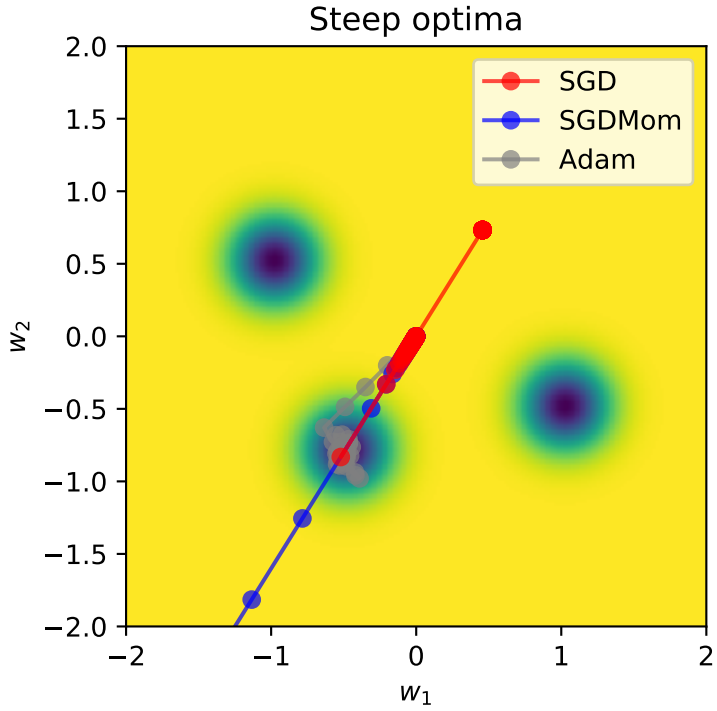
A second type of challenging loss surfaces are steep optima. In those, we have a larger part of the surface having very small gradients while around the optimum, we have very large gradients. For instance, take the following loss surfaces:

[32]:
```
def bivar_gaussian(w1, w2, x_mean=0.0, y_mean=0.0, x_sig=1.0, y_sig=1.0):
    norm = 1 / (2 * np.pi * x_sig * y_sig)
    x_exp = (-1 * (w1 - x_mean)**2) / (2 * x_sig**2)
    y_exp = (-1 * (w2 - y_mean)**2) / (2 * y_sig**2)
    return norm * jnp.exp(x_exp + y_exp)

def comb_func(w1, w2):
    z = -bivar_gaussian(w1, w2, x_mean=1.0, y_mean=-0.5, x_sig=0.2, y_sig=0.2)
    z -= bivar_gaussian(w1, w2, x_mean=-1.0, y_mean=0.5, x_sig=0.2, y_sig=0.2)
    z -= bivar_gaussian(w1, w2, x_mean=-0.5, y_mean=-0.8, x_sig=0.2, y_sig=0.2)
    return z

_ = plot_curve(comb_func, x_range=(-2,2), y_range=(-2,2), plot_3d=True, title="Steep␣
↪optima")
```



Most of the loss surface has very little to no gradients. However, close to the optima, we have very steep gradients. To reach the minimum when starting in a region with lower gradients, we expect an adaptive learning rate to be crucial. To verify this hypothesis, we can run our three optimizers on the surface:

[33]:
```
SGD_points = train_curve(sgd(lr=.5), comb_func, init=[0,0])
SGDMom_points = train_curve(sgd_momentum(lr=1, momentum=0.9), comb_func, init=[0,0])
Adam_points = train_curve(adam(lr=0.2), comb_func, init=[0,0])

all_points = np.concatenate([SGD_points, SGDMom_points, Adam_points], axis=0)
ax = plot_curve(comb_func,
                x_range=(-2, 2),
                y_range=(-2, 2),
                plot_3d=False,
                title="Steep optima")
ax.plot(SGD_points[:,0], SGD_points[:,1], color="red", marker="o", zorder=3, label="SGD",
↪ alpha=0.7)
ax.plot(SGDMom_points[:,0], SGDMom_points[:,1], color="blue", marker="o", zorder=2,␣
↪label="SGDMom", alpha=0.7)
ax.plot(Adam_points[:,0], Adam_points[:,1], color="grey", marker="o", zorder=1, label=
↪"Adam", alpha=0.7)
ax.set_xlim(-2, 2)
ax.set_ylim(-2, 2)
plt.legend()
plt.show()
```



SGD first takes very small steps until it touches the border of the optimum. First reaching a point around $(-0.75, -0.5)$, the gradient direction has changed and pushes the parameters to $(0.8, 0.5)$ from which SGD cannot recover anymore (only with many, many steps). A similar problem has SGD with momentum, only that it continues the direction of the touch of the optimum. The gradients from this time step are so much larger than any other point that the momentum m_t is overpowered by it. Finally, Adam is able to converge in the optimum showing the importance of adaptive learning rates.

What optimizer to take

After seeing the results on optimization, what is our conclusion? Should we always use Adam and never look at SGD anymore? The short answer: no. There are many papers saying that in certain situations, SGD (with momentum) generalizes better where Adam often tends to overfit [5,6]. This is related to the idea of finding wider optima. For instance, see the illustration of different optima below (credit: Keskar et al., 2017):

The black line represents the training loss surface, while the dotted red line is the test loss. Finding sharp, narrow minima can be helpful for finding the minimal training loss. However, this doesn't mean that it also minimizes the test loss as especially flat minima have shown to generalize better. You can imagine that the test dataset has a slightly shifted loss surface due to the different examples than in the training set. A small change can have a significant influence for sharp minima, while flat minima are generally more robust to this change.

In the next tutorial, we will see that some network types can still be better optimized with SGD and learning rate scheduling than Adam. Nevertheless, Adam is the most commonly used optimizer in Deep Learning as it usually performs better than other optimizers, especially for deep networks.

4.32.4 Conclusion

In this tutorial, we have looked at initialization and optimization techniques for neural networks. We have seen that a good initialization has to balance the preservation of the gradient variance as well as the activation variance. This can be achieved with the Xavier initialization for tanh-based networks, and the Kaiming initialization for ReLU-based networks. In optimization, concepts like momentum and adaptive learning rate can help with challenging loss surfaces but don't guarantee an increase in performance for neural networks.

4.32.5 References

[1] Glorot, Xavier, and Yoshua Bengio. "Understanding the difficulty of training deep feedforward neural networks." Proceedings of the thirteenth international conference on artificial intelligence and statistics. 2010. link

[2] He, Kaiming, et al. "Delving deep into rectifiers: Surpassing human-level performance on imagenet classification." Proceedings of the IEEE international conference on computer vision. 2015. link

[3] Kingma, Diederik P. & Ba, Jimmy. "Adam: A Method for Stochastic Optimization." Proceedings of the third international conference for learning representations (ICLR). 2015. link

[4] Keskar, Nitish Shirish, et al. "On large-batch training for deep learning: Generalization gap and sharp minima." Proceedings of the fifth international conference for learning representations (ICLR). 2017. link

[5] Wilson, Ashia C., et al. "The Marginal Value of Adaptive Gradient Methods in Machine Learning." Advances in neural information processing systems. 2017. link

[6] Ruder, Sebastian. "An overview of gradient descent optimization algorithms." arXiv preprint. 2017. link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.33 Tutorial 5 (JAX): Inception, ResNet and DenseNet

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We note the training times for all models in the PyTorch and the JAX implementation below (PyTorch v1.11, JAX v0.3.13). The models were trained on the same hardware (NVIDIA RTX3090, 24 core CPU) and we slightly adjusted the tutorials to use the exact same training settings (200 epochs, data loading parameters, evaluation schedule, etc.). Overall, the JAX implementation is about *2.5-3.4x faster* than PyTorch! However, with larger models, larger batch sizes, or smaller GPUs, the speed up is expected to become considerably smaller.

Models	PyTorch	JAX
GoogleNet	53min 50sec	16min 10sec
ResNet	20min 47sec	7min 51sec
Pre-Activation ResNet	20min 57sec	8min 25sec
DenseNet	49min 23sec	20min 1sec

In this tutorial, we will implement and discuss variants of modern CNN architectures. There have been many different architectures been proposed over the past few years. Some of the most impactful ones, and still relevant today, are the following: GoogleNet/Inception architecture (winner of ILSVRC 2014), ResNet (winner of ILSVRC 2015), and DenseNet (best paper award CVPR 2017). All of them were state-of-the-art models when being proposed, and the core ideas of these networks are the foundations for most current state-of-the-art architectures. Thus, it is important to understand these architectures in detail and learn how to implement them.

Let's start with importing our standard libraries here.

[1]:
```
## Standard libraries
import os
import numpy as np
from PIL import Image
from typing import Any
from collections import defaultdict
import time

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## Progress bar
from tqdm.auto import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)
```

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```
## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch
import torch
import torch.utils.data as data
from torch.utils.tensorboard import SummaryWriter
import torchvision
from torchvision import transforms
from torchvision.datasets import CIFAR10
```

We will use the same path variables `DATASET_PATH` and `CHECKPOINT_PATH` as in the previous tutorials. Adjust the paths if necessary.

[2]:
```
# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial5_jax"

print("Device:", jax.devices()[0])
```

```
Device: gpu:0
```

We also have pretrained models and TensorBoards (more on this later) for this tutorial, and download them below.

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial5/"
# Files to download
pretrained_files = ["GoogleNet.ckpt", "ResNet.ckpt", "PreActResNet.ckpt", "DenseNet.ckpt
↪",
                    "tensorboards/GoogleNet/events.out.tfevents.googlenet",
                    "tensorboards/ResNet/events.out.tfevents.resnet",
                    "tensorboards/PreActResNet/events.out.tfevents.preactresnet",
                    "tensorboards/DenseNet/events.out.tfevents.densenet"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)
```

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```
# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

Throughout this tutorial, we will train and evaluate the models on the CIFAR10 dataset. This allows you to compare the results obtained here with the model you have implemented in the first assignment. As we have learned from the previous tutorial about initialization, it is important to have the data preprocessed with a zero mean. Therefore, as a first step, we will calculate the mean and standard deviation of the CIFAR dataset:

[4]:
```
train_dataset = CIFAR10(root=DATASET_PATH, train=True, download=True)
DATA_MEANS = (train_dataset.data / 255.0).mean(axis=(0,1,2))
DATA_STD = (train_dataset.data / 255.0).std(axis=(0,1,2))
print("Data mean", DATA_MEANS)
print("Data std", DATA_STD)
```

```
Files already downloaded and verified
Data mean [0.49139968 0.48215841 0.44653091]
Data std [0.24703223 0.24348513 0.26158784]
```

We will use this information to normalize our data accordingly. Additionally, we will use transformations from the package `torchvision` to implement data augmentations during training. This reduces the risk of overfitting and helps CNNs to generalize better. Specifically, we will apply two random augmentations.

First, we will flip each image horizontally by a chance of 50% (`transforms.RandomHorizontalFlip`). The object class usually does not change when flipping an image, and we don't expect any image information to be dependent on the horizontal orientation. This would be however different if we would try to detect digits or letters in an image, as those have a certain orientation.

The second augmentation we use is called `transforms.RandomResizedCrop`. This transformation crops the image in a small range, eventually changing the aspect ratio, and scaling it back afterward to the previous size. Therefore, the actual pixel values change while the content or overall semantics of the image stays the same.

We will randomly split the training dataset into a training and a validation set. The validation set will be used for determining early stopping. After finishing the training, we test the models on the CIFAR test set.

[5]:
```
# Transformations applied on each image => bring them into a numpy array
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    img = (img / 255. - DATA_MEANS) / DATA_STD
    return img

# We need to stack the batch elements
def numpy_collate(batch):
```

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```
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)


test_transform = image_to_numpy
# For training, we add some augmentation. Networks are too powerful and would overfit.
train_transform = transforms.Compose([transforms.RandomHorizontalFlip(),
                                      transforms.RandomResizedCrop((32,32),scale=(0.8,1.
↪0),ratio=(0.9,1.1)),
                                      image_to_numpy
                                     ])
# Loading the training dataset. We need to split it into a training and validation part
# We need to do a little trick because the validation set should not use the␣
↪augmentation.
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=train_transform,␣
↪download=True)
val_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=test_transform,␣
↪download=True)
train_set, _ = torch.utils.data.random_split(train_dataset, [45000, 5000],␣
↪generator=torch.Generator().manual_seed(42))
_, val_set = torch.utils.data.random_split(val_dataset, [45000, 5000], generator=torch.
↪Generator().manual_seed(42))

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=test_transform,␣
↪download=True)

# We define a set of data loaders that we can use for training and validation
train_loader = data.DataLoader(train_set,
                               batch_size=128,
                               shuffle=True,
                               drop_last=True,
                               collate_fn=numpy_collate,
                               num_workers=8,
                               persistent_workers=True)
val_loader   = data.DataLoader(val_set,
                               batch_size=128,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate,
                               num_workers=4,
                               persistent_workers=True)
test_loader  = data.DataLoader(test_set,
                               batch_size=128,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate,
```

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```
                                num_workers=4,
                                persistent_workers=True)
```

```
Files already downloaded and verified
Files already downloaded and verified
Files already downloaded and verified
```

To verify that our normalization works, we can print out the mean and standard deviation of the single batch. The mean should be close to 0 and the standard deviation close to 1 for each channel:

[6]:
```
imgs, _ = next(iter(train_loader))
print("Batch mean", imgs.mean(axis=(0,1,2)))
print("Batch std", imgs.std(axis=(0,1,2)))
```

```
Batch mean [-0.05225317 -0.06281322 -0.11905593]
Batch std [0.95375352 0.92699525 0.91463391]
```

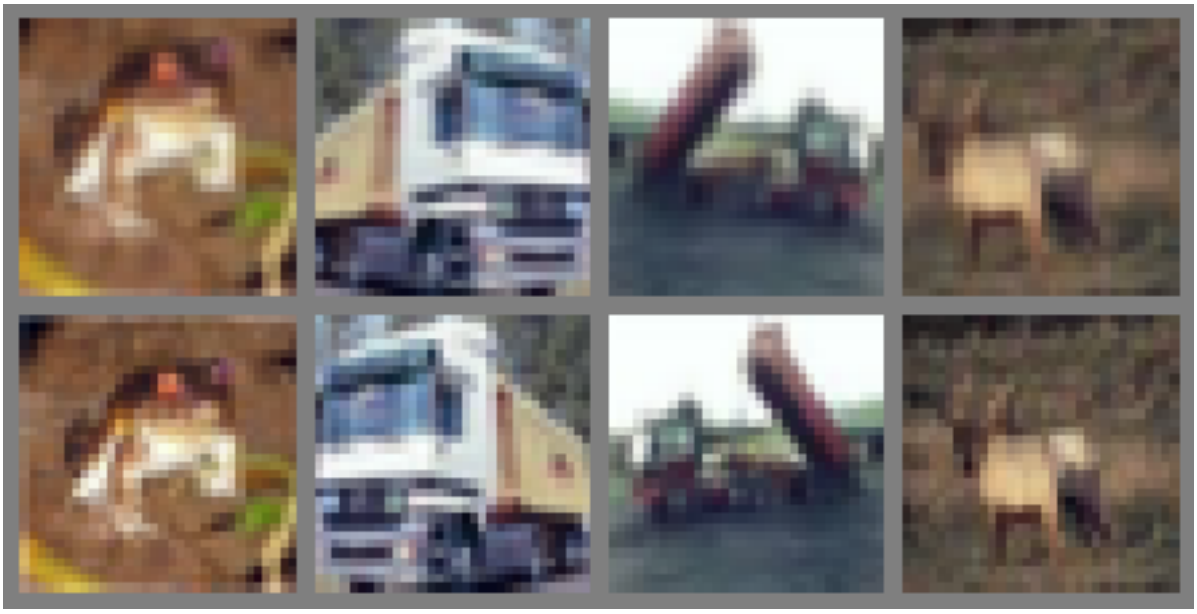
Finally, let's visualize a few images from the training set, and how they look like after random data augmentation:

[7]:
```
NUM_IMAGES = 4
images = [train_dataset[idx][0] for idx in range(NUM_IMAGES)]
orig_images = [Image.fromarray(train_dataset.data[idx]) for idx in range(NUM_IMAGES)]
orig_images = [test_transform(img) for img in orig_images]

imgs = np.stack(images + orig_images, axis=0)
imgs = torch.from_numpy(imgs).permute(0, 3, 1, 2)
img_grid = torchvision.utils.make_grid(imgs, nrow=4, normalize=True, pad_value=0.5)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Augmentation examples on CIFAR10 (Top: augmented, bottom: original)")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

Augmentation examples on CIFAR10 (Top: augmented, bottom: original)



4.33.1 Trainer Module

In the PyTorch version of this tutorial, we would now introduce the framework PyTorch Lightning which simplifies the overall training of a model. So far (June 2022), there is no clear equivalent of it for JAX. Some basic training functionalities are implemented in `flax.training` (documentation), and predefined training modules are implemented in `trax` (documentation), but neither provide a complete, flexible training package yet like PyTorch Lightning. Hence, we need to write our own small training loop.

For this, we take inspiration from PyTorch Lightning and build a trainer module/object with the following main functionalities:

1. *Storing model and parameters*: In order to train multiple models with different hyperparameters, the trainer module creates an instance of the model class, and keeps the parameters in the same class. This way, we can easily apply a model with its parameters on new inputs.
2. *Initialization of model and training state*: During initialization of the trainer, we initialize the model parameters and a new train state, which includes the optimizer and possible learning rate schedulers.
3. *Training, validation and test loops*: Similar to PyTorch Lightning, we implement simple training, validation and test loops, where subclasses of this trainer could overwrite the respective training, validation or test steps. Since in this tutorial, all models will have the same objective, i.e. classification on CIFAR10, we will pre-specify them in the trainer module below.
4. *Logging, saving and loading of models*: To keep track of the training, we implement functionalities to log the training progress and save the best model on the validation set. Afterwards, this model can be loaded from the disk.

Before starting to implement a trainer module with these functionalities, we need to take one prior step. The networks we will implement in this tutorial use BatchNormalization, which carries an exponential average of the prior batch statistics (mean and std) to apply during evaluation. In PyTorch, this is simply tracked by an object attribute of an object of the class `nn.BatchNorm2d`, but in JAX, we only work with functions. Hence, we need to take care of the batch statistics ourselves, similar to the parameters, and enter them during every forward pass. To simplify this a little, we overwrite the `train_state.TrainState` class of Flax by adding a field for the batch statistics:

[8]:
```
class TrainState(train_state.TrainState):
    # A simple extension of TrainState to also include batch statistics
    batch_stats: Any
```

With this, the training state contains both the training parameters and the batch statistics, which makes it easier to keep everything in one place.

Now that the batch statistics are sorted out, we can implement our full training module:

[9]:
```
class TrainerModule:

    def __init__(self,
                 model_name : str,
                 model_class : nn.Module,
                 model_hparams : dict,
                 optimizer_name : str,
                 optimizer_hparams : dict,
                 exmp_imgs : Any,
                 seed=42):
        """
        Module for summarizing all training functionalities for classification on␣
↪CIFAR10.

        Inputs:
            model_name - String of the class name, used for logging and saving
            model_class - Class implementing the neural network
            model_hparams - Hyperparameters of the model, used as input to model␣
↪constructor
            optimizer_name - String of the optimizer name, supporting ['sgd', 'adam', 'adamw
↪']
            optimizer_hparams - Hyperparameters of the optimizer, including learning␣
↪rate as 'lr'
            exmp_imgs - Example imgs, used as input to initialize the model
            seed - Seed to use in the model initialization
        """
        super().__init__()
        self.model_name = model_name
        self.model_class = model_class
        self.model_hparams = model_hparams
        self.optimizer_name = optimizer_name
        self.optimizer_hparams = optimizer_hparams
        self.seed = seed
        # Create empty model. Note: no parameters yet
        self.model = self.model_class(**self.model_hparams)
        # Prepare logging
        self.log_dir = os.path.join(CHECKPOINT_PATH, self.model_name)
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model(exmp_imgs)

    def create_functions(self):
```

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```
        # Function to calculate the classification loss and accuracy for a model
        def calculate_loss(params, batch_stats, batch, train):
            imgs, labels = batch
            # Run model. During training, we need to update the BatchNorm statistics.
            outs = self.model.apply({'params': params, 'batch_stats': batch_stats},
                                    imgs,
                                    train=train,
                                    mutable=['batch_stats'] if train else False)
            logits, new_model_state = outs if train else (outs, None)
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).mean()
            return loss, (acc, new_model_state)
        # Training function
        def train_step(state, batch):
            loss_fn = lambda params: calculate_loss(params, state.batch_stats, batch,␣
↪train=True)
            # Get loss, gradients for loss, and other outputs of loss function
            ret, grads = jax.value_and_grad(loss_fn, has_aux=True)(state.params)
            loss, acc, new_model_state = ret[0], *ret[1]
            # Update parameters and batch statistics
            state = state.apply_gradients(grads=grads, batch_stats=new_model_state[
↪'batch_stats'])
            return state, loss, acc
        # Eval function
        def eval_step(state, batch):
            # Return the accuracy for a single batch
            _, (acc, _) = calculate_loss(state.params, state.batch_stats, batch,␣
↪train=False)
            return acc
        # jit for efficiency
        self.train_step = jax.jit(train_step)
        self.eval_step = jax.jit(eval_step)

    def init_model(self, exmp_imgs):
        # Initialize model
        init_rng = jax.random.PRNGKey(self.seed)
        variables = self.model.init(init_rng, exmp_imgs, train=True)
        self.init_params, self.init_batch_stats = variables['params'], variables['batch_
↪stats']
        self.state = None

    def init_optimizer(self, num_epochs, num_steps_per_epoch):
        # Initialize learning rate schedule and optimizer
        if self.optimizer_name.lower() == 'adam':
            opt_class = optax.adam
        elif self.optimizer_name.lower() == 'adamw':
            opt_class = optax.adamw
        elif self.optimizer_name.lower() == 'sgd':
            opt_class = optax.sgd
        else:
            assert False, f'Unknown optimizer "{opt_class}"'
        # We decrease the learning rate by a factor of 0.1 after 60% and 85% of the␣
↪training
```

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```
        lr_schedule = optax.piecewise_constant_schedule(
            init_value=self.optimizer_hparams.pop('lr'),
            boundaries_and_scales=
                {int(num_steps_per_epoch*num_epochs*0.6): 0.1,
                 int(num_steps_per_epoch*num_epochs*0.85): 0.1}
        )
        # Clip gradients at max value, and evt. apply weight decay
        transf = [optax.clip(1.0)]
        if opt_class == optax.sgd and 'weight_decay' in self.optimizer_hparams:  # wd is␣
↪integrated in adamw
            transf.append(optax.add_decayed_weights(self.optimizer_hparams.pop('weight_
↪decay')))
        optimizer = optax.chain(
            *transf,
            opt_class(lr_schedule, **self.optimizer_hparams)
        )
        # Initialize training state
        self.state = TrainState.create(apply_fn=self.model.apply,
                                       params=self.init_params if self.state is None␣
↪else self.state.params,
                                       batch_stats=self.init_batch_stats if self.state␣
↪is None else self.state.batch_stats,
                                       tx=optimizer)

    def train_model(self, train_loader, val_loader, num_epochs=200):
        # Train model for defined number of epochs
        # We first need to create optimizer and the scheduler for the given number of␣
↪epochs
        self.init_optimizer(num_epochs, len(train_loader))
        # Track best eval accuracy
        best_eval = 0.0
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(train_loader, epoch=epoch_idx)
            if epoch_idx % 2 == 0:
                eval_acc = self.eval_model(val_loader)
                self.logger.add_scalar('val/acc', eval_acc, global_step=epoch_idx)
                if eval_acc >= best_eval:
                    best_eval = eval_acc
                    self.save_model(step=epoch_idx)
                self.logger.flush()

    def train_epoch(self, train_loader, epoch):
        # Train model for one epoch, and log avg loss and accuracy
        metrics = defaultdict(list)
        for batch in tqdm(train_loader, desc='Training', leave=False):
            self.state, loss, acc = self.train_step(self.state, batch)
            metrics['loss'].append(loss)
            metrics['acc'].append(acc)
        for key in metrics:
            avg_val = np.stack(jax.device_get(metrics[key])).mean()
            self.logger.add_scalar('train/'+key, avg_val, global_step=epoch)
```

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```
    def eval_model(self, data_loader):
        # Test model on all images of a data loader and return avg loss
        correct_class, count = 0, 0
        for batch in data_loader:
            acc = self.eval_step(self.state, batch)
            correct_class += acc * batch[0].shape[0]
            count += batch[0].shape[0]
        eval_acc = (correct_class / count).item()
        return eval_acc

    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir,
                                    target={'params': self.state.params,
                                            'batch_stats': self.state.batch_stats},
                                    step=step,
                                    overwrite=True)

    def load_model(self, pretrained=False):
        # Load model. We use different checkpoint for pretrained models
        if not pretrained:
            state_dict = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir,␣
↪target=None)
        else:
            state_dict = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'{self.model_name}.ckpt'), target=None)
        self.state = TrainState.create(apply_fn=self.model.apply,
                                       params=state_dict['params'],
                                       batch_stats=state_dict['batch_stats'],
                                       tx=self.state.tx if self.state else optax.sgd(0.
↪1)   # Default optimizer
                                      )

    def checkpoint_exists(self):
        # Check whether a pretrained model exist for this autoencoder
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'{self.model_name}.ckpt'))
```

Next, we can use this trainer module to create a compact training function:

[10]:
```
def train_classifier(*args, num_epochs=200, **kwargs):
    # Create a trainer module with specified hyperparameters
    trainer = TrainerModule(*args, **kwargs)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(train_loader, val_loader, num_epochs=num_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    # Test trained model
    val_acc = trainer.eval_model(val_loader)
    test_acc = trainer.eval_model(test_loader)
    return trainer, {'val': val_acc, 'test': test_acc}
```

Finally, we can focus on the Convolutional Neural Networks we want to implement today: GoogleNet, ResNet, and

DenseNet.

4.33.2 Inception

The GoogleNet, proposed in 2014, won the ImageNet Challenge because of its usage of the Inception modules. In general, we will mainly focus on the concept of Inception in this tutorial instead of the specifics of the GoogleNet, as based on Inception, there have been many follow-up works (Inception-v2, Inception-v3, Inception-v4, Inception-ResNet,...). The follow-up works mainly focus on increasing efficiency and enabling very deep Inception networks. However, for a fundamental understanding, it is sufficient to look at the original Inception block.

An Inception block applies four convolution blocks separately on the same feature map: a 1x1, 3x3, and 5x5 convolution, and a max pool operation. This allows the network to look at the same data with different receptive fields. Of course, learning only 5x5 convolution would be theoretically more powerful. However, this is not only more computation and memory heavy but also tends to overfit much easier. The overall inception block looks like below (figure credit - Szegedy et al.):

The additional 1x1 convolutions before the 3x3 and 5x5 convolutions are used for dimensionality reduction. This is especially crucial as the feature maps of all branches are merged afterward, and we don't want any explosion of feature size. As 5x5 convolutions are 25 times more expensive than 1x1 convolutions, we can save a lot of computation and parameters by reducing the dimensionality before the large convolutions.

We can now try to implement the Inception Block ourselves:

[11]:
```
googlenet_kernel_init = nn.initializers.kaiming_normal()

class InceptionBlock(nn.Module):
    c_red : dict  # Dictionary of reduced dimensionalities with keys "1x1", "3x3", "5x5",
↪ and "max"
    c_out : dict  # Dictionary of output feature sizes with keys "1x1", "3x3", "5x5",␣
↪and "max"
    act_fn : callable   # Activation function

    @nn.compact
    def __call__(self, x, train=True):
        # 1x1 convolution branch
        x_1x1 = nn.Conv(self.c_out["1x1"], kernel_size=(1, 1), kernel_init=googlenet_
↪kernel_init, use_bias=False)(x)
        x_1x1 = nn.BatchNorm()(x_1x1, use_running_average=not train)
        x_1x1 = self.act_fn(x_1x1)

        # 3x3 convolution branch
        x_3x3 = nn.Conv(self.c_red["3x3"], kernel_size=(1, 1), kernel_init=googlenet_
↪kernel_init, use_bias=False)(x)
        x_3x3 = nn.BatchNorm()(x_3x3, use_running_average=not train)
        x_3x3 = self.act_fn(x_3x3)
        x_3x3 = nn.Conv(self.c_out["3x3"], kernel_size=(3, 3), kernel_init=googlenet_
↪kernel_init, use_bias=False)(x_3x3)
        x_3x3 = nn.BatchNorm()(x_3x3, use_running_average=not train)
        x_3x3 = self.act_fn(x_3x3)

        # 5x5 convolution branch
        x_5x5 = nn.Conv(self.c_red["5x5"], kernel_size=(1, 1), kernel_init=googlenet_
↪kernel_init, use_bias=False)(x)
```

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```
        x_5x5 = nn.BatchNorm()(x_5x5, use_running_average=not train)
        x_5x5 = self.act_fn(x_5x5)
        x_5x5 = nn.Conv(self.c_out["5x5"], kernel_size=(5, 5), kernel_init=googlenet_
↪kernel_init, use_bias=False)(x_5x5)
        x_5x5 = nn.BatchNorm()(x_5x5, use_running_average=not train)
        x_5x5 = self.act_fn(x_5x5)

        # Max-pool branch
        x_max = nn.max_pool(x, (3, 3), strides=(2, 2))
        x_max = nn.Conv(self.c_out["max"], kernel_size=(1, 1), kernel_init=googlenet_
↪kernel_init, use_bias=False)(x)
        x_max = nn.BatchNorm()(x_max, use_running_average=not train)
        x_max = self.act_fn(x_max)

        x_out = jnp.concatenate([x_1x1, x_3x3, x_5x5, x_max], axis=-1)
        return x_out
```

The GoogleNet architecture consists of stacking multiple Inception blocks with occasional max pooling to reduce the height and width of the feature maps. The original GoogleNet was designed for image sizes of ImageNet (224x224 pixels) and had almost 7 million parameters. As we train on CIFAR10 with image sizes of 32x32, we don't require such a heavy architecture, and instead, apply a reduced version. The number of channels for dimensionality reduction and output per filter (1x1, 3x3, 5x5, and max pooling) need to be manually specified and can be changed if interested. The general intuition is to have the most filters for the 3x3 convolutions, as they are powerful enough to take the context into account while requiring almost a third of the parameters of the 5x5 convolution.

[12]:
```
class GoogleNet(nn.Module):
    num_classes : int
    act_fn : callable

    @nn.compact
    def __call__(self, x, train=True):
        # A first convolution on the original image to scale up the channel size
        x = nn.Conv(64, kernel_size=(3, 3), kernel_init=googlenet_kernel_init, use_
↪bias=False)(x)
        x = nn.BatchNorm()(x, use_running_average=not train)
        x = self.act_fn(x)

        # Stacking inception blocks
        inception_blocks = [
            InceptionBlock(c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 16, "3x3": 32,
↪"5x5": 8, "max": 8}, act_fn=self.act_fn),
            InceptionBlock(c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 24, "3x3": 48,
↪"5x5": 12, "max": 12}, act_fn=self.act_fn),
            lambda inp: nn.max_pool(inp, (3, 3), strides=(2, 2)),  # 32x32 => 16x16
            InceptionBlock(c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 24, "3x3": 48,
↪"5x5": 12, "max": 12}, act_fn=self.act_fn),
            InceptionBlock(c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 16, "3x3": 48,
↪"5x5": 16, "max": 16}, act_fn=self.act_fn),
            InceptionBlock(c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 16, "3x3": 48,
↪"5x5": 16, "max": 16}, act_fn=self.act_fn),
            InceptionBlock(c_red={"3x3": 32, "5x5": 16}, c_out={"1x1": 32, "3x3": 48,
↪"5x5": 24, "max": 24}, act_fn=self.act_fn),
```

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```
            lambda inp: nn.max_pool(inp, (3, 3), strides=(2, 2)),  # 16x16 => 8x8
            InceptionBlock(c_red={"3x3": 48, "5x5": 16}, c_out={"1x1": 32, "3x3": 64,
↪"5x5": 16, "max": 16}, act_fn=self.act_fn),
            InceptionBlock(c_red={"3x3": 48, "5x5": 16}, c_out={"1x1": 32, "3x3": 64,
↪"5x5": 16, "max": 16}, act_fn=self.act_fn)
        ]
        for block in inception_blocks:
            x = block(x, train=train) if isinstance(block, InceptionBlock) else block(x)

        # Mapping to classification output
        x = x.mean(axis=(1, 2))
        x = nn.Dense(self.num_classes)(x)
        return x
```

The training of the model is handled by our previously implemented training function, and we just have to define the command to start. Note that we train for 200 epochs, which takes about 15mins on a RTX3090. We would recommend using the saved models and train your own model if you are interested.

[13]:
```
googlenet_trainer, googlenet_results = train_classifier(model_class=GoogleNet,
                                                         model_name="GoogleNet",
                                                         model_hparams={"num_classes": 10,
                                                                        "act_fn": nn.relu}
↪,
                                                         optimizer_name="adamw",
                                                         optimizer_hparams={"lr": 1e-3,
                                                                            "weight_decay
↪": 1e-4},
                                                         exmp_imgs=jax.device_put(
                                                             next(iter(train_loader))[0]),
                                                         num_epochs=200)
```

We will compare the results later in the notebooks, but we can already print them here for a first glance:

[14]:
```
print("GoogleNet Results", googlenet_results)
```

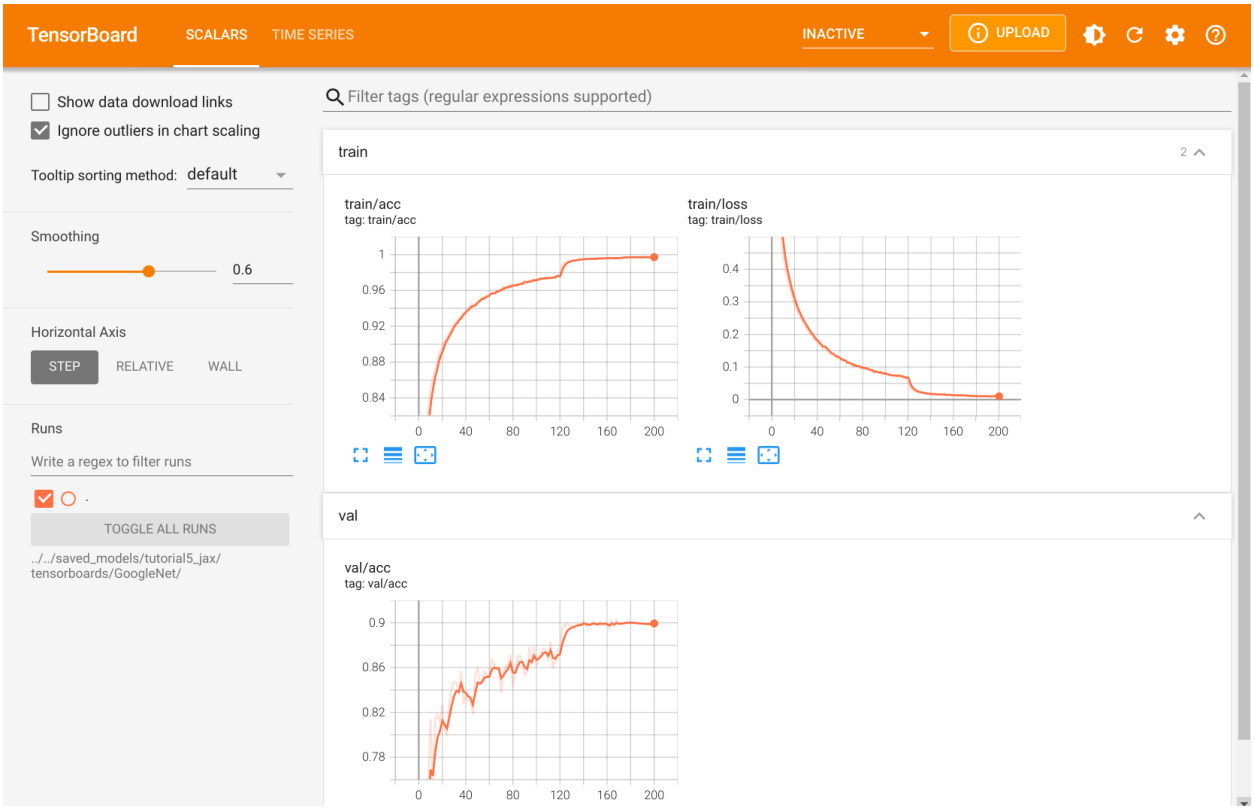
```
GoogleNet Results {'val': 0.9022000432014465, 'test': 0.8911000490188599}
```

Tensorboard log

For logging our results, we have used TensorBoard. To give you a better intuition of what TensorBoard can be used for, we can look at the board that our training of the GoogleNet has generated. TensorBoard provides an inline functionality for Jupyter notebooks, and we use it here:

[15]:
```
# Load tensorboard extension
%load_ext tensorboard
```

[16]:
```
# Opens tensorboard in notebook.
%tensorboard --logdir $CHECKPOINT_PATH/tensorboards/GoogleNet/
```



TensorBoard is organized in multiple tabs. The main tab is the scalar tab where we can log the development of single numbers. For example, we have plotted the training loss, accuracy, learning rate, etc. If we look at the training or validation accuracy, we can really see the impact of using a learning rate scheduler. Reducing the learning rate gives our model a nice increase in training performance. Similarly, when looking at the training loss, we see a sudden decrease at this point. However, the high numbers on the training set compared to validation indicate that our model was overfitting which is inevitable for such large networks.

4.33.3 ResNet

The ResNet paper is one of the most cited AI papers, and has been the foundation for neural networks with more than 1,000 layers. Despite its simplicity, the idea of residual connections is highly effective as it supports stable gradient propagation through the network. Instead of modeling $x_{l+1} = F(x_l)$, we model $x_{l+1} = x_l + F(x_l)$ where F is a non-linear mapping (usually a sequence of NN modules likes convolutions, activation functions, and normalizations). If we do backpropagation on such residual connections, we obtain:

$$\frac{\partial x_{l+1}}{\partial x_l} = \mathbf{I} + \frac{\partial F(x_l)}{\partial x_l}$$

The bias towards the identity matrix guarantees a stable gradient propagation being less effected by F itself. There have been many variants of ResNet proposed, which mostly concern the function F, or operations applied on the sum. In this tutorial, we look at two of them: the original ResNet block, and the Pre-Activation ResNet block. We visually compare the blocks below (figure credit - He et al.):

The original ResNet block applies a non-linear activation function, usually ReLU, after the skip connection. In contrast, the pre-activation ResNet block applies the non-linearity at the beginning of F. Both have their advantages and disadvantages. For very deep network, however, the pre-activation ResNet has shown to perform better as the gradient flow

is guaranteed to have the identity matrix as calculated above, and is not harmed by any non-linear activation applied to it. For comparison, in this notebook, we implement both ResNet types as shallow networks.

Let's start with the original ResNet block. The visualization above already shows what layers are included in F. One special case we have to handle is when we want to reduce the image dimensions in terms of width and height. The basic ResNet block requires $F(x_l)$ to be of the same shape as x_l. Thus, we need to change the dimensionality of x_l as well before adding to $F(x_l)$. The original implementation used an identity mapping with stride 2 and padded additional feature dimensions with 0. However, the more common implementation is to use a 1x1 convolution with stride 2 as it allows us to change the feature dimensionality while being efficient in parameter and computation cost. The code for the ResNet block is relatively simple, and shown below:

[17]:
```
# Conv initialized with kaiming int, but uses fan-out instead of fan-in mode
# Fan-out focuses on the gradient distribution, and is commonly used in ResNets
resnet_kernel_init = nn.initializers.variance_scaling(2.0, mode='fan_out', distribution=
↪'normal')

class ResNetBlock(nn.Module):
    act_fn : callable  # Activation function
    c_out : int   # Output feature size
    subsample : bool = False  # If True, we apply a stride inside F

    @nn.compact
    def __call__(self, x, train=True):
        # Network representing F
        z = nn.Conv(self.c_out, kernel_size=(3, 3),
                    strides=(1, 1) if not self.subsample else (2, 2),
                    kernel_init=resnet_kernel_init,
                    use_bias=False)(x)
        z = nn.BatchNorm()(z, use_running_average=not train)
        z = self.act_fn(z)
        z = nn.Conv(self.c_out, kernel_size=(3, 3),
                    kernel_init=resnet_kernel_init,
                    use_bias=False)(z)
        z = nn.BatchNorm()(z, use_running_average=not train)

        if self.subsample:
            x = nn.Conv(self.c_out, kernel_size=(1, 1), strides=(2, 2), kernel_
↪init=resnet_kernel_init)(x)

        x_out = self.act_fn(z + x)
        return x_out
```

The second block we implement is the pre-activation ResNet block. For this, we have to change the order of layers, and do not apply an activation function on the output. Additionally, the downsampling operation has to apply a non-linearity as well as the input, x_l, has not been processed by a non-linearity yet. Hence, the block looks as follows:

[18]:
```
class PreActResNetBlock(ResNetBlock):

    @nn.compact
    def __call__(self, x, train=True):
        # Network representing F
        z = nn.BatchNorm()(x, use_running_average=not train)
        z = self.act_fn(z)
        z = nn.Conv(self.c_out, kernel_size=(3, 3),
```

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```
                    strides=(1, 1) if not self.subsample else (2, 2),
                    kernel_init=resnet_kernel_init,
                    use_bias=False)(z)
        z = nn.BatchNorm()(z, use_running_average=not train)
        z = self.act_fn(z)
        z = nn.Conv(self.c_out, kernel_size=(3, 3),
                    kernel_init=resnet_kernel_init,
                    use_bias=False)(z)

        if self.subsample:
            x = nn.BatchNorm()(x, use_running_average=not train)
            x = self.act_fn(x)
            x = nn.Conv(self.c_out,
                        kernel_size=(1, 1),
                        strides=(2, 2),
                        kernel_init=resnet_kernel_init,
                        use_bias=False)(x)

        x_out = z + x
        return x_out
```

The overall ResNet architecture consists of stacking multiple ResNet blocks, of which some are downsampling the input. When talking about ResNet blocks in the whole network, we usually group them by the same output shape. Hence, if we say the ResNet has `[3,3,3]` blocks, it means that we have 3 times a group of 3 ResNet blocks, where a subsampling is taking place in the fourth and seventh block. The ResNet with `[3,3,3]` blocks on CIFAR10 is visualized below.

The three groups operate on the resolutions 32×32, 16×16 and 8×8 respectively. The blocks in orange denote ResNet blocks with downsampling. The same notation is used by many other implementations such as in the torchvision library from PyTorch or flaxmodels (pretrained ResNets and more for JAX). Thus, our code looks as follows:

[19]:
```
class ResNet(nn.Module):
    num_classes : int
    act_fn : callable
    block_class : nn.Module
    num_blocks : tuple = (3, 3, 3)
    c_hidden : tuple = (16, 32, 64)

    @nn.compact
    def __call__(self, x, train=True):
        # A first convolution on the original image to scale up the channel size
        x = nn.Conv(self.c_hidden[0], kernel_size=(3, 3), kernel_init=resnet_kernel_init,
↪ use_bias=False)(x)
        if self.block_class == ResNetBlock:  # If pre-activation block, we do not apply␣
↪non-linearities yet
            x = nn.BatchNorm()(x, use_running_average=not train)
            x = self.act_fn(x)

        # Creating the ResNet blocks
        for block_idx, block_count in enumerate(self.num_blocks):
            for bc in range(block_count):
                # Subsample the first block of each group, except the very first one.
```

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```
                subsample = (bc == 0 and block_idx > 0)
                # ResNet block
                x = self.block_class(c_out=self.c_hidden[block_idx],
                                     act_fn=self.act_fn,
                                     subsample=subsample)(x, train=train)

        # Mapping to classification output
        x = x.mean(axis=(1, 2))
        x = nn.Dense(self.num_classes)(x)
        return x
```

Finally, we can train our ResNet models. One difference to the GoogleNet training is that we explicitly use SGD with Momentum as optimizer instead of Adam. Adam often leads to a slightly worse accuracy on plain, shallow ResNets. It is not 100% clear why Adam performs worse in this context, but one possible explanation is related to ResNet's loss surface. ResNet has been shown to produce smoother loss surfaces than networks without skip connection (see Li et al., 2018 for details). A possible visualization of the loss surface with/out skip connections is below (figure credit - Li et al.):

The x and y axis shows a projection of the parameter space, and the z axis shows the loss values achieved by different parameter values. On smooth surfaces like the one on the right, we might not require an adaptive learning rate as Adam provides. Instead, Adam can get stuck in local optima while SGD finds the wider minima that tend to generalize better. However, to answer this question in detail, we would need an extra tutorial because it is not easy to answer. For now, we conclude: for ResNet architectures, consider the optimizer to be an important hyperparameter, and try training with both Adam and SGD. Let's train the model below with SGD:

[20]:
```
resnet_trainer, resnet_results = train_classifier(model_name="ResNet",
                                                  model_class=ResNet,
                                                  model_hparams={"num_classes": 10,
                                                                 "c_hidden": (16, 32,␣
↪64),
                                                                 "num_blocks": (3, 3, 3),
                                                                 "act_fn": nn.relu,
                                                                 "block_class":␣
↪ResNetBlock},
                                                  optimizer_name="SGD",
                                                  optimizer_hparams={"lr": 0.1,
                                                                     "momentum": 0.9,
                                                                     "weight_decay": 1e-
↪4},
                                                  exmp_imgs=jax.device_put(
                                                      next(iter(train_loader))[0]),
                                                  num_epochs=200)
```

Let's also train the pre-activation ResNet as comparison:

[21]:
```
preactresnet_trainer, preactresnet_results = train_classifier(model_name="PreActResNet",
                                                              model_class=ResNet,
                                                              model_hparams={"num_classes
↪": 10,
                                                                             "c_hidden":␣
↪(16, 32, 64),
```

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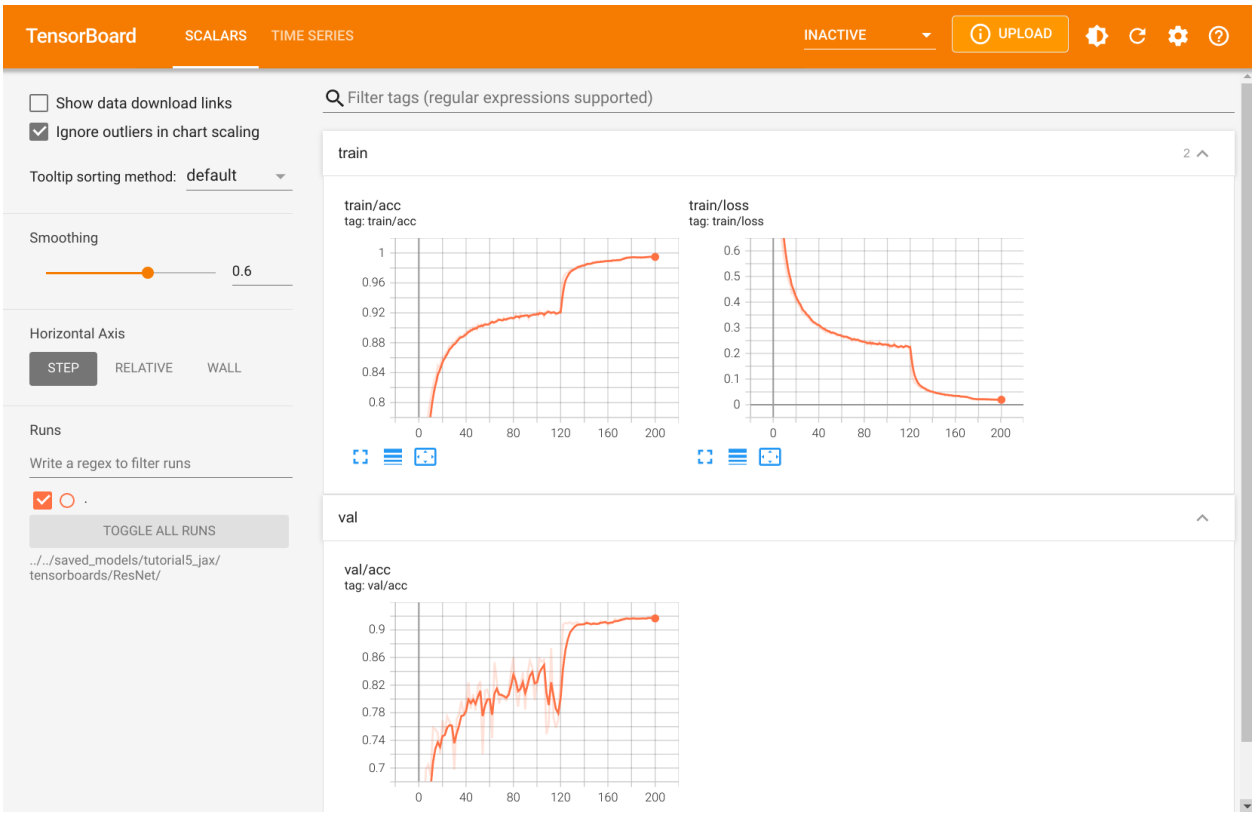
```
                                                                    "num_blocks
↪": (3, 3, 3),
                                                                    "act_fn":␣
↪nn.relu,
                                                                    "block_class
↪": PreActResNetBlock},
                                                          optimizer_name="SGD",
                                                          optimizer_hparams={"lr": 0.
↪1,
↪"momentum": 0.9,
                                                                              "weight_
↪decay": 1e-4},
                                                          exmp_imgs=jax.device_put(
                                                              next(iter(train_
↪loader))[0]),
                                                          num_epochs=200)
```

Tensorboard log

Similarly to our GoogleNet model, we also have a TensorBoard log for the ResNet model. We can open it below.

[22]:
```
# Opens tensorboard in notebook. Feel free to change "ResNet" to "PreActResNet"
%tensorboard --logdir $CHECKPOINT_PATH/tensorboards/ResNet/ --port 6007
```



Feel free to explore the TensorBoard yourself, including the computation graph. In general, we can see that with SGD,

the ResNet has a higher training loss than the GoogleNet in the first stage of the training. After reducing the learning rate however, the model achieves even higher validation accuracies. We compare the precise scores at the end of the notebook.

4.33.4 DenseNet

DenseNet is another architecture for enabling very deep neural networks and takes a slightly different perspective on residual connections. Instead of modeling the difference between layers, DenseNet considers residual connections as a possible way to reuse features across layers, removing any necessity to learn redundant feature maps. If we go deeper into the network, the model learns abstract features to recognize patterns. However, some complex patterns consist of a combination of abstract features (e.g. hand, face, etc.), and low-level features (e.g. edges, basic color, etc.). To find these low-level features in the deep layers, standard CNNs have to learn copy such feature maps, which wastes a lot of parameter complexity. DenseNet provides an efficient way of reusing features by having each convolution depends on all previous input features, but add only a small amount of filters to it. See the figure below for an illustration (figure credit - Hu et al.):

The last layer, called the transition layer, is responsible for reducing the dimensionality of the feature maps in height, width, and channel size. Although those technically break the identity backpropagation, there are only a few in a network so that it doesn't affect the gradient flow much.

We split the implementation of the layers in DenseNet into three parts: a `DenseLayer`, and a `DenseBlock`, and a `TransitionLayer`. The module `DenseLayer` implements a single layer inside a dense block. It applies a 1x1 convolution for dimensionality reduction with a subsequential 3x3 convolution. The output channels are concatenated to the originals and returned. Note that we apply the Batch Normalization as the first layer of each block. This allows slightly different activations for the same features to different layers, depending on what is needed. Overall, we can implement it as follows:

[23]:
```
densenet_kernel_init = nn.initializers.kaiming_normal()

class DenseLayer(nn.Module):
    bn_size : int  # Bottleneck size (factor of growth rate) for the output of the 1x1␣
↪convolution
    growth_rate : int  # Number of output channels of the 3x3 convolution
    act_fn : callable  # Activation function

    @nn.compact
    def __call__(self, x, train=True):
        z = nn.BatchNorm()(x, use_running_average=not train)
        z = self.act_fn(z)
        z = nn.Conv(self.bn_size * self.growth_rate,
                    kernel_size=(1, 1),
                    kernel_init=densenet_kernel_init,
                    use_bias=False)(z)
        z = nn.BatchNorm()(z, use_running_average=not train)
        z = self.act_fn(z)
        z = nn.Conv(self.growth_rate,
                    kernel_size=(3, 3),
                    kernel_init=densenet_kernel_init,
                    use_bias=False)(z)
        x_out = jnp.concatenate([x, z], axis=-1)
        return x_out
```

The module `DenseBlock` summarizes multiple dense layers applied in sequence. Each dense layer takes as input the original input concatenated with all previous layers' feature maps:

[24]:
```
class DenseBlock(nn.Module):
    num_layers : int  # Number of dense layers to apply in the block
    bn_size : int  # Bottleneck size to use in the dense layers
    growth_rate : int  # Growth rate to use in the dense layers
    act_fn : callable  # Activation function to use in the dense layers

    @nn.compact
    def __call__(self, x, train=True):
        for _ in range(self.num_layers):
            x = DenseLayer(bn_size=self.bn_size,
                           growth_rate=self.growth_rate,
                           act_fn=self.act_fn)(x, train=train)
        return x
```

Finally, the `TransitionLayer` takes as input the final output of a dense block and reduces its channel dimensionality using a 1x1 convolution. To reduce the height and width dimension, we take a slightly different approach than in ResNet and apply an average pooling with kernel size 2 and stride 2. This is because we don't have an additional connection to the output that would consider the full 2x2 patch instead of a single value. Besides, it is more parameter efficient than using a 3x3 convolution with stride 2. Thus, the layer is implemented as follows:

[25]:
```
class TransitionLayer(nn.Module):
    c_out : int  # Output feature size
    act_fn : callable  # Activation function

    @nn.compact
    def __call__(self, x, train=True):
        x = nn.BatchNorm()(x, use_running_average=not train)
        x = self.act_fn(x)
        x = nn.Conv(self.c_out,
                    kernel_size=(1, 1),
                    kernel_init=densenet_kernel_init,
                    use_bias=False)(x)
        x = nn.avg_pool(x, (2, 2), strides=(2, 2))
        return x
```

Now we can put everything together and create our DenseNet. To specify the number of layers, we use a similar notation as in ResNets and pass on a list of ints representing the number of layers per block. After each dense block except the last one, we apply a transition layer to reduce the dimensionality by 2.

[26]:
```
class DenseNet(nn.Module):
    num_classes : int
    act_fn : callable = nn.relu
    num_layers : tuple = (6, 6, 6, 6)
    bn_size : int = 2
    growth_rate : int = 16

    @nn.compact
    def __call__(self, x, train=True):
        c_hidden = self.growth_rate * self.bn_size  # The start number of hidden channels

        x = nn.Conv(c_hidden,
```

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```
                    kernel_size=(3, 3),
                    kernel_init=densenet_kernel_init)(x)

        for block_idx, num_layers in enumerate(self.num_layers):
            x = DenseBlock(num_layers=num_layers,
                           bn_size=self.bn_size,
                           growth_rate=self.growth_rate,
                           act_fn=self.act_fn)(x, train=train)
            c_hidden += num_layers * self.growth_rate
            if block_idx < len(self.num_layers)-1:  # Don't apply transition layer on␣
↪last block
                x = TransitionLayer(c_out=c_hidden//2,
                                    act_fn=self.act_fn)(x, train=train)
                c_hidden //= 2

        x = nn.BatchNorm()(x, use_running_average=not train)
        x = self.act_fn(x)
        x = x.mean(axis=(1, 2))
        x = nn.Dense(self.num_classes)(x)
        return x
```

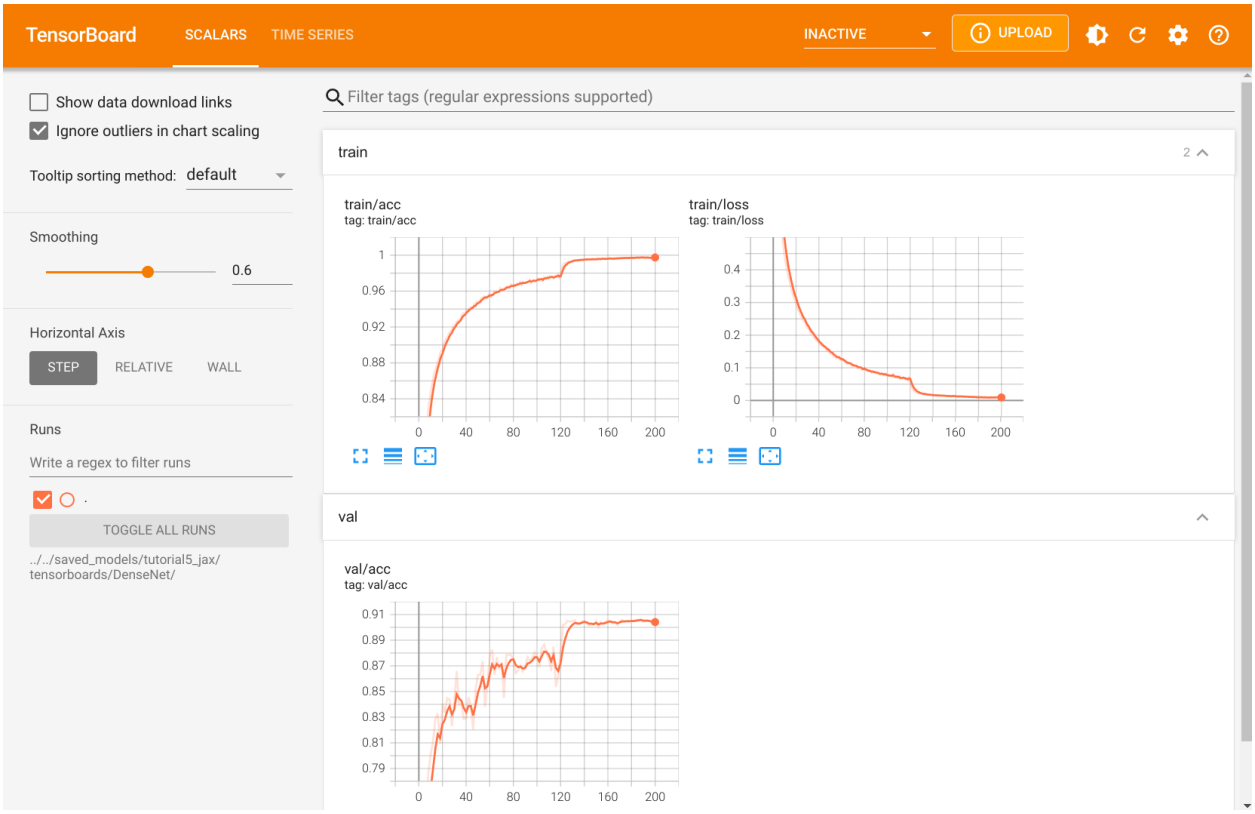
Lastly, we train our network. In contrast to ResNet, DenseNet does not show any issues with Adam, and hence we train it with this optimizer. The other hyperparameters are chosen to result in a network with a similar parameter size as the ResNet and GoogleNet. Commonly, when designing very deep networks, DenseNet is more parameter efficient than ResNet while achieving a similar or even better performance.

[27]:
```
densenet_trainer, densenet_results = train_classifier(model_name="DenseNet",
                                                      model_class=DenseNet,
                                                      model_hparams={"num_classes": 10,
                                                                     "num_layers": [6, 6,
↪ 6, 6],
                                                                     "bn_size": 2,
                                                                     "growth_rate": 16,
                                                                     "act_fn": nn.relu},
                                                      optimizer_name="adamw",
                                                      optimizer_hparams={"lr": 1e-3,
                                                                         "weight_decay":␣
↪1e-4},
                                                      exmp_imgs=jax.device_put(
                                                          next(iter(train_loader))[0]),
                                                      num_epochs=200)
```

Tensorboard log

Finally, we also have another TensorBoard for the DenseNet training. We take a look at it below:

[28]:
```
# Opens tensorboard in notebook.
%tensorboard --logdir $CHECKPOINT_PATH/tensorboards/DenseNet/ --port 6008
```



The overall course of the validation accuracy and training loss resemble the training of GoogleNet, which is also related to training the network with Adam. Feel free to explore the training metrics yourself.

4.33.5 Conclusion and Comparison

After discussing each model separately, and training all of them, we can finally compare them. First, let's organize the results of all models in a table:

[29]:
```
%%html
<!-- Some HTML code to increase font size in the following table -->
<style>
th {font-size: 120%;}
td {font-size: 120%;}
</style>
```

```
<IPython.core.display.HTML object>
```

[30]:
```
import tabulate
from IPython.display import display, HTML
all_models = [
```

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```
    ("GoogleNet", googlenet_results, googlenet_trainer),
    ("ResNet", resnet_results, resnet_trainer),
    ("PreActResNet", preactresnet_results, preactresnet_trainer),
    ("DenseNet", densenet_results, densenet_trainer)
]
table = [[model_name,
          f"{100.0*model_results['val']:4.2f}%",
          f"{100.0*model_results['test']:4.2f}%",
          "{:,}".format(sum([np.prod(p.shape) for p in jax.tree_leaves(model.state.
↪params)]))]
         for model_name, model_results, model in all_models]
display(HTML(tabulate.tabulate(table, tablefmt='html', headers=["Model", "Val Accuracy",
↪"Test Accuracy", "Num Parameters"])))
```

```
<IPython.core.display.HTML object>
```

First of all, we see that all models are performing reasonably well. Simple models as you have implemented them in the practical achieve considerably lower performance, which is beside the lower number of parameters also attributed to the architecture design choice. GoogleNet is the model to obtain the lowest performance on the validation and test set, although it is very close to DenseNet. A proper hyperparameter search over all the channel sizes in GoogleNet would likely improve the accuracy of the model to a similar level, but this is also expensive given a large number of hyperparameters. ResNet outperforms both DenseNet and GoogleNet by more than 1% on the validation set, while there is a minor difference between both versions, original and pre-activation. We can conclude that for shallow networks, the place of the activation function does not seem to be crucial, although papers have reported the contrary for very deep networks (e.g. He et al.).

In general, we can conclude that ResNet is a simple, but powerful architecture. If we would apply the models on more complex tasks with larger images and more layers inside the networks, we would likely see a bigger gap between GoogleNet and skip-connection architectures like ResNet and DenseNet. A comparison with deeper models on CIFAR10 can be for example found here. Interestingly, DenseNet outperforms the original ResNet on their setup but comes closely behind the Pre-Activation ResNet. The best model, a Dual Path Network (Chen et. al), is actually a combination of ResNet and DenseNet showing that both offer different advantages.

Which model should I choose for my task?

We have reviewed four different models. So, which one should we choose if have given a new task? Usually, starting with a ResNet is a good idea given the superior performance of the CIFAR dataset and its simple implementation. Besides, for the parameter number we have chosen here, ResNet is the fastest as DenseNet and GoogleNet have many more layers that are applied in sequence in our primitive implementation. However, if you have a really difficult task, such as semantic segmentation on HD images, more complex variants of ResNet and DenseNet are recommended.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.34 Tutorial 6 (JAX): Transformers and Multi-Head Attention

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We note the training times for all models in the PyTorch and the JAX implementation below (PyTorch v1.11, JAX v0.3.13). The models were trained on the same hardware (NVIDIA RTX3090, 24 core CPU) and we slightly adjusted the tutorials to use the exact same training settings (same data loading parameters, evaluation schedule, etc.). Overall, the JAX implementation is almost *4x faster* than PyTorch! However, this is mostly due to the small model and input sizes, and the code has not been explicitly designed for benchmarking. With larger models, larger batch sizes, or smaller GPUs, the speed up is expected to become considerably smaller (see e.g. Tutorial 15).

Models	PyTorch	JAX
Reverse Sequence	0min 26sec	0min 7sec
Anomaly Detection	16min 34sec	3min 45sec

In this tutorial, we will discuss one of the most impactful architectures of the last 2 years: the Transformer model. Since the paper Attention Is All You Need by Vaswani et al. had been published in 2017, the Transformer architecture has continued to beat benchmarks in many domains, most importantly in Natural Language Processing. Transformers with an incredible amount of parameters can generate long, convincing essays, and opened up new application fields of AI. As the hype of the Transformer architecture seems not to come to an end in the next years, it is important to understand how it works, and have implemented it yourself, which we will do in this notebook.

Despite the huge success of Transformers in NLP, we will *not* include the NLP domain in our notebook here. Why? Firstly, the Master AI at UvA offers many great NLP courses that will take a closer look at the application of the Transformer architecture in NLP (NLP2, Advanced Topics in Computational Semantics). Secondly, assignment 2 takes already a closer look at language generation on character level, on which you could easily apply our transformer architecture. Finally, and most importantly, there is so much more to the Transformer architecture. NLP is the domain the Transformer architecture has been originally proposed for and had the greatest impact on, but it also accelerated research in other domains, recently even Computer Vision. Thus, we focus here on what makes the Transformer and self-attention so powerful in general. In Tutorial 15, we will discuss the application of Transformers in Computer Vision.

Below, we import our standard libraries. We use JAX as acceleration backend, Flax for implementing neural networks, and Optax to optimize the models.

[1]:
```
## Standard libraries
import os
import numpy as np
import math
import json
from functools import partial

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## tqdm for loading bars
from tqdm.auto import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch
import torch
import torch.utils.data as data
from torch.utils.tensorboard import SummaryWriter
```

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```
import torchvision
from torchvision import transforms
from torchvision.datasets import CIFAR100

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial6_jax"

print("Device:", jax.devices()[0])
```

```
Device: gpu:0
```

Two pre-trained models are downloaded below. Make sure to have adjusted your `CHECKPOINT_PATH` before running this code if not already done.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial6/"
# Files to download
pretrained_files = ["ReverseTask.ckpt", "SetAnomalyTask.ckpt"]

# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.34.1 The Transformer architecture

In the first part of this notebook, we will implement the Transformer architecture by hand. As the architecture is so popular, its main components are already integrated into Flax (SelfAttention, MultiHeadAttention) and there exist several implementations (e.g. in Trax) and pre-trained models (e.g. on Hugging Face). However, we will implement it here ourselves, to get through to the smallest details.

There are of course many more tutorials out there about attention and Transformers. Below, we list a few that are worth exploring if you are interested in the topic and might want yet another perspective on the topic after this one:

- Transformer: A Novel Neural Network Architecture for Language Understanding (Jakob Uszkoreit, 2017) - The original Google blog post about the Transformer paper, focusing on the application in machine translation.

- The Illustrated Transformer (Jay Alammar, 2018) - A very popular and great blog post intuitively explaining the Transformer architecture with many nice visualizations. The focus is on NLP.
- Attention? Attention! (Lilian Weng, 2018) - A nice blog post summarizing attention mechanisms in many domains including vision.
- Illustrated: Self-Attention (Raimi Karim, 2019) - A nice visualization of the steps of self-attention. Recommended going through if the explanation below is too abstract for you.
- The Transformer family (Lilian Weng, 2020) - A very detailed blog post reviewing more variants of Transformers besides the original one.

What is Attention?

The attention mechanism describes a recent new group of layers in neural networks that has attracted a lot of interest in the past few years, especially in sequence tasks. There are a lot of different possible definitions of "attention" in the literature, but the one we will use here is the following: *the attention mechanism describes a weighted average of (sequence) elements with the weights dynamically computed based on an input query and elements' keys*. So what does this exactly mean? The goal is to take an average over the features of multiple elements. However, instead of weighting each element equally, we want to weight them depending on their actual values. In other words, we want to dynamically decide on which inputs we want to "attend" more than others. In particular, an attention mechanism has usually four parts we need to specify:

- **Query**: The query is a feature vector that describes what we are looking for in the sequence, i.e. what would we maybe want to pay attention to.
- **Keys**: For each input element, we have a key which is again a feature vector. This feature vector roughly describes what the element is "offering", or when it might be important. The keys should be designed such that we can identify the elements we want to pay attention to based on the query.
- **Values**: For each input element, we also have a value vector. This feature vector is the one we want to average over.
- **Score function**: To rate which elements we want to pay attention to, we need to specify a score function f_{attn}. The score function takes the query and a key as input, and output the score/attention weight of the query-key pair. It is usually implemented by simple similarity metrics like a dot product, or a small MLP.

The weights of the average are calculated by a softmax over all score function outputs. Hence, we assign those value vectors a higher weight whose corresponding key is most similar to the query. If we try to describe it with pseudo-math, we can write:

$$\alpha_i = \frac{\exp\left(f_{attn}\left(\text{key}_i, \text{query}\right)\right)}{\sum_j \exp\left(f_{attn}\left(\text{key}_j, \text{query}\right)\right)}, \qquad \text{out} = \sum_i \alpha_i \cdot \text{value}_i$$

Visually, we can show the attention over a sequence of words as follows:

For every word, we have one key and one value vector. The query is compared to all keys with a score function (in this case the dot product) to determine the weights. The softmax is not visualized for simplicity. Finally, the value vectors of all words are averaged using the attention weights.

Most attention mechanisms differ in terms of what queries they use, how the key and value vectors are defined, and what score function is used. The attention applied inside the Transformer architecture is called **self-attention**. In self-attention, each sequence element provides a key, value, and query. For each element, we perform an attention layer where based on its query, we check the similarity of the all sequence elements' keys, and returned a different, averaged value vector for each element. We will now go into a bit more detail by first looking at the specific implementation of the attention mechanism which is in the Transformer case the scaled dot product attention.

Scaled Dot Product Attention

The core concept behind self-attention is the scaled dot product attention. Our goal is to have an attention mechanism with which any element in a sequence can attend to any other while still being efficient to compute. The dot product attention takes as input a set of queries $Q \in \mathbb{R}^{T \times d_k}$, keys $K \in \mathbb{R}^{T \times d_k}$ and values $V \in \mathbb{R}^{T \times d_v}$ where T is the sequence length, and d_k and d_v are the hidden dimensionality for queries/keys and values respectively. For simplicity, we neglect the batch dimension for now. The attention value from element i to j is based on its similarity of the query Q_i and key K_j, using the dot product as the similarity metric. In math, we calculate the dot product attention as follows:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

The matrix multiplication QK^T performs the dot product for every possible pair of queries and keys, resulting in a matrix of the shape $T \times T$. Each row represents the attention logits for a specific element i to all other elements in the sequence. On these, we apply a softmax and multiply with the value vector to obtain a weighted mean (the weights being determined by the attention). Another perspective on this attention mechanism offers the computation graph which is visualized below (figure credit - Vaswani et al., 2017).

One aspect we haven't discussed yet is the scaling factor of $1/\sqrt{d_k}$. This scaling factor is crucial to maintain an appropriate variance of attention values after initialization. Remember that we intialize our layers with the intention of having equal variance throughout the model, and hence, Q and K might also have a variance close to 1. However, performing a dot product over two vectors with a variance σ^2 results in a scalar having d_k-times higher variance:

$$q_i \sim \mathcal{N}(0, \sigma^2), k_i \sim \mathcal{N}(0, \sigma^2) \rightarrow \text{Var}\left(\sum_{i=1}^{d_k} q_i \cdot k_i\right) = \sigma^4 \cdot d_k$$

If we do not scale down the variance back to $\sim \sigma^2$, the softmax over the logits will already saturate to 1 for one random element and 0 for all others. The gradients through the softmax will be close to zero so that we can't learn the parameters appropriately. Note that the extra factor of σ^2, i.e., having σ^4 instead of σ^2, is usually not an issue, since we keep the original variance σ^2 close to 1 anyways.

The block `Mask (opt.)` in the diagram above represents the optional masking of specific entries in the attention matrix. This is for instance used if we stack multiple sequences with different lengths into a batch. To still benefit from parallelization in PyTorch, we pad the sentences to the same length and mask out the padding tokens during the calculation of the attention values. This is usually done by setting the respective attention logits to a very low value.

After we have discussed the details of the scaled dot product attention block, we can write a function below which computes the output features given the triple of queries, keys, and values:

[3]:
```
def scaled_dot_product(q, k, v, mask=None):
    d_k = q.shape[-1]
    attn_logits = jnp.matmul(q, jnp.swapaxes(k, -2, -1))
    attn_logits = attn_logits / math.sqrt(d_k)
    if mask is not None:
        attn_logits = jnp.where(mask == 0, -9e15, attn_logits)
    attention = nn.softmax(attn_logits, axis=-1)
    values = jnp.matmul(attention, v)
    return values, attention
```

Note that our code above supports any additional dimensionality in front of the sequence length so that we can also use it for batches. However, for a better understanding, let's generate a few random queries, keys, and value vectors, and calculate the attention outputs:

[4]:
```
seq_len, d_k = 3, 2
main_rng, rand1 = random.split(main_rng)
qkv = random.normal(rand1, (3, seq_len, d_k))
q, k, v = qkv[0], qkv[1], qkv[2]
values, attention = scaled_dot_product(q, k, v)
print("Q\n", q)
print("K\n", k)
print("V\n", v)
print("Values\n", values)
print("Attention\n", attention)
```

```
Q
 [[-0.6613315   0.70056266]
 [ 0.08239268 -1.7793142 ]
 [-0.04378588  1.0965251 ]]
K
 [[ 1.7257481   0.35568172]
 [ 1.3034704   1.2873708 ]
 [ 1.6871481  -0.5714404 ]]
V
 [[ 1.5129997   1.1050899 ]
 [ 0.27949408 -0.46224892]
 [-1.1003422  -1.1437942 ]]
Values
 [[ 0.376226   -0.14656176]
 [-0.42778552 -0.5989564 ]
 [ 0.4362476  -0.11678296]]
Attention
 [[0.27963293 0.54049295 0.17987415]
 [0.22194655 0.06706189 0.71099156]
 [0.27977085 0.58373076 0.13649833]]
```

Before continuing, make sure you can follow the calculation of the specific values here, and also check it by hand. It is important to fully understand how the scaled dot product attention is calculated.

Multi-Head Attention

The scaled dot product attention allows a network to attend over a sequence. However, often there are multiple different aspects a sequence element wants to attend to, and a single weighted average is not a good option for it. This is why we extend the attention mechanisms to multiple heads, i.e. multiple different query-key-value triplets on the same features. Specifically, given a query, key, and value matrix, we transform those into h sub-queries, sub-keys, and sub-values, which we pass through the scaled dot product attention independently. Afterward, we concatenate the heads and combine them with a final weight matrix. Mathematically, we can express this operation as:

$$\text{Multihead}(Q, K, V) = \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O$$

$$\text{where head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

We refer to this as Multi-Head Attention layer with the learnable parameters $W^Q_{1...h} \in \mathbb{R}^{D\times d_k}$, $W^K_{1...h} \in \mathbb{R}^{D\times d_k}$, $W^V_{1...h} \in \mathbb{R}^{D\times d_v}$, and $W^O \in \mathbb{R}^{h\cdot d_v \times d_{out}}$ (D being the input dimensionality). Expressed in a computational graph, we can visualize it as below (figure credit - Vaswani et al., 2017).

How are we applying a Multi-Head Attention layer in a neural network, where we don't have an arbitrary query, key, and value vector as input? Looking at the computation graph above, a simple but effective implementation is to set

the current feature map in a NN, $X \in \mathbb{R}^{B \times T \times d_{\text{model}}}$, as Q, K and V (B being the batch size, T the sequence length, d_{model} the hidden dimensionality of X). The consecutive weight matrices W^Q, W^K, and W^V can transform X to the corresponding feature vectors that represent the queries, keys, and values of the input. Note that commonly, these weight matrices are initialized with the Xavier initialization. However, the layer is usually not too sensitive to the initialization, as long as the variance of Q and K do not become too large. With this in mind, we can implement the Multi-Head Attention module below.

[ ]:
```
# Helper function to support different mask shapes.
# Output shape supports (batch_size, number of heads, seq length, seq length)
# If 2D: broadcasted over batch size and number of heads
# If 3D: broadcasted over number of heads
# If 4D: leave as is
def expand_mask(mask):
    assert mask.ndim >= 2, "Mask must be at least 2-dimensional with seq_length x seq_
↪length"
    if mask.ndim == 3:
        mask = mask.unsqueeze(1)
    while mask.ndim < 4:
        mask = mask.unsqueeze(0)
    return mask
```

[5]:
```
class MultiheadAttention(nn.Module):
    embed_dim : int  # Output dimension
    num_heads : int  # Number of parallel heads (h)

    def setup(self):
        # Stack all weight matrices 1...h and W^Q, W^K, W^V together for efficiency
        # Note that in many implementations you see "bias=False" which is optional
        self.qkv_proj = nn.Dense(3*self.embed_dim,
                                 kernel_init=nn.initializers.xavier_uniform(),  #␣
↪Weights with Xavier uniform init
                                 bias_init=nn.initializers.zeros  # Bias init with zeros
                                )
        self.o_proj = nn.Dense(self.embed_dim,
                               kernel_init=nn.initializers.xavier_uniform(),
                               bias_init=nn.initializers.zeros)

    def __call__(self, x, mask=None):
        batch_size, seq_length, embed_dim = x.shape
        if mask is not None:
            mask = expand_mask(mask)
        qkv = self.qkv_proj(x)

        # Separate Q, K, V from linear output
        qkv = qkv.reshape(batch_size, seq_length, self.num_heads, -1)
        qkv = qkv.transpose(0, 2, 1, 3) # [Batch, Head, SeqLen, Dims]
        q, k, v = jnp.array_split(qkv, 3, axis=-1)

        # Determine value outputs
        values, attention = scaled_dot_product(q, k, v, mask=mask)
        values = values.transpose(0, 2, 1, 3) # [Batch, SeqLen, Head, Dims]
        values = values.reshape(batch_size, seq_length, embed_dim)
        o = self.o_proj(values)
```

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```
        return o, attention
```

[6]:
```
## Test MultiheadAttention implementation
# Example features as input
main_rng, x_rng = random.split(main_rng)
x = random.normal(x_rng, (3, 16, 128))
# Create attention
mh_attn = MultiheadAttention(embed_dim=128, num_heads=4)
# Initialize parameters of attention with random key and inputs
main_rng, init_rng = random.split(main_rng)
params = mh_attn.init(init_rng, x)['params']
# Apply attention with parameters on the inputs
out, attn = mh_attn.apply({'params': params}, x)
print('Out', out.shape, 'Attention', attn.shape)

del mh_attn, params
```

```
Out (3, 16, 128) Attention (3, 4, 16, 16)
```

One crucial characteristic of the multi-head attention is that it is permutation-equivariant with respect to its inputs. This means that if we switch two input elements in the sequence, e.g. $X_1 \leftrightarrow X_2$ (neglecting the batch dimension for now), the output is exactly the same besides the elements 1 and 2 switched. Hence, the multi-head attention is actually looking at the input not as a sequence, but as a set of elements. This property makes the multi-head attention block and the Transformer architecture so powerful and widely applicable! But what if the order of the input is actually important for solving the task, like language modeling? The answer is to encode the position in the input features, which we will take a closer look at later (topic *Positional encodings* below).

Before moving on to creating the Transformer architecture, we can compare the self-attention operation with our other common layer competitors for sequence data: convolutions and recurrent neural networks. Below you can find a table by Vaswani et al. (2017) on the complexity per layer, the number of sequential operations, and maximum path length. The complexity is measured by the upper bound of the number of operations to perform, while the maximum path length represents the maximum number of steps a forward or backward signal has to traverse to reach any other position. The lower this length, the better gradient signals can backpropagate for long-range dependencies. Let's take a look at the table below:

n is the sequence length, d is the representation dimension and k is the kernel size of convolutions. In contrast to recurrent networks, the self-attention layer can parallelize all its operations making it much faster to execute for smaller sequence lengths. However, when the sequence length exceeds the hidden dimensionality, self-attention becomes more expensive than RNNs. One way of reducing the computational cost for long sequences is by restricting the self-attention to a neighborhood of inputs to attend over, denoted by r. Nevertheless, there has been recently a lot of work on more efficient Transformer architectures that still allow long dependencies, of which you can find an overview in the paper by Tay et al. (2020) if interested.

Transformer Encoder

Next, we will look at how to apply the multi-head attention block inside the Transformer architecture. Originally, the Transformer model was designed for machine translation. Hence, it got an encoder-decoder structure where the encoder takes as input the sentence in the original language and generates an attention-based representation. On the other hand, the decoder attends over the encoded information and generates the translated sentence in an autoregressive manner, as in a standard RNN. While this structure is extremely useful for Sequence-to-Sequence tasks with the necessity of autoregressive decoding, we will focus here on the encoder part. Many advances in NLP have been made using pure encoder-based Transformer models (if interested, models include the BERT-family, the Vision Transformer, and more), and in our tutorial, we will also mainly focus on the encoder part. If you have understood the encoder architecture, the decoder is a very small step to implement as well. The full Transformer architecture looks as follows (figure credit - Vaswani et al., 2017).:

The encoder consists of N identical blocks that are applied in sequence. Taking as input x, it is first passed through a Multi-Head Attention block as we have implemented above. The output is added to the original input using a residual connection, and we apply a consecutive Layer Normalization on the sum. Overall, it calculates $\text{LayerNorm}(x + \text{Multihead}(x, x, x))$ (x being Q, K and V input to the attention layer). The residual connection is crucial in the Transformer architecture for two reasons:

1. Similar to ResNets, Transformers are designed to be very deep. Some models contain more than 24 blocks in the encoder. Hence, the residual connections are crucial for enabling a smooth gradient flow through the model.
2. Without the residual connection, the information about the original sequence is lost. Remember that the Multi-Head Attention layer ignores the position of elements in a sequence, and can only learn it based on the input features. Removing the residual connections would mean that this information is lost after the first attention layer (after initialization), and with a randomly initialized query and key vector, the output vectors for position i has no relation to its original input. All outputs of the attention are likely to represent similar/same information, and there is no chance for the model to distinguish which information came from which input element. An alternative option to residual connection would be to fix at least one head to focus on its original input, but this is very inefficient and does not have the benefit of the improved gradient flow.

The Layer Normalization also plays an important role in the Transformer architecture as it enables faster training and provides small regularization. Additionally, it ensures that the features are in a similar magnitude among the elements in the sequence. We are not using Batch Normalization because it depends on the batch size which is often small with Transformers (they require a lot of GPU memory), and BatchNorm has shown to perform particularly bad in language as the features of words tend to have a much higher variance (there are many, very rare words which need to be considered for a good distribution estimate).

Additionally to the Multi-Head Attention, a small fully connected feed-forward network is added to the model, which is applied to each position separately and identically. Specifically, the model uses a Linear→ReLU→Linear MLP. The full transformation including the residual connection can be expressed as:

$$\begin{aligned}\text{FFN}(x) &= \max(0, xW_1 + b_1)W_2 + b_2\\ x &= \text{LayerNorm}(x + \text{FFN}(x))\end{aligned}$$

This MLP adds extra complexity to the model and allows transformations on each sequence element separately. You can imagine as this allows the model to "post-process" the new information added by the previous Multi-Head Attention, and prepare it for the next attention block. Usually, the inner dimensionality of the MLP is 2-8× larger than d_{model}, i.e. the dimensionality of the original input x. The general advantage of a wider layer instead of a narrow, multi-layer MLP is the faster, parallelizable execution.

Finally, after looking at all parts of the encoder architecture, we can start implementing it below. We first start by implementing a single encoder block. Additionally to the layers described above, we will add dropout layers in the MLP and on the output of the MLP and Multi-Head Attention for regularization.

[7]:
```
class EncoderBlock(nn.Module):
    input_dim : int  # Input dimension is needed here since it is equal to the output␣
↪dimension (residual connection)
    num_heads : int
    dim_feedforward : int
    dropout_prob : float

    def setup(self):
        # Attention layer
        self.self_attn = MultiheadAttention(embed_dim=self.input_dim,
                                            num_heads=self.num_heads)
        # Two-layer MLP
        self.linear = [
            nn.Dense(self.dim_feedforward),
            nn.Dropout(self.dropout_prob),
            nn.relu,
            nn.Dense(self.input_dim)
        ]
        # Layers to apply in between the main layers
        self.norm1 = nn.LayerNorm()
        self.norm2 = nn.LayerNorm()
        self.dropout = nn.Dropout(self.dropout_prob)

    def __call__(self, x, mask=None, train=True):
        # Attention part
        attn_out, _ = self.self_attn(x, mask=mask)
        x = x + self.dropout(attn_out, deterministic=not train)
        x = self.norm1(x)

        # MLP part
        linear_out = x
        for l in self.linear:
            linear_out = l(linear_out) if not isinstance(l, nn.Dropout) else l(linear_
↪out, deterministic=not train)
        x = x + self.dropout(linear_out, deterministic=not train)
        x = self.norm2(x)

        return x
```

[8]:
```
## Test EncoderBlock implementation
# Example features as input
main_rng, x_rng = random.split(main_rng)
x = random.normal(x_rng, (3, 16, 128))
# Create encoder block
encblock = EncoderBlock(input_dim=128, num_heads=4, dim_feedforward=512, dropout_prob=0.
↪1)
# Initialize parameters of encoder block with random key and inputs
main_rng, init_rng, dropout_init_rng = random.split(main_rng, 3)
params = encblock.init({'params': init_rng, 'dropout': dropout_init_rng}, x, train=True)[
↪'params']
# Apply encoder block with parameters on the inputs
# Since dropout is stochastic, we need to pass a rng to the forward
```

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```
main_rng, dropout_apply_rng = random.split(main_rng)
out = encblock.apply({'params': params}, x, train=True, rngs={'dropout': dropout_apply_
↪rng})
print('Out', out.shape)

del encblock, params
```

```
Out (3, 16, 128)
```

Based on this block, we can implement a module for the full Transformer encoder. Additionally to a forward function that iterates through the sequence of encoder blocks, we also provide a function called `get_attention_maps`. The idea of this function is to return the attention probabilities for all Multi-Head Attention blocks in the encoder. This helps us in understanding, and in a sense, explaining the model. However, the attention probabilities should be interpreted with a grain of salt as it does not necessarily reflect the true interpretation of the model (there is a series of papers about this, including Attention is not Explanation and Attention is not not Explanation).

[9]:
```
class TransformerEncoder(nn.Module):
    num_layers : int
    input_dim : int
    num_heads : int
    dim_feedforward : int
    dropout_prob : float

    def setup(self):
        self.layers = [EncoderBlock(self.input_dim, self.num_heads, self.dim_feedforward,
↪ self.dropout_prob) for _ in range(self.num_layers)]

    def __call__(self, x, mask=None, train=True):
        for l in self.layers:
            x = l(x, mask=mask, train=train)
        return x

    def get_attention_maps(self, x, mask=None, train=True):
        # A function to return the attention maps within the model for a single␣
↪application
        # Used for visualization purpose later
        attention_maps = []
        for l in self.layers:
            _, attn_map = l.self_attn(x, mask=mask)
            attention_maps.append(attn_map)
            x = l(x, mask=mask, train=train)
        return attention_maps
```

[10]:
```
## Test TransformerEncoder implementation
# Example features as input
main_rng, x_rng = random.split(main_rng)
x = random.normal(x_rng, (3, 16, 128))
# Create Transformer encoder
transenc = TransformerEncoder(num_layers=5,
                              input_dim=128,
                              num_heads=4,
                              dim_feedforward=256,
```

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```
                                dropout_prob=0.15)
# Initialize parameters of transformer with random key and inputs
main_rng, init_rng, dropout_init_rng = random.split(main_rng, 3)
params = transenc.init({'params': init_rng, 'dropout': dropout_init_rng}, x, train=True)[
↪'params']
# Apply transformer with parameters on the inputs
# Since dropout is stochastic, we need to pass a rng to the forward
main_rng, dropout_apply_rng = random.split(main_rng)
# Instead of passing params and rngs every time to a function call, we can bind them to␣
↪the module
binded_mod = transenc.bind({'params': params}, rngs={'dropout': dropout_apply_rng})
out = binded_mod(x, train=True)
print('Out', out.shape)
attn_maps = binded_mod.get_attention_maps(x, train=True)
print('Attention maps', len(attn_maps), attn_maps[0].shape)

del transenc, binded_mod, params
```

```
Out (3, 16, 128)
Attention maps 5 (3, 4, 16, 16)
```

Positional encoding

We have discussed before that the Multi-Head Attention block is permutation-equivariant, and cannot distinguish whether an input comes before another one in the sequence or not. In tasks like language understanding, however, the position is important for interpreting the input words. The position information can therefore be added via the input features. We could learn a embedding for every possible position, but this would not generalize to a dynamical input sequence length. Hence, the better option is to use feature patterns that the network can identify from the features and potentially generalize to larger sequences. The specific pattern chosen by Vaswani et al. are sine and cosine functions of different frequencies, as follows:

$$PE_{(pos,i)} = \begin{cases} \sin\left(\frac{pos}{10000^{i/d_{\text{model}}}}\right) & \text{if} \quad i \bmod 2 = 0 \\ \cos\left(\frac{pos}{10000^{(i-1)/d_{\text{model}}}}\right) & \text{otherwise} \end{cases}$$

$PE_{(pos,i)}$ represents the position encoding at position pos in the sequence, and hidden dimensionality i. These values, concatenated for all hidden dimensions, are added to the original input features (in the Transformer visualization above, see "Positional encoding"), and constitute the position information. We distinguish between even ($i \bmod 2 = 0$) and uneven ($i \bmod 2 = 1$) hidden dimensionalities where we apply a sine/cosine respectively. The intuition behind this encoding is that you can represent $PE_{(pos+k,:)}$ as a linear function of $PE_{(pos,:)}$, which might allow the model to easily attend to relative positions. The wavelengths in different dimensions range from 2π to $10000 \cdot 2\pi$.

The positional encoding is implemented below.

[11]:
```
class PositionalEncoding(nn.Module):
    d_model : int         # Hidden dimensionality of the input.
    max_len : int = 5000  # Maximum length of a sequence to expect.

    def setup(self):
        # Create matrix of [SeqLen, HiddenDim] representing the positional encoding for␣
↪max_len inputs
        pe = np.zeros((self.max_len, self.d_model))
        position = np.arange(0, self.max_len, dtype=np.float32)[:,None]
```

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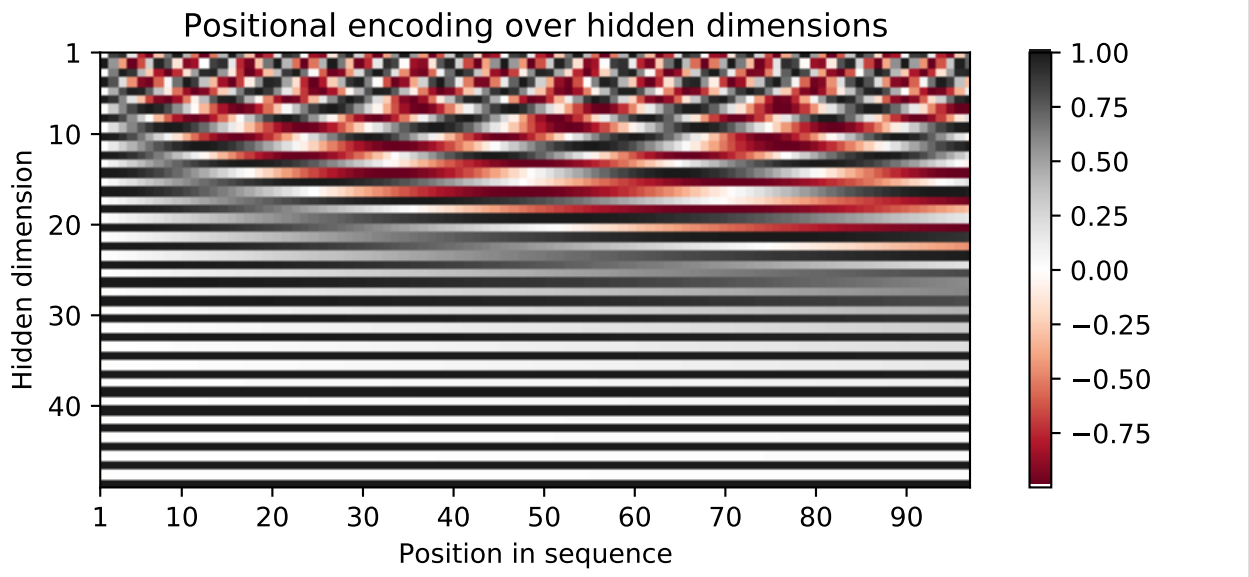
```
        div_term = np.exp(np.arange(0, self.d_model, 2) * (-math.log(10000.0) / self.d_
↪model))
        pe[:, 0::2] = np.sin(position * div_term)
        pe[:, 1::2] = np.cos(position * div_term)
        pe = pe[None]
        self.pe = jax.device_put(pe)

    def __call__(self, x):
        x = x + self.pe[:, :x.shape[1]]
        return x
```

To understand the positional encoding, we can visualize it below. We will generate an image of the positional encoding over hidden dimensionality and position in a sequence. Each pixel, therefore, represents the change of the input feature we perform to encode the specific position. Let's do it below.

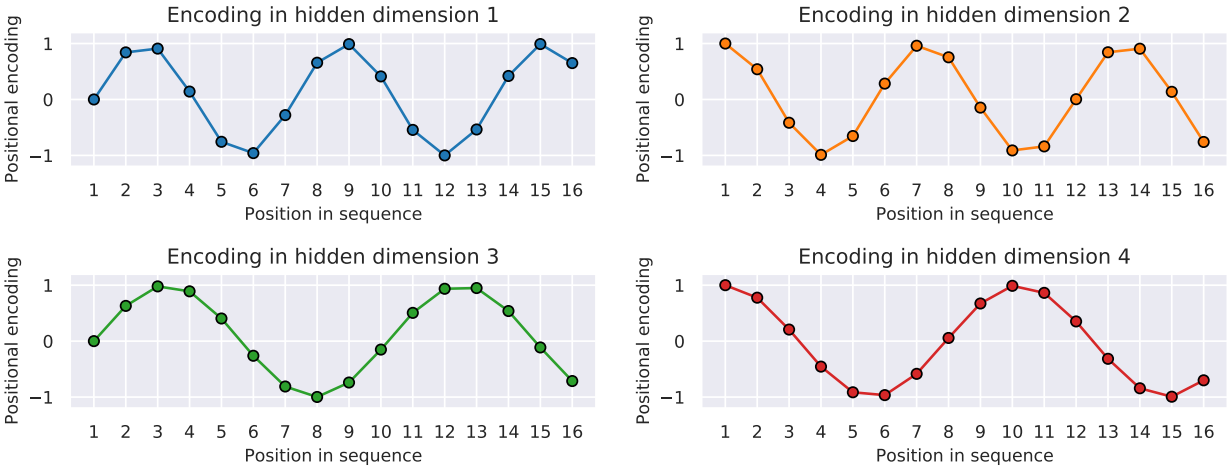
[12]:
```
# Create encoding block, bind to access positional encoding (module has no parameters)
encod_block = PositionalEncoding(d_model=48, max_len=96).bind({})
# Obtain positional encodings as numpy array
pe = jax.device_get(encod_block.pe.squeeze().T)

fig, ax = plt.subplots(nrows=1, ncols=1, figsize=(8,3))
pos = ax.imshow(pe, cmap="RdGy", extent=(1,pe.shape[1]+1,pe.shape[0]+1,1))
fig.colorbar(pos, ax=ax)
ax.set_xlabel("Position in sequence")
ax.set_ylabel("Hidden dimension")
ax.set_title("Positional encoding over hidden dimensions")
ax.set_xticks([1]+[i*10 for i in range(1,1+pe.shape[1]//10)])
ax.set_yticks([1]+[i*10 for i in range(1,1+pe.shape[0]//10)])
plt.show()
```



You can clearly see the sine and cosine waves with different wavelengths that encode the position in the hidden dimensions. Specifically, we can look at the sine/cosine wave for each hidden dimension separately, to get a better intuition of the pattern. Below we visualize the positional encoding for the hidden dimensions 1, 2, 3 and 4.

[13]:
```
sns.set_theme()
fig, ax = plt.subplots(2, 2, figsize=(12,4))
ax = [a for a_list in ax for a in a_list]
for i in range(len(ax)):
    ax[i].plot(np.arange(1,17), pe[i,:16], color=f'C{i}', marker="o", markersize=6,␣
↪markeredgecolor="black")
    ax[i].set_title(f"Encoding in hidden dimension {i+1}")
    ax[i].set_xlabel("Position in sequence", fontsize=10)
    ax[i].set_ylabel("Positional encoding", fontsize=10)
    ax[i].set_xticks(np.arange(1,17))
    ax[i].tick_params(axis='both', which='major', labelsize=10)
    ax[i].tick_params(axis='both', which='minor', labelsize=8)
    ax[i].set_ylim(-1.2, 1.2)
fig.subplots_adjust(hspace=0.8)
sns.reset_orig()
plt.show()
```



As we can see, the patterns between the hidden dimension 1 and 2 only differ in the starting angle. The wavelength is 2π, hence the repetition after position 6. The hidden dimensions 2 and 3 have about twice the wavelength.

Learning rate warm-up

One commonly used technique for training a Transformer is learning rate warm-up. This means that we gradually increase the learning rate from 0 on to our originally specified learning rate in the first few iterations. Thus, we slowly start learning instead of taking very large steps from the beginning. In fact, training a deep Transformer without learning rate warm-up can make the model diverge and achieve a much worse performance on training and testing. Take for instance the following plot by Liu et al. (2019) comparing Adam-vanilla (i.e. Adam without warm-up) vs Adam with a warm-up:

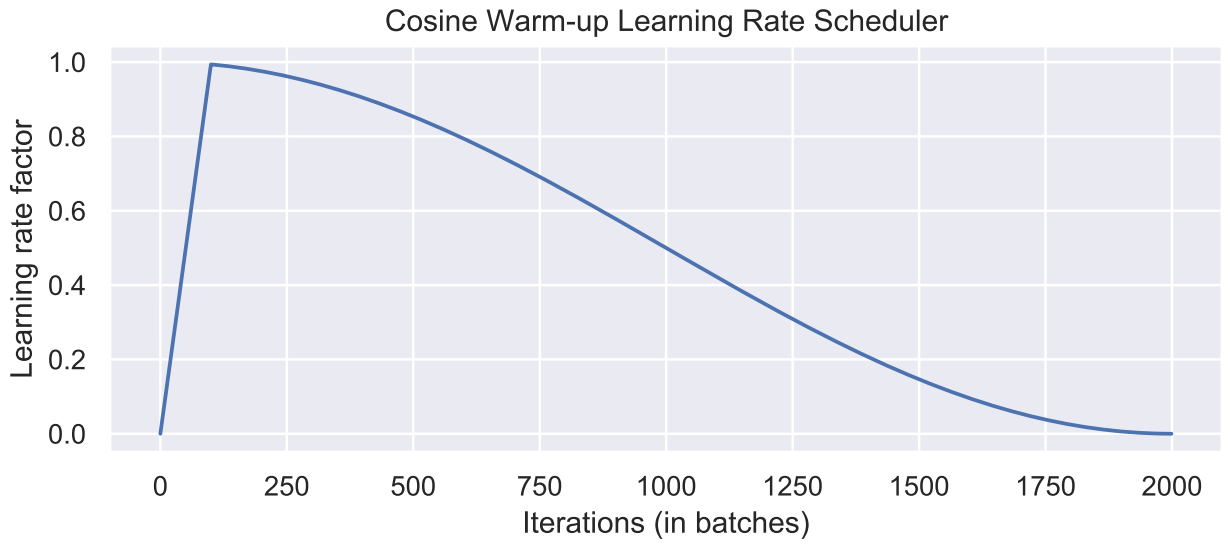
Clearly, the warm-up is a crucial hyperparameter in the Transformer architecture. Why is it so important? There are currently two common explanations. Firstly, Adam uses the bias correction factors which however can lead to a higher variance in the adaptive learning rate during the first iterations. Improved optimizers like RAdam have been shown to overcome this issue, not requiring warm-up for training Transformers. Secondly, the iteratively applied Layer Normalization across layers can lead to very high gradients during the first iterations, which can be solved by using Pre-Layer Normalization (similar to Pre-Activation ResNet), or replacing Layer Normalization by other techniques (Adaptive Normalization, Power Normalization).

Nevertheless, many applications and papers still use the original Transformer architecture with Adam, because warm-up is a simple, yet effective way of solving the gradient problem in the first iterations. There are many different schedulers we could use. For instance, the original Transformer paper used an exponential decay scheduler with a warm-up. However, the currently most popular scheduler is the cosine warm-up scheduler, which combines warm-up with a cosine-shaped learning rate decay. In Optax, this learning rate scheduler is also implemented in `optax.warmup_cosine_decay_schedule`, but let's manually implement it below, and visualize the learning rate factor over epochs.

[14]:
```
def cosine_warmup_schedule(base_lr: float, warmup: int, max_iters: int):
    assert warmup > 0 and max_iters > 0
    # Create function to return lr based on iteration count
    def get_lr(train_iter):
        lr_factor = 0.5 * (1 + np.cos(np.pi * train_iter / max_iters))
        if train_iter <= warmup:
            lr_factor *= train_iter * 1.0 / warmup
        return lr_factor * base_lr
    return get_lr
```

[15]:
```
lr_scheduler = cosine_warmup_schedule(base_lr=1.0, warmup=100, max_iters=2000)

# Plotting
epochs = list(range(2000))
sns.set()
plt.figure(figsize=(8,3))
plt.plot(epochs, [lr_scheduler(e) for e in epochs])
plt.ylabel("Learning rate factor")
plt.xlabel("Iterations (in batches)")
plt.title("Cosine Warm-up Learning Rate Scheduler")
plt.show()
sns.reset_orig()
```



In the first 100 iterations, we increase the learning rate factor from 0 to 1, whereas for all later iterations, we decay it using the cosine wave.

Full Transformer model

Finally, we can embed the Transformer architecture into a full architecture. We will implement a template for a classifier based on the Transformer encoder. Thereby, we have a prediction output per sequence element. If we would need a classifier over the whole sequence, the common approach is to add an additional `[CLS]` token to the sequence, representing the classifier token. However, here we focus on tasks where we have one output per element.

Additionally to the Transformer architecture, we add a small input network (maps input dimensions to model dimensions), the positional encoding, and an output network (transforms output encodings to predictions). We also add the learning rate scheduler, which takes a step each iteration instead of once per epoch. This is needed for the warmup and the smooth cosine decay. The training, validation, and test step is left empty for now and will be filled for our task-specific models.

[16]:
```
class TransformerPredictor(nn.Module):
    model_dim : int                   # Hidden dimensionality to use inside the␣
↪Transformer
    num_classes : int                 # Number of classes to predict per sequence element
    num_heads : int                   # Number of heads to use in the Multi-Head␣
↪Attention blocks
    num_layers : int                  # Number of encoder blocks to use
    dropout_prob : float = 0.0        # Dropout to apply inside the model
    input_dropout_prob : float = 0.0  # Dropout to apply on the input features

    def setup(self):
        # Input dim -> Model dim
        self.input_dropout = nn.Dropout(self.input_dropout_prob)
        self.input_layer = nn.Dense(self.model_dim)
        # Positional encoding for sequences
        self.positional_encoding = PositionalEncoding(self.model_dim)
        # Transformer
        self.transformer = TransformerEncoder(num_layers=self.num_layers,
                                              input_dim=self.model_dim,
                                              dim_feedforward=2*self.model_dim,
                                              num_heads=self.num_heads,
                                              dropout_prob=self.dropout_prob)
        # Output classifier per sequence lement
        self.output_net = [
            nn.Dense(self.model_dim),
            nn.LayerNorm(),
            nn.relu,
            nn.Dropout(self.dropout_prob),
            nn.Dense(self.num_classes)
        ]

    def __call__(self, x, mask=None, add_positional_encoding=True, train=True):
        """
        Inputs:
            x - Input features of shape [Batch, SeqLen, input_dim]
            mask - Mask to apply on the attention outputs (optional)
            add_positional_encoding - If True, we add the positional encoding to the␣
↪input.
                                      Might not be desired for some tasks.
            train - If True, dropout is stochastic
        """
```

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```
        x = self.input_dropout(x, deterministic=not train)
        x = self.input_layer(x)
        if add_positional_encoding:
            x = self.positional_encoding(x)
        x = self.transformer(x, mask=mask, train=train)
        for l in self.output_net:
            x = l(x) if not isinstance(l, nn.Dropout) else l(x, deterministic=not train)
        return x

    def get_attention_maps(self, x, mask=None, add_positional_encoding=True, train=True):
        """
        Function for extracting the attention matrices of the whole Transformer for a␣
↪single batch.
        Input arguments same as the forward pass.
        """
        x = self.input_dropout(x, deterministic=not train)
        x = self.input_layer(x)
        if add_positional_encoding:
            x = self.positional_encoding(x)
        attention_maps = self.transformer.get_attention_maps(x, mask=mask, train=train)
        return attention_maps
```

[17]:
```
## Test TransformerPredictor implementation
# Example features as input
main_rng, x_rng = random.split(main_rng)
x = random.normal(x_rng, (3, 16, 64))
# Create Transformer encoder
transpre = TransformerPredictor(num_layers=5,
                                model_dim=128,
                                num_classes=10,
                                num_heads=4,
                                dropout_prob=0.15,
                                input_dropout_prob=0.05)
# Initialize parameters of transformer predictor with random key and inputs
main_rng, init_rng, dropout_init_rng = random.split(main_rng, 3)
params = transpre.init({'params': init_rng, 'dropout': dropout_init_rng}, x, train=True)[
↪'params']
# Apply transformer predictor with parameters on the inputs
# Since dropout is stochastic, we need to pass a rng to the forward
main_rng, dropout_apply_rng = random.split(main_rng)
# Instead of passing params and rngs every time to a function call, we can bind them to␣
↪the module
binded_mod = transpre.bind({'params': params}, rngs={'dropout': dropout_apply_rng})
out = binded_mod(x, train=True)
print('Out', out.shape)
attn_maps = binded_mod.get_attention_maps(x, train=True)
print('Attention maps', len(attn_maps), attn_maps[0].shape)

del transpre, binded_mod, params
```

```
Out (3, 16, 10)
Attention maps 5 (3, 4, 16, 16)
```

Trainer module

Finally, we add the missing parts needed for training a model in JAX and Flax. Note that we leave the specific loss function unimplemented, since this function depends on different tasks we do below.

In the optimization, we use the Adam optimizer with our previously discussed cosine scheduler. Additionally, we use the optax transformation `optax.clip_by_global_norm` (documentation). This clips the norm of the gradients for all parameters before taking an optimizer step and prevents the model from diverging if we obtain very high gradients at, for instance, sharp loss surfaces (see many good blog posts on gradient clipping, like DeepAI glossary). For Transformers, gradient clipping can help to further stabilize the training during the first few iterations, and also afterward. The clip value is usually between 0.5 and 10, depending on how harsh you want to clip large gradients.

[18]:
```
class TrainerModule:

    def __init__(self, model_name, exmp_batch, max_iters, lr=1e-3, warmup=100, seed=42,␣
↪**model_kwargs):
        """
        Inputs:
            model_name - Name of the model. Used for saving and checkpointing
            exmp_batch - Example batch to the model for initialization
            max_iters - Number of maximum iterations the model is trained for. This is␣
↪needed for the CosineWarmup scheduler
            lr - Learning rate in the optimizer
            warmup - Number of warmup steps. Usually between 50 and 500
            seed - Seed to use for model init
        """
        super().__init__()
        self.model_name = model_name
        self.max_iters = max_iters
        self.lr = lr
        self.warmup = warmup
        self.seed = seed
        # Create empty model. Note: no parameters yet
        self.model = TransformerPredictor(**model_kwargs)
        # Prepare logging
        self.log_dir = os.path.join(CHECKPOINT_PATH, self.model_name)
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model(exmp_batch)

    def batch_to_input(self, exmp_batch):
        # Map batch to input data to the model
        # To be implemented in a task specific sub-class
        raise NotImplementedError

    def get_loss_function(self):
        # Return a function that calculates the loss for a batch
        # To be implemented in a task specific sub-class
        raise NotImplementedError

    def create_functions(self):
        # Create jitted train and eval functions
```

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```
        calculate_loss = self.get_loss_function()

        # Training function
        def train_step(state, rng, batch):
            loss_fn = lambda params: calculate_loss(params, rng, batch, train=True)
            ret, grads = jax.value_and_grad(loss_fn, has_aux=True)(state.params)
            loss, acc, rng = ret[0], *ret[1]
            state = state.apply_gradients(grads=grads)
            return state, rng, loss, acc
        self.train_step = jax.jit(train_step)

        # Evaluation function
        def eval_step(state, rng, batch):
            _, (acc, rng) = calculate_loss(state.params, rng, batch, train=False)
            return acc, rng
        self.eval_step = jax.jit(eval_step)

    def init_model(self, exmp_batch):
        # Initialize model
        self.rng = jax.random.PRNGKey(self.seed)
        self.rng, init_rng, dropout_init_rng = jax.random.split(self.rng, 3)
        exmp_input = self.batch_to_input(exmp_batch)
        params = self.model.init({'params': init_rng, 'dropout': dropout_init_rng}, exmp_
↪input, train=True)['params']
        # Initialize learning rate schedule and optimizer
        lr_schedule = optax.warmup_cosine_decay_schedule(
            init_value=0.0,
            peak_value=self.lr,
            warmup_steps=self.warmup,
            decay_steps=self.max_iters,
            end_value=0.0
        )
        optimizer = optax.chain(
            optax.clip_by_global_norm(1.0),  # Clip gradients at norm 1
            optax.adam(lr_schedule)
        )
        # Initialize training state
        self.state = train_state.TrainState.create(apply_fn=self.model.apply,␣
↪params=params, tx=optimizer)

    def train_model(self, train_loader, val_loader, num_epochs=500):
        # Train model for defined number of epochs
        best_acc = 0.0
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(train_loader, epoch=epoch_idx)
            if epoch_idx % 5 == 0:
                eval_acc = self.eval_model(val_loader)
                self.logger.add_scalar('val/accuracy', eval_acc, global_step=epoch_idx)
                if eval_acc >= best_acc:
                    best_acc = eval_acc
                    self.save_model(step=epoch_idx)
                self.logger.flush()
```

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```
    def train_epoch(self, train_loader, epoch):
        # Train model for one epoch, and log avg loss and accuracy
        accs, losses = [], []
        for batch in tqdm(train_loader, desc='Training', leave=False):
            self.state, self.rng, loss, accuracy = self.train_step(self.state, self.rng,␣
↪batch)
            losses.append(loss)
            accs.append(accuracy)
        avg_loss = np.stack(jax.device_get(losses)).mean()
        avg_acc = np.stack(jax.device_get(accs)).mean()
        self.logger.add_scalar('train/loss', avg_loss, global_step=epoch)
        self.logger.add_scalar('train/accuracy', avg_acc, global_step=epoch)

    def eval_model(self, data_loader):
        # Test model on all data points of a data loader and return avg accuracy
        correct_class, count = 0, 0
        for batch in data_loader:
            acc, self.rng = self.eval_step(self.state, self.rng, batch)
            correct_class += acc * batch[0].shape[0]
            count += batch[0].shape[0]
        eval_acc = (correct_class / count).item()
        return eval_acc

    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir, target=self.state.params,␣
↪step=step)

    def load_model(self, pretrained=False):
        # Load model. We use different checkpoint for the pretrained model
        if not pretrained:
            params = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir, target=self.
↪state.params)
        else:
            params = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'{self.model_name}.ckpt'), target=self.state.params)
        self.state = train_state.TrainState.create(apply_fn=self.model.apply,␣
↪params=params, tx=self.state.tx)

    def checkpoint_exists(self):
        # Check whether a pretrained model exist for this Transformer
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'{self.model_name}.ckpt'))
```

4.34.2 Experiments

After having finished the implementation of the Transformer architecture, we can start experimenting and apply it to various tasks. In this notebook, we will focus on two tasks: parallel Sequence-to-Sequence, and set anomaly detection. The two tasks focus on different properties of the Transformer architecture, and we go through them below.

Sequence to Sequence

A Sequence-to-Sequence task represents a task where the input *and* the output is a sequence, not necessarily of the same length. Popular tasks in this domain include machine translation and summarization. For this, we usually have a Transformer encoder for interpreting the input sequence, and a decoder for generating the output in an autoregressive manner. Here, however, we will go back to a much simpler example task and use only the encoder. Given a sequence of N numbers between 0 and M, the task is to reverse the input sequence. In Numpy notation, if our input is x, the output should be x[::-1]. Although this task sounds very simple, RNNs can have issues with such because the task requires long-term dependencies. Transformers are built to support such, and hence, we expect it to perform very well.

First, let's create a dataset class below.

[19]:
```
class ReverseDataset(data.Dataset):

    def __init__(self, num_categories, seq_len, size, np_rng):
        super().__init__()
        self.num_categories = num_categories
        self.seq_len = seq_len
        self.size = size
        self.np_rng = np_rng

        self.data = self.np_rng.integers(self.num_categories, size=(self.size, self.seq_
↪len))

    def __len__(self):
        return self.size

    def __getitem__(self, idx):
        inp_data = self.data[idx]
        labels = np.flip(inp_data, axis=0)
        return inp_data, labels
```

We create an arbitrary number of random sequences of numbers between 0 and `num_categories-1`. The label is simply the tensor flipped over the sequence dimension. We can create the corresponding data loaders using PyTorch below.

[20]:
```
# Combine batch elements (all numpy) by stacking
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

dataset = partial(ReverseDataset, 10, 16)
```

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```
rev_train_loader = data.DataLoader(dataset(50000, np_rng=np.random.default_rng(42)),
                                   batch_size=128,
                                   shuffle=True,
                                   drop_last=True,
                                   collate_fn=numpy_collate)
rev_val_loader   = data.DataLoader(dataset(1000, np_rng=np.random.default_rng(43)),
                                   batch_size=128,
                                   collate_fn=numpy_collate)
rev_test_loader  = data.DataLoader(dataset(10000, np_rng=np.random.default_rng(44)),
                                   batch_size=128,
                                   collate_fn=numpy_collate)
```

Remember that these data loaders return numpy arrays instead of PyTorch tensors, as we define in the `numpy_collate` function which combines individual elements to a batch. As the data set is so simple and the `__getitem__` finishes a neglectable time, we don't need subprocesses, i.e. workers, to provide us the data (in fact, more workers can slow down the training as we have communication overhead among processes/threads).

Now, let's look at an arbitrary sample of the dataset:

[21]:
```
inp_data, labels = rev_train_loader.dataset[0]
print("Input data:", inp_data)
print("Labels:    ", labels)
```

```
Input data: [0 7 6 4 4 8 0 6 2 0 5 9 7 7 7 7]
Labels:     [7 7 7 7 9 5 0 2 6 0 8 4 4 6 7 0]
```

During training, we pass the input sequence through the Transformer encoder and predict the output for each input token. We use the standard Cross-Entropy loss to perform this. Every number is represented as a one-hot vector. Remember that representing the categories as single scalars decreases the expressiveness of the model extremely as 0 and 1 are not closer related than 0 and 9 in our example. An alternative to a one-hot vector is using a learned embedding vector as it is provided by an `nn.Embed` module (documentation). However, using a one-hot vector with an additional linear layer as in our case has the same effect as an embedding layer (`self.input_net` maps one-hot vector to a dense vector, where each row of the weight matrix represents the embedding for a specific category).

To implement the training dynamic, we create a new class inheriting from `TrainerModule` and defining the loss function as follows:

[22]:
```
class ReverseTrainer(TrainerModule):

    def batch_to_input(self, batch):
        inp_data, _ = batch
        inp_data = jax.nn.one_hot(inp_data, num_classes=self.model.num_classes)
        return inp_data

    def get_loss_function(self):
        # Function for calculating loss and accuracy for a batch
        def calculate_loss(params, rng, batch, train):
            inp_data, labels = batch
            inp_data = jax.nn.one_hot(inp_data, num_classes=self.model.num_classes)
            rng, dropout_apply_rng = random.split(rng)
            logits = self.model.apply({'params': params}, inp_data, train=train, rngs={
↪'dropout': dropout_apply_rng})
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).mean()
```

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```
            return loss, (acc, rng)
        return calculate_loss
```

Finally, we can create a training function, similar to ones we have seen before. We create a `ReverseTrainer` object, run the training for N epochs while logging in TensorBoard, and saving our best model based on the validation. Afterward, we test our models on the test set.

[23]:
```
def train_reverse(max_epochs=10, **model_args):
    num_train_iters = len(rev_train_loader) * max_epochs
    # Create a trainer module with specified hyperparameters
    trainer = ReverseTrainer(model_name='ReverseTask',
                             exmp_batch=next(iter(rev_train_loader)),
                             max_iters=num_train_iters,
                             **model_args)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(rev_train_loader, rev_val_loader, num_epochs=max_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    val_acc = trainer.eval_model(rev_val_loader)
    test_acc = trainer.eval_model(rev_test_loader)
    # Bind parameters to model for easier inference
    trainer.model_bd = trainer.model.bind({'params': trainer.state.params})
    return trainer, {'val_acc': val_acc, 'test_acc': test_acc}
```

Finally, we can train the model. In this setup, we will use a single encoder block and a single head in the Multi-Head Attention. This is chosen because of the simplicity of the task, and in this case, the attention can actually be interpreted as an "explanation" of the predictions (compared to the other papers above dealing with deep Transformers).

[24]:
```
reverse_trainer, reverse_result = train_reverse(model_dim=32,
                                                num_heads=1,
                                                num_classes=rev_train_loader.dataset.num_
↪categories,
                                                num_layers=1,
                                                dropout_prob=0.0,
                                                lr=5e-4,
                                                warmup=50)
```

First, let's print the results:

[25]:
```
print(f"Val accuracy:  {(100.0 * reverse_result['val_acc']):4.2f}%")
print(f"Test accuracy: {(100.0 * reverse_result['test_acc']):4.2f}%")
```

```
Val accuracy:  100.00%
Test accuracy: 100.00%
```

As we would have expected, the Transformer can correctly solve the task. However, how does the attention in the Multi-Head Attention block looks like for an arbitrary input? Let's try to visualize it below.

[26]:
```
data_input, labels = next(iter(rev_val_loader))
inp_data = jax.nn.one_hot(data_input, num_classes=reverse_trainer.model.num_classes)
attention_maps = reverse_trainer.model_bd.get_attention_maps(inp_data)
```

The object `attention_maps` is a list of length N where N is the number of layers. Each element is a tensor of shape

[Batch, Heads, SeqLen, SeqLen], which we can verify below.

[27]:
```
attention_maps[0].shape
```

[27]:
```
(128, 1, 16, 16)
```

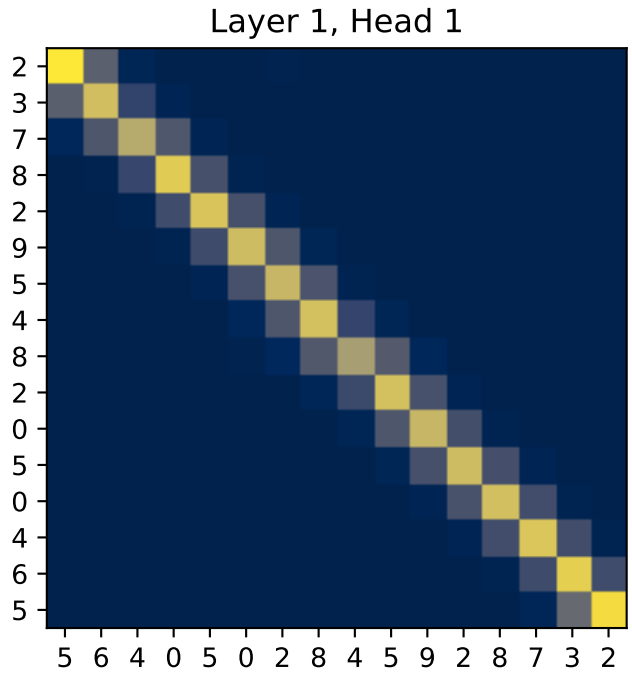
Next, we will write a plotting function that takes as input the sequences, attention maps, and an index indicating for which batch element we want to visualize the attention map. We will create a plot where over rows, we have different layers, while over columns, we show the different heads. Remember that the softmax has been applied for each row separately.

[28]:
```
def plot_attention_maps(input_data, attn_maps, idx=0):
    if input_data is not None:
        input_data = jax.device_get(input_data[idx])
    else:
        input_data = np.arange(attn_maps[0][idx].shape[-1])
    attn_maps = [jax.device_get(m[idx]) for m in attn_maps]

    num_heads = attn_maps[0].shape[0]
    num_layers = len(attn_maps)
    seq_len = input_data.shape[0]
    fig_size = 4 if num_heads == 1 else 3
    fig, ax = plt.subplots(num_layers, num_heads, figsize=(num_heads*fig_size, num_
↪layers*fig_size))
    if num_layers == 1:
        ax = [ax]
    if num_heads == 1:
        ax = [[a] for a in ax]
    for row in range(num_layers):
        for column in range(num_heads):
            ax[row][column].imshow(attn_maps[row][column], origin='lower', vmin=0)
            ax[row][column].set_xticks(list(range(seq_len)))
            ax[row][column].set_xticklabels(input_data.tolist())
            ax[row][column].set_yticks(list(range(seq_len)))
            ax[row][column].set_yticklabels(input_data.tolist())
            ax[row][column].set_title(f"Layer {row+1}, Head {column+1}")
    fig.subplots_adjust(hspace=0.5)
    plt.show()
```

Finally, we can plot the attention map of our trained Transformer on the reverse task:

[29]:
```
plot_attention_maps(data_input, attention_maps, idx=0)
```

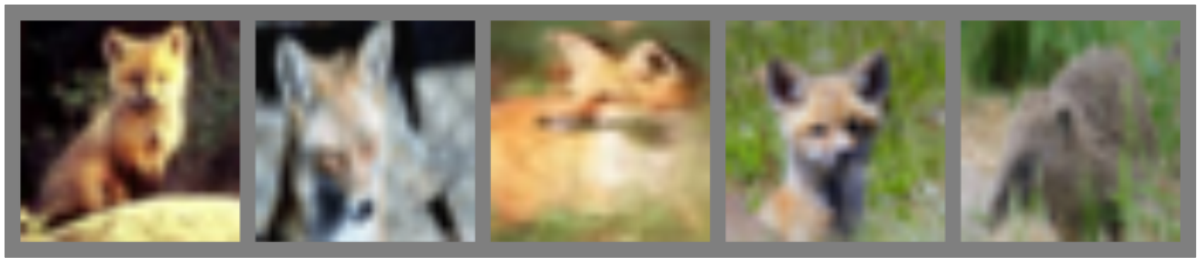


The model has learned to attend to the token that is on the flipped index of itself. Hence, it actually does what we intended it to do. We see that it however also pays some attention to values close to the flipped index. This is because the model doesn't need the perfect, hard attention to solve this problem, but is fine with this approximate, noisy attention map. The close-by indices are caused by the similarity of the positional encoding, which we also intended with the positional encoding.

Set Anomaly Detection

Besides sequences, sets are another data structure that is relevant for many applications. In contrast to sequences, elements are unordered in a set. RNNs can only be applied on sets by assuming an order in the data, which however biases the model towards a non-existing order in the data. Vinyals et al. (2015) and other papers have shown that the assumed order can have a significant impact on the model's performance, and hence, we should try to not use RNNs on sets. Ideally, our model should be permutation-equivariant/invariant such that the output is the same no matter how we sort the elements in a set.

Transformers offer the perfect architecture for this as the Multi-Head Attention is permutation-equivariant, and thus, outputs the same values no matter in what order we enter the inputs (inputs and outputs are permuted equally). The task we are looking at for sets is *Set Anomaly Detection* which means that we try to find the element(s) in a set that does not fit the others. In the research community, the common application of anomaly detection is performed on a set of images, where $N - 1$ images belong to the same category/have the same high-level features while one belongs to another category. Note that category does not necessarily have to relate to a class in a standard classification problem, but could be the combination of multiple features. For instance, on a face dataset, this could be people with glasses, male, beard, etc. An example of distinguishing different animals can be seen below. The first four images show foxes, while the last represents a different animal. We want to recognize that the last image shows a different animal, but it is not relevant which class of animal it is.



In this tutorial, we will use the CIFAR100 dataset. CIFAR100 has 600 images for 100 classes each with a resolution of 32x32, similar to CIFAR10. The larger amount of classes requires the model to attend to specific features in the images instead of coarse features as in CIFAR10, therefore making the task harder. We will show the model a set of 9 images of one class, and 1 image from another class. The task is to find the image that is from a different class than the other images. Using the raw images directly as input to the Transformer is not a good idea, because it is not translation invariant as a CNN, and would need to learn to detect image features from high-dimensional input first of all. Instead, we will use a pre-trained ResNet34 model from the package `flaxmodels` (link) to obtain high-level, low-dimensional features of the images. The ResNet model has been pre-trained on the ImageNet dataset which contains 1 million images of 1k classes and varying resolutions. However, during training and testing, the images are usually scaled to a resolution of 224x224, and hence we rescale our CIFAR images to this resolution as well. Below, we will load the dataset, and prepare the data for being processed by the ResNet model.

[30]:
```
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    img = img / 255.   # Normalization is done in the ResNet
    return img

# Resize to 224x224, and map to JAX
transform = transforms.Compose([transforms.Resize((224,224)),
                                image_to_numpy
                               ])
# Loading the training dataset.
train_set = CIFAR100(root=DATASET_PATH, train=True, transform=transform, download=True)

# Loading the test set
test_set = CIFAR100(root=DATASET_PATH, train=False, transform=transform, download=True)

# For later, keep a dictionary mapping class indices to class names
class_idx_to_name = {val: key for key, val in train_set.class_to_idx.items()}
```

```
Files already downloaded and verified
Files already downloaded and verified
```

Next, we want to run the pre-trained ResNet model on the images, and extract the features before the classification layer. These are the most high-level features, and should sufficiently describe the images. CIFAR100 has some similarity to ImageNet, and thus we are not retraining the ResNet model in any form. However, if you would want to get the best performance and have a very large dataset, it would be better to add the ResNet to the computation graph during training and finetune its parameters as well. As we don't have a large enough dataset and want to train our model efficiently, we will extract the features beforehand. Let's load and prepare the model below.

[31]:
```
# Import and install flaxmodels if needed
try:
    import flaxmodels
except ModuleNotFoundError:
    !pip install --upgrade git+https://github.com/matthias-wright/flaxmodels.git
```

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```
    import flaxmodels

# Pretrained ResNet34 on ImageNet
resnet34 = flaxmodels.ResNet34(output='activations', pretrained='imagenet',␣
↪normalize=True)
main_rng, resnet_rng = random.split(main_rng, 2)
resnet_params = resnet34.init(resnet_rng, jnp.zeros((1, 224, 224, 3)))
# Jit its forward pass for efficiency
apply_resnet = jax.jit(lambda imgs: resnet34.apply(resnet_params, imgs, train=False))
```

We will now write a extraction function for the features below. This cell requires access to a GPU, as the model is rather deep and the images relatively large. The GPUs on GoogleColab are sufficient, but running this cell can take 2-3 minutes. Once it is run, the features are exported on disk so they don't have to be recalculated every time you run the notebook. However, this requires >150MB free disk space. So it is recommended to run this only on a local computer if you have enough free disk and a GPU (GoogleColab is fine for this). If you do not have a GPU, you can download the features from the GoogleDrive folder.

[32]:
```
def extract_features(dataset, save_file):
    if not os.path.isfile(save_file):
        data_loader = data.DataLoader(dataset, batch_size=128, shuffle=False, drop_
↪last=False,
                                      collate_fn=lambda batch: np.stack([b[0] for b in␣
↪batch], axis=0))
        extracted_features = []
        for imgs in tqdm(data_loader):
            feats = apply_resnet(imgs)
            # Average pooling on the last conv features to obtain a image-level feature␣
↪vector
            feats = feats['block4_2'].mean(axis=(1,2))
            extracted_features.append(feats)
        extracted_features = jnp.concatenate(extracted_features, axis=0)
        extracted_features = jax.device_get(extracted_features)
        np.savez_compressed(save_file, feats=extracted_features)
    else:
        extracted_features = np.load(save_file)['feats']
    return extracted_features

train_feat_file = os.path.join(CHECKPOINT_PATH, "train_set_features.npz")
train_set_feats = extract_features(train_set, train_feat_file)

test_feat_file = os.path.join(CHECKPOINT_PATH, "test_set_features.npz")
test_feats = extract_features(test_set, test_feat_file)
```

Let's verify the feature shapes below. The training should have 50k elements, and the test 10k images. The feature dimension is 512 for the ResNet34. If you experiment with other models, you likely see a different feature dimension.

[33]:
```
print("Train:", train_set_feats.shape)
print("Test: ", test_feats.shape)
```

```
Train: (50000, 512)
Test:  (10000, 512)
```

As usual, we want to create a validation set to detect when we should stop training. In this case, we will split the training set into 90% training, 10% validation. However, the difficulty is here that we need to ensure that the validation set has

the same number of images for all 100 labels. Otherwise, we have a class imbalance which is not good for creating the image sets. Hence, we take 10% of the images for each class, and move them into the validation set. The code below does exactly this.

[34]:
```
## Split train into train+val
# Get labels from train set
labels = np.array(train_set.targets, dtype=np.int32)

# Get indices of images per class
num_labels = labels.max()+1
sorted_indices = np.argsort(labels).reshape(num_labels, -1) # [classes, num_imgs per␣
↪class]

# Determine number of validation images per class
num_val_exmps = sorted_indices.shape[1] // 10

# Get image indices for validation and training
val_indices   = sorted_indices[:,:num_val_exmps].reshape(-1)
train_indices = sorted_indices[:,num_val_exmps:].reshape(-1)

# Group corresponding image features and labels
train_feats, train_labels = train_set_feats[train_indices], labels[train_indices]
val_feats,   val_labels   = train_set_feats[val_indices],   labels[val_indices]
```

Now we can prepare a dataset class for the set anomaly task. We define an epoch to be the sequence in which each image has been exactly once as an "anomaly". Hence, the length of the dataset is the number of images in it. For the training set, each time we access an item with `__getitem__`, we sample a random, different class than the image at the corresponding index `idx` has. In a second step, we sample $N-1$ images of this sampled class. The set of 10 images is finally returned. The randomness in the `__getitem__` allows us to see a slightly different set during each iteration. However, we can't use the same strategy for the test set as we want the test dataset to be the same every time we iterate over it. Hence, we sample the sets in the `__init__` method, and return those in `__getitem__`. The code below implements exactly this dynamic.

[35]:
```
class SetAnomalyDataset(data.Dataset):

    def __init__(self, img_feats, labels, np_rng, set_size=10, train=True):
        """
        Inputs:
            img_feats - Tensor of shape [num_imgs, img_dim]. Represents the high-level␣
↪features.
            labels - Tensor of shape [num_imgs], containing the class labels for the␣
↪images
            set_size - Number of elements in a set. N-1 are sampled from one class, and␣
↪one from another one.
            train - If True, a new set will be sampled every time __getitem__ is called.
        """
        super().__init__()
        self.img_feats = img_feats
        self.labels = labels
        self.np_rng = np_rng
        self.set_size = set_size-1  # The set size is here the number of images from the␣
↪same class per set
        self.train = train
```

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```
        # Tensors with indices of the images per class
        self.num_labels = labels.max()+1
        self.img_idx_by_label = np.argsort(self.labels).reshape(self.num_labels, -1)

        if not train:
            self.test_sets = self._create_test_sets()

    def _create_test_sets(self):
        # Pre-generates the sets for each image for the test set
        test_sets = []
        num_imgs = self.img_feats.shape[0]
        test_sets = [self.sample_img_set(self.labels[idx]) for idx in range(num_imgs)]
        test_sets = np.stack(test_sets, axis=0)
        return test_sets

    def sample_img_set(self, anomaly_label):
        """
        Samples a new set of images, given the label of the anomaly.
        The sampled images come from a different class than anomaly_label
        """
        # Sample class from 0,...,num_classes-1 while skipping anomaly_label as class
        set_label = self.np_rng.integers(self.num_labels-1)
        if set_label >= anomaly_label:
            set_label += 1

        # Sample images from the class determined above
        img_indices = self.np_rng.choice(self.img_idx_by_label.shape[1], size=self.set_
↪size, replace=False)
        img_indices = self.img_idx_by_label[set_label, img_indices]
        return img_indices

    def __len__(self):
        return self.img_feats.shape[0]

    def __getitem__(self, idx):
        anomaly = self.img_feats[idx]
        if self.train: # If train => sample
            img_indices = self.sample_img_set(self.labels[idx])
        else: # If test => use pre-generated ones
            img_indices = self.test_sets[idx]

        # Concatenate images. The anomaly is always the last image for simplicity
        img_set = np.concatenate([self.img_feats[img_indices], anomaly[None]], axis=0)
        indices = np.concatenate([img_indices, np.array([idx], dtype=np.int32)], axis=0)
        label = img_set.shape[0]-1

        # We return the indices of the images for visualization purpose. "Label" is the␣
↪index of the anomaly
        return img_set, indices, label
```

Next, we can setup our datasets and data loaders below. Here, we will use a set size of 10, i.e. 9 images from one category + 1 anomaly. Feel free to change it if you want to experiment with the sizes.

[36]:
```
SET_SIZE = 10
test_labels = np.array(test_set.targets, dtype=np.int32)

anom_train_dataset = SetAnomalyDataset(train_feats, train_labels, np_rng=np.random.
↪default_rng(42), set_size=SET_SIZE, train=True)
anom_val_dataset   = SetAnomalyDataset(val_feats,   val_labels,   np_rng=np.random.
↪default_rng(43), set_size=SET_SIZE, train=False)
anom_test_dataset  = SetAnomalyDataset(test_feats,  test_labels,  np_rng=np.random.
↪default_rng(123), set_size=SET_SIZE, train=False)

anom_train_loader = data.DataLoader(anom_train_dataset, batch_size=64, shuffle=True, ␣
↪drop_last=True,  collate_fn=numpy_collate)
anom_val_loader   = data.DataLoader(anom_val_dataset,   batch_size=64, shuffle=False,␣
↪drop_last=False, collate_fn=numpy_collate)
anom_test_loader  = data.DataLoader(anom_test_dataset,  batch_size=64, shuffle=False,␣
↪drop_last=False, collate_fn=numpy_collate)
```

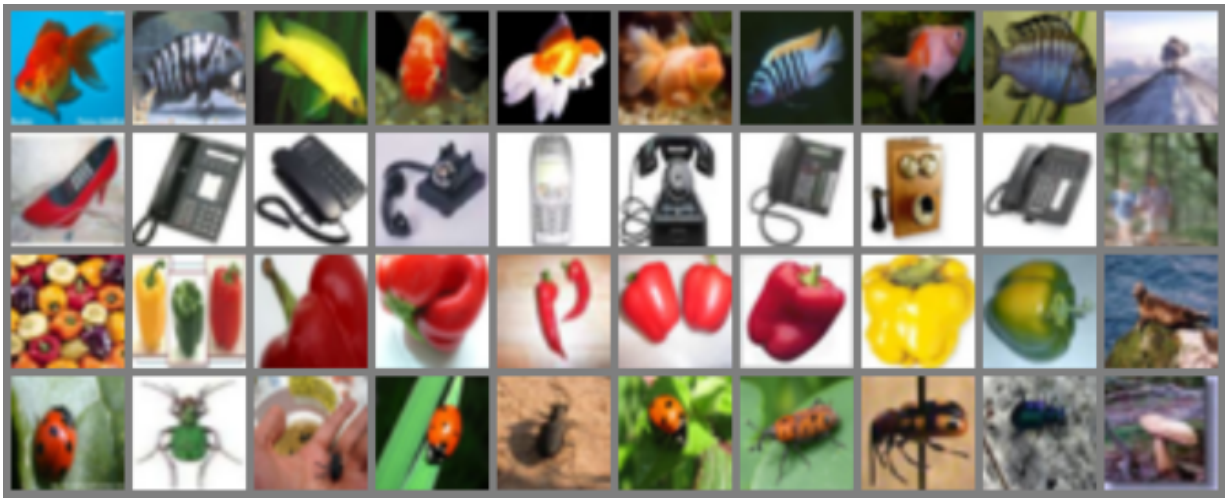
To understand the dataset a little better, we can plot below a few sets from the test dataset. Each row shows a different input set, where the first 9 are from the same class.

[37]:
```
def visualize_exmp(indices, orig_dataset):
    images = [orig_dataset[idx][0] for idx in indices.reshape(-1)]
    images = jax.device_get(jnp.stack(images, axis=0)).astype(np.float32)
    images = torch.from_numpy(images)
    images = images.permute(0, 3, 1, 2)
    img_grid = torchvision.utils.make_grid(images, nrow=SET_SIZE, normalize=True, pad_
↪value=0.5, padding=16)
    img_grid = img_grid.permute(1, 2, 0)

    plt.figure(figsize=(12,8))
    plt.title("Anomaly examples on CIFAR100")
    plt.imshow(img_grid)
    plt.axis('off')
    plt.show()
    plt.close()

_, indices, _ = next(iter(anom_test_loader))
visualize_exmp(indices[:4], test_set)
```

Anomaly examples on CIFAR100



We can already see that for some sets the task might be easier than for others. Difficulties can especially arise if the anomaly is in a different, but yet visually similar class (e.g. insect vs mushroom, train vs bus, etc.).

After having prepared the data, we can look closer at the model. Here, we have a classification of the whole set. For the prediction to be permutation-equivariant, we will output one logit for each image. Over these logits, we apply a softmax and train the anomaly image to have the highest score/probability. This is a bit different than a standard classification layer as the softmax is applied over images, not over output classes in the classical sense. However, if we swap two images in their position, we effectively swap their position in the output softmax. Hence, the prediction is equivariant with respect to the input. Furthermore, we need to remove the positional encoding since these features would break the permutation equivariance. We implement this setup below in the subclass of the Trainer module.

[38]:
```
class AnomalyTrainer(TrainerModule):

    def batch_to_input(self, batch):
        inp_data, _, _ = batch
        return inp_data

    def get_loss_function(self):
        # Function for calculating loss and accuracy for a batch
        def calculate_loss(params, rng, batch, train):
            inp_data, _, labels = batch
            rng, dropout_apply_rng = random.split(rng)
            logits = self.model.apply({'params': params}, inp_data,
                                      add_positional_encoding=False,  # No positional␣
↪encoding since this is a permutation equivariant task
                                      train=train,
                                      rngs={'dropout': dropout_apply_rng})
            logits = logits.squeeze(axis=-1)
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).astype(jnp.float32).mean()
            return loss, (acc, rng)
        return calculate_loss
```

Finally, we write our train function below. It has the exact same structure as the reverse task one, hence not much of an explanation is needed here.

[39]:
```
def train_anomaly(max_epochs=100, **model_args):
    num_train_iters = len(anom_train_loader) * max_epochs
    # Create a trainer module with specified hyperparameters
    trainer = AnomalyTrainer(model_name='SetAnomalyTask',
                             exmp_batch=next(iter(anom_train_loader)),
                             max_iters=num_train_iters,
                             **model_args)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(anom_train_loader, anom_val_loader, num_epochs=max_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    train_acc = trainer.eval_model(anom_train_loader)
    val_acc = trainer.eval_model(anom_val_loader)
    test_acc = trainer.eval_model(anom_test_loader)
    # Bind parameters to model for easier inference
    trainer.model_bd = trainer.model.bind({'params': trainer.state.params})
    return trainer, {'train_acc': train_acc, 'val_acc': val_acc, 'test_acc': test_acc}
```

Let's finally train our model. We will use 4 layers with 4 attention heads each. The hidden dimensionality of the model is 256, and we use a dropout of 0.1 throughout the model for good regularization. Note that we also apply the dropout on the input features, as this makes the model more robust against image noise and generalizes better. Again, we use warmup to slowly start our model training.

[40]:
```
anomaly_trainer, anomaly_result = train_anomaly(model_dim=256,
                                                num_heads=4,
                                                num_classes=1,
                                                num_layers=4,
                                                dropout_prob=0.1,
                                                input_dropout_prob=0.1,
                                                lr=5e-4,
                                                warmup=100)
```

We can print the achieved accuracy below.

[41]:
```
print(f"Train accuracy: {(100.0*anomaly_result['train_acc']):4.2f}%")
print(f"Val accuracy:   {(100.0*anomaly_result['val_acc']):4.2f}%")
print(f"Test accuracy:  {(100.0*anomaly_result['test_acc']):4.2f}%")
```

```
Train accuracy: 98.37%
Val accuracy:   94.50%
Test accuracy:  94.66%
```

With ~94% validation and test accuracy, the model generalizes quite well. It should be noted that you might see slightly different scores depending on what computer/device you are running this notebook. This is because despite setting the seed before generating the test dataset, it may not always be the same across platforms and numpy versions. Nevertheless, we can conclude that the model performs quite well and can solve the task for most sets. Before trying to interpret the model, let's verify that our model is permutation-equivariant, and assigns the same predictions for different permutations of the input set. For this, we sample a batch from the test set and run it through the model to obtain the probabilities.

[42]:
```
inp_data, indices, labels = next(iter(anom_test_loader))
preds = anomaly_trainer.model_bd(inp_data, add_positional_encoding=False, train=False)
preds = jax.nn.softmax(preds.squeeze(axis=-1))
```

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```
permut = np.random.permutation(inp_data.shape[1])
permut_inp_data = inp_data[:,permut]
perm_preds = anomaly_trainer.model_bd(permut_inp_data, add_positional_encoding=False,␣
↪train=False)
perm_preds = jax.nn.softmax(perm_preds.squeeze(axis=-1))

preds = jax.device_get(preds)
perm_preds = jax.device_get(perm_preds)

assert np.abs(preds[:,permut] - perm_preds).max() < 1e-5, "Predictions are not␣
↪permutation equivariant"

print("Preds\n", preds[0,permut])
print("Permuted preds\n", perm_preds[0])
```

```
Preds
 [1.3902171e-07 4.3522828e-08 5.2554757e-08 1.2441276e-08 2.7709259e-08
 9.9999952e-01 5.5640967e-08 3.5155960e-08 1.4563368e-08 4.8264688e-08]
Permuted preds
 [1.3902175e-07 4.3522839e-08 5.2554768e-08 1.2441279e-08 2.7709264e-08
 9.9999976e-01 5.5640978e-08 3.5155971e-08 1.4563372e-08 4.8264699e-08]
```

You can see that the predictions are almost exactly the same, and only differ because of slight numerical differences inside the network operation.

To interpret the model a little more, we can plot the attention maps inside the model. This will give us an idea of what information the model is sharing/communicating between images, and what each head might represent. First, we need to extract the attention maps for the test batch above, and determine the discrete predictions for simplicity.

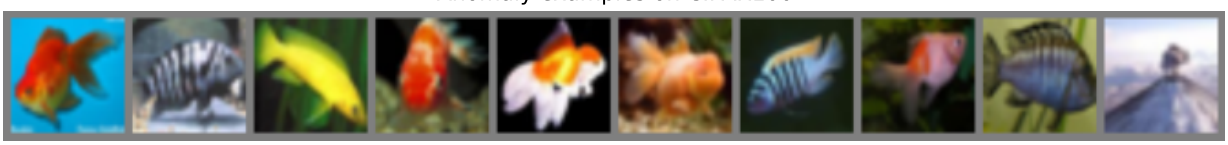
[43]:
```
attention_maps = anomaly_trainer.model_bd.get_attention_maps(inp_data, add_positional_
↪encoding=False, train=False)
predictions = preds.argmax(axis=-1)
```

Below we write a plot function which plots the images in the input set, the prediction of the model, and the attention maps of the different heads on layers of the transformer. Feel free to explore the attention maps for different input examples as well.

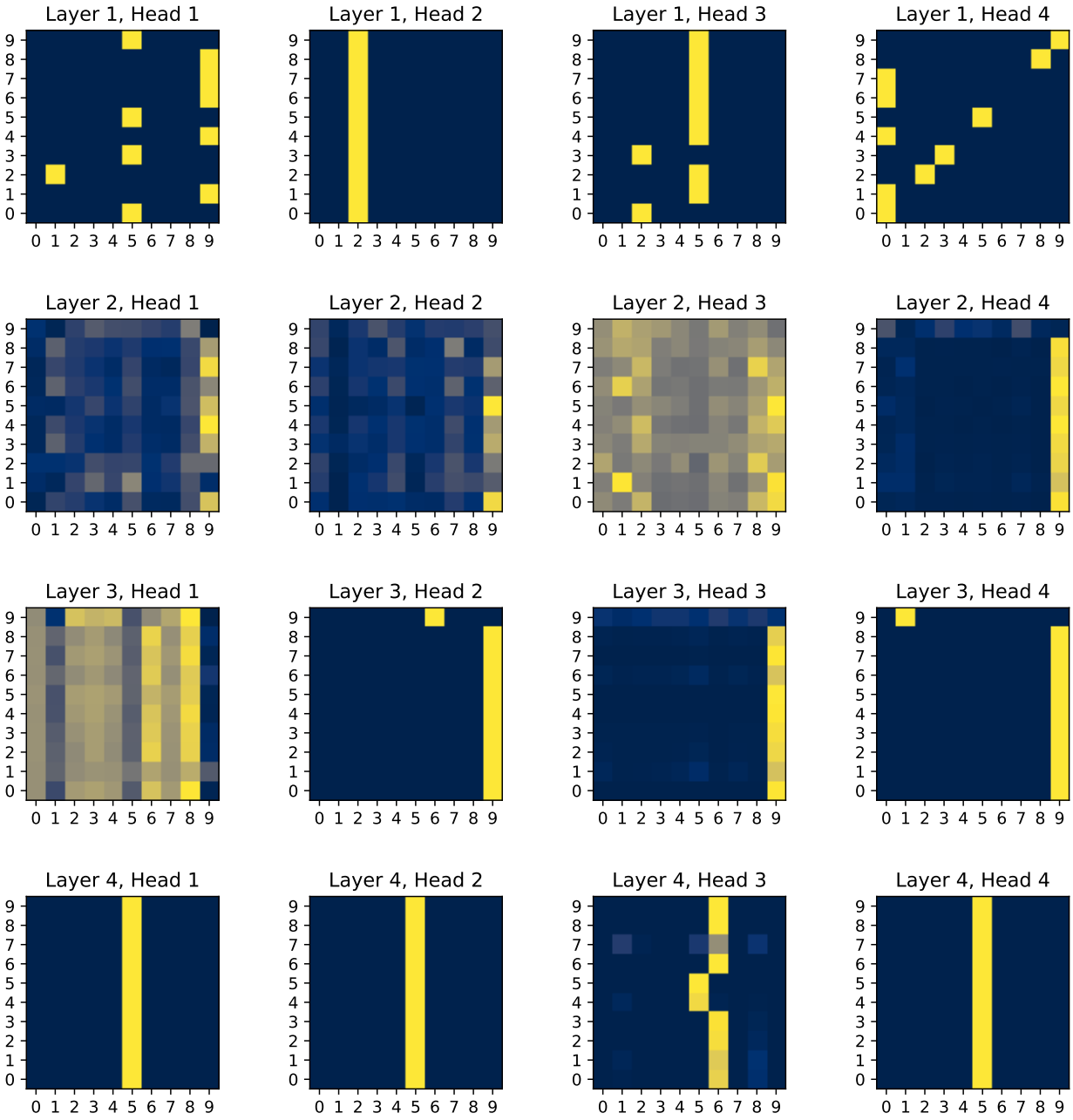
[44]:
```
def visualize_prediction(idx):
    visualize_exmp(indices[idx:idx+1], test_set)
    print(f'Main class: {class_idx_to_name[test_labels[indices[idx,0]]]}, Anomaly class:
↪{class_idx_to_name[test_labels[indices[idx,-1]]]}')
    print(f'Prediction: image {predictions[idx].item()}')
    plot_attention_maps(input_data=None, attn_maps=attention_maps, idx=idx)

visualize_prediction(0)
```

Anomaly examples on CIFAR100



```
Main class: aquarium_fish, Anomaly class: mountain
Prediction: image 9
```



Depending on the random seed, you might see a slightly different input set. For the version on the website, we compare 9 aquarium fish images with a volcano/mountain. We see that multiple heads, for instance, Layer 2 Head 1, Layer 2 Head 4, and Layer 3 Head 2-4 focus on the last image. Additionally, the heads in Layer 4 all seem to ignore the last image and assign a very low attention probability to it. This shows that the model has indeed recognized that the image doesn't fit the setting, and hence predicted it to be the anomaly. Layer 2 Head 3 and Layer 3 Head 1 seems to take a slightly weighted average of all images. That might indicate that the model extracts the "average" information of all images, to compare it to the image features itself.

Let's try to find where the model actually makes a mistake. We can do this by identifying the sets where the model

predicts something else than 9, as in the dataset, we ensured that the anomaly is always at the last position in the set.

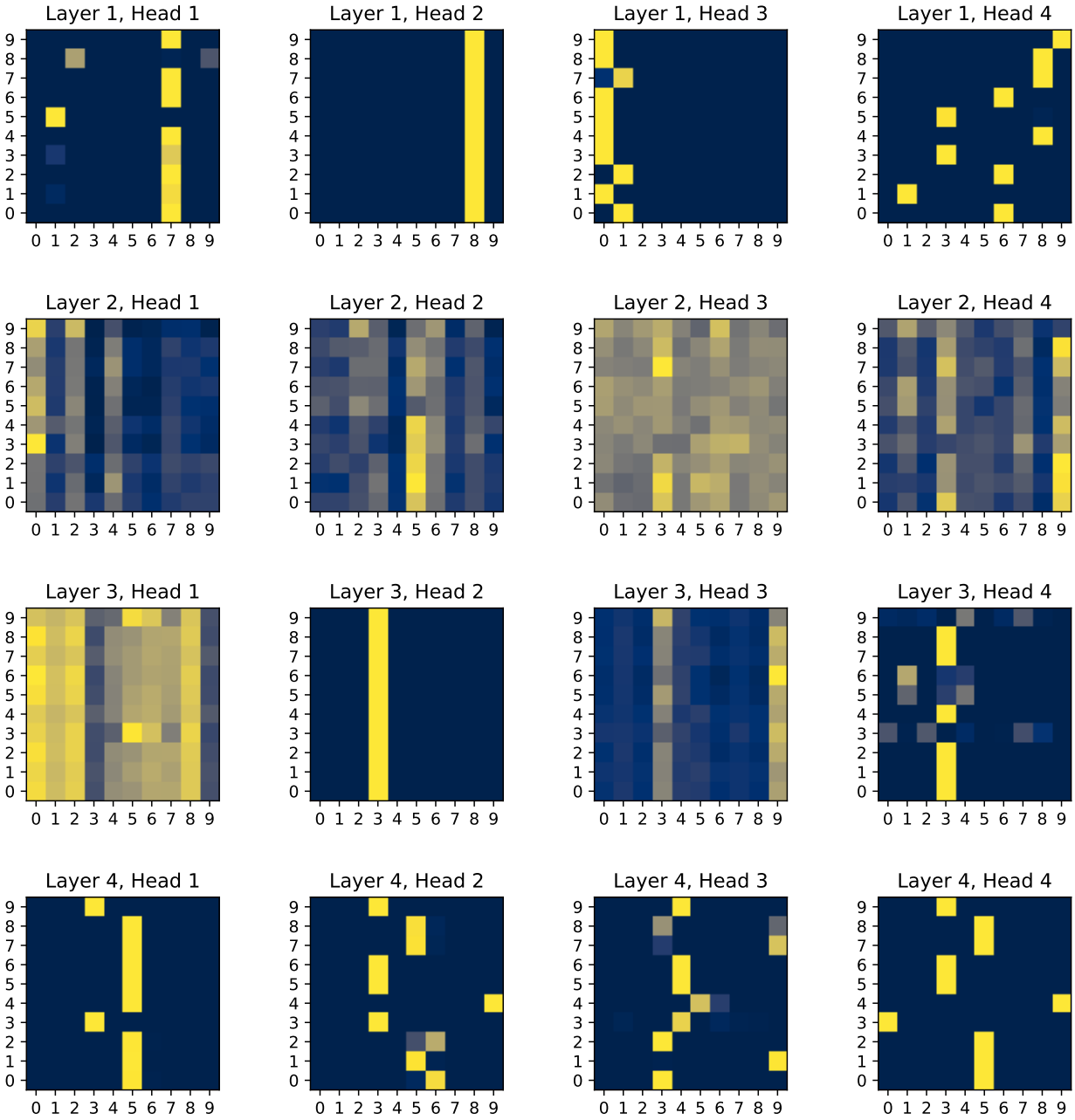
[45]:
```
mistakes = np.where(predictions != 9)[0]
print("Indices with mistake:", mistakes)
```

```
Indices with mistake: [10 58]
```

As our model achieves ~94% accuracy, we only have very little number of mistakes in a batch of 64 sets. Still, let's visualize one of them, for example the last one:

[46]:
```
visualize_prediction(mistakes[0])
print("Probabilities:")
for i, p in enumerate(preds[mistakes[0]]):
    print(f"Image {i}: {100.0*p:4.2f}%")
```


```
Main class: forest, Anomaly class: sea
Prediction: image 3
```




```
Probabilities:
Image 0: 0.84%
Image 1: 1.53%
Image 2: 1.00%
Image 3: 54.88%
Image 4: 2.39%
Image 5: 6.54%
Image 6: 4.91%
Image 7: 1.44%
Image 8: 1.39%
Image 9: 25.09%
```

In this example, the model confuses a picture of a sea with a forest, giving a probability of ~55% to image 3, and 25% to the actual anomaly. However, the difficulty here is that the picture of the sea actually contains trees in the foreground, which makes the image a bit of an ambiguous class. It is possible a picture of a sea taken out of a forest, which confuses the model. Nevertheless, in general, the model performs quite well.

4.34.3 Conclusion

In this tutorial, we took a closer look at the Multi-Head Attention layer which uses a scaled dot product between queries and keys to find correlations and similarities between input elements. The Transformer architecture is based on the Multi-Head Attention layer and applies multiple of them in a ResNet-like block. The Transformer is a very important, recent architecture that can be applied to many tasks and datasets. Although it is best known for its success in NLP, there is so much more to it. We have seen its application on sequence-to-sequence tasks and set anomaly detection. Its property of being permutation-equivariant if we do not provide any positional encodings, allows it to generalize to many settings. Hence, it is important to know the architecture, but also its possible issues such as the gradient problem during the first iterations solved by learning rate warm-up. If you are interested in continuing with the study of the Transformer architecture, please have a look at the blog posts listed at the beginning of the tutorial notebook.

If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.35 Tutorial 7 (JAX): Graph Neural Networks

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

In this tutorial, we will discuss the application of neural networks on graphs. Graph Neural Networks (GNNs) have recently gained increasing popularity in both applications and research, including domains such as social networks, knowledge graphs, recommender systems, and bioinformatics. While the theory and math behind GNNs might first seem complicated, the implementation of those models is quite simple and helps in understanding the methodology. Therefore, we will discuss the implementation of basic network layers of a GNN, namely graph convolutions, and attention layers.

Below, we will start by importing our standard libraries. We will use JAX, Flax and Optax for training our models.

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
import time

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()
sns.set()

## Progress bar
from tqdm.notebook import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch
import torch
import torch.utils.data as data
import torchvision
```

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```
from torchvision.datasets import CIFAR10
from torchvision import transforms

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial7_jax"

print("Device:", jax.devices()[0])
```

```
/tmp/ipykernel_2384472/156319451.py:12: DeprecationWarning: `set_matplotlib_formats` is␣
↪deprecated since IPython 7.23, directly use `matplotlib_inline.backend_inline.set_
↪matplotlib_formats()`
  set_matplotlib_formats('svg', 'pdf') # For export
```

```
Device: gpu:0
```

We also have a few pre-trained models we download below.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial7/"
# Files to download
pretrained_files = []

# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please contact the author with the full output␣
↪including the following error:\n", e)
```

4.35.1 Graph Neural Networks

Graph representation

Before starting the discussion of specific neural network operations on graphs, we should consider how to represent a graph. Mathematically, a graph $\mathcal{G}$ is defined as a tuple of a set of nodes/vertices V, and a set of edges/links E: $\mathcal{G} = (V, E)$. Each edge is a pair of two vertices, and represents a connection between them. For instance, let's look at the following graph:

The vertices are $V = \{1, 2, 3, 4\}$, and edges $E = \{(1, 2), (2, 3), (2, 4), (3, 4)\}$. Note that for simplicity, we assume the graph to be undirected and hence don't add mirrored pairs like $(2, 1)$. In application, vertices and edge can often have specific attributes, and edges can even be directed. The question is how we could represent this diversity in an efficient way for matrix operations. Usually, for the edges, we decide between two variants: an adjacency matrix, or a list of paired vertex indices.

The **adjacency matrix** A is a square matrix whose elements indicate whether pairs of vertices are adjacent, i.e. connected, or not. In the simplest case, A_{ij} is 1 if there is a connection from node i to j, and otherwise 0. If we have edge attributes or different categories of edges in a graph, this information can be added to the matrix as well. For an undirected graph, keep in mind that A is a symmetric matrix ($A_{ij} = A_{ji}$). For the example graph above, we have the following adjacency matrix:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

While expressing a graph as a list of edges is more efficient in terms of memory and (possibly) computation, using an adjacency matrix is more intuitive and simpler to implement. In our implementations below, we will rely on the adjacency matrix to keep the code simple. However, common libraries use edge lists, which we will discuss later more.

Graph Convolutions

Graph Convolutional Networks have been introduced by Kipf et al. in 2016 at the University of Amsterdam. He also wrote a great blog post about this topic, which is recommended if you want to read about GCNs from a different perspective. GCNs are similar to convolutions in images in the sense that the "filter" parameters are typically shared over all locations in the graph. At the same time, GCNs rely on message passing methods, which means that vertices exchange information with the neighbors, and send "messages" to each other. Before looking at the math, we can try to visually understand how GCNs work. The first step is that each node creates a feature vector that represents the message it wants to send to all its neighbors. In the second step, the messages are sent to the neighbors, so that a node receives one message per adjacent node. Below we have visualized the two steps for our example graph.

If we want to formulate that in more mathematical terms, we need to first decide how to combine all the messages a node receives. As the number of messages vary across nodes, we need an operation that works for any number. Hence, the usual way to go is to sum or take the mean. Given the previous features of nodes $H^{(l)}$, the GCN layer is defined as follows:

$$H^{(l+1)} = \sigma\left(\hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}H^{(l)}W^{(l)}\right)$$

$W^{(l)}$ is the weight parameters with which we transform the input features into messages ($H^{(l)}W^{(l)}$). To the adjacency matrix A we add the identity matrix so that each node sends its own message also to itself: $\hat{A} = A + I$. Finally, to take the average instead of summing, we calculate the matrix $\hat{D}$ which is a diagonal matrix with D_{ii} denoting the number of neighbors node i has. σ represents an arbitrary activation function, and not necessarily the sigmoid (usually a ReLU-based activation function is used in GNNs).

When implementing the GCN layer in JAX/Flax, we can take advantage of the flexible operations on tensors. Instead of defining a matrix $\hat{D}$, we can simply divide the summed messages by the number of neighbors afterward. Additionally, we replace the weight matrix with a linear layer, which additionally allows us to add a bias. Written as a Flax module, the GCN layer is defined as follows:

[3]:
```
class GCNLayer(nn.Module):
    c_out : int  # Output feature size
```

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```
    @nn.compact
    def __call__(self, node_feats, adj_matrix):
        """
        Inputs:
            node_feats - Array with node features of shape [batch_size, num_nodes, c_in]
            adj_matrix - Batch of adjacency matrices of the graph. If there is an edge␣
↪from i to j, adj_matrix[b,i,j]=1 else 0.
                         Supports directed edges by non-symmetric matrices. Assumes to␣
↪already have added the identity connections.
                         Shape: [batch_size, num_nodes, num_nodes]
        """
        # Num neighbours = number of incoming edges
        num_neighbours = adj_matrix.sum(axis=-1, keepdims=True)
        node_feats = nn.Dense(features=self.c_out, name='projection')(node_feats)
        node_feats = jax.lax.batch_matmul(adj_matrix, node_feats)
        node_feats = node_feats / num_neighbours
        return node_feats
```

To further understand the GCN layer, we can apply it to our example graph above. First, let's specify some node features and the adjacency matrix with added self-connections:

[4]:
```
node_feats = jnp.arange(8, dtype=jnp.float32).reshape((1, 4, 2))
adj_matrix = jnp.array([[[1, 1, 0, 0],
                         [1, 1, 1, 1],
                         [0, 1, 1, 1],
                         [0, 1, 1, 1]]]).astype(jnp.float32)

print("Node features:\n", node_feats)
print("\nAdjacency matrix:\n", adj_matrix)
```

```
Node features:
 [[[0. 1.]
  [2. 3.]
  [4. 5.]
  [6. 7.]]]

Adjacency matrix:
 [[[1. 1. 0. 0.]
  [1. 1. 1. 1.]
  [0. 1. 1. 1.]
  [0. 1. 1. 1.]]]
```

Next, let's apply a GCN layer to it. For simplicity, we initialize the linear weight matrix as an identity matrix so that the input features are equal to the messages. This makes it easier for us to verify the message passing operation.

[5]:
```
layer = GCNLayer(c_out=2)
# We define our own parameters here instead of using random initialization
params = {'projection': {
    'kernel': jnp.array([[1., 0.], [0., 1.]]),
    'bias': jnp.array([0., 0.])
}}
out_feats = layer.apply({'params': params}, node_feats, adj_matrix)
```

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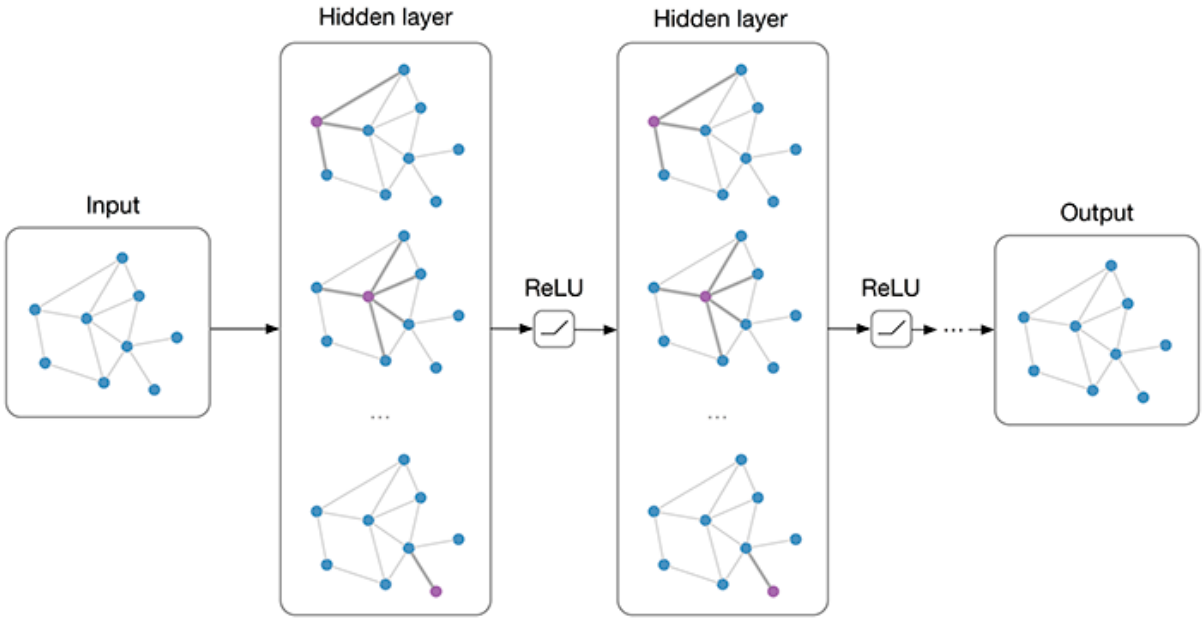
```
print("Adjacency matrix", adj_matrix)
print("Input features", node_feats)
print("Output features", out_feats)
```

```
Adjacency matrix [[[1. 1. 0. 0.]
  [1. 1. 1. 1.]
  [0. 1. 1. 1.]
  [0. 1. 1. 1.]]]
Input features [[[0. 1.]
  [2. 3.]
  [4. 5.]
  [6. 7.]]]
Output features [[[1. 2.]
  [3. 4.]
  [4. 5.]
  [4. 5.]]]
```

As we can see, the first node's output values are the average of itself and the second node. Similarly, we can verify all other nodes. However, in a GNN, we would also want to allow feature exchange between nodes beyond its neighbors. This can be achieved by applying multiple GCN layers, which gives us the final layout of a GNN. The GNN can be build up by a sequence of GCN layers and non-linearities such as ReLU. For a visualization, see below (figure credit - Thomas Kipf, 2016).



However, one issue we can see from looking at the example above is that the output features for nodes 3 and 4 are the same because they have the same adjacent nodes (including itself). Therefore, GCN layers can make the network forget node-specific information if we just take a mean over all messages. Multiple possible improvements have been proposed. While the simplest option might be using residual connections, the more common approach is to either weigh the self-connections higher or define a separate weight matrix for the self-connections. Alternatively, we can re-visit a concept from the last tutorial: attention.

Graph Attention

If you remember from the last tutorial, attention describes a weighted average of multiple elements with the weights dynamically computed based on an input query and elements' keys (if you haven't read Tutorial 6 yet, it is recommended to at least go through the very first section called What is Attention?). This concept can be similarly applied to graphs, one of such is the Graph Attention Network (called GAT, proposed by Velickovic et al., 2017). Similarly to the GCN, the graph attention layer creates a message for each node using a linear layer/weight matrix. For the attention part, it uses the message from the node itself as a query, and the messages to average as both keys and values (note that this also includes the message to itself). The score function f_{attn} is implemented as a one-layer MLP which maps the query and key to a single value. The MLP looks as follows (figure credit - Velickovic et al.):

h_i and h_j are the original features from node i and j respectively, and represent the messages of the layer with $\mathbf{W}$ as weight matrix. $\mathbf{a}$ is the weight matrix of the MLP, which has the shape $[1, 2 \times d_{\text{message}}]$, and α_{ij} the final attention weight from node i to j. The calculation can be described as follows:

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_j\right]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_k\right]\right)\right)}$$

The operator $||$ represents the concatenation, and $\mathcal{N}_i$ the indices of the neighbors of node i. Note that in contrast to usual practice, we apply a non-linearity (here LeakyReLU) before the softmax over elements. Although it seems like a minor change at first, it is crucial for the attention to depend on the original input. Specifically, let's remove the non-linearity for a second, and try to simplify the expression:

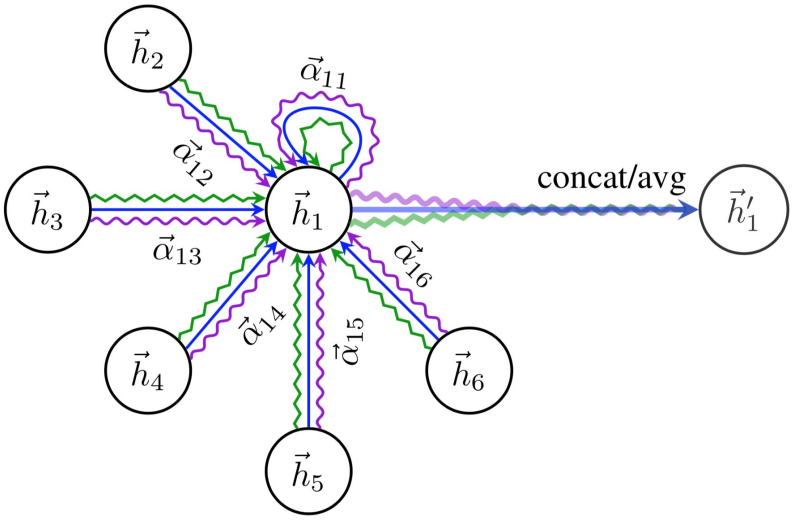
$$\begin{aligned}
\alpha_{ij} &= \frac{\exp\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_j\right]\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}\left[\mathbf{W}h_i||\mathbf{W}h_k\right]\right)}\\
&= \frac{\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i + \mathbf{a}_{:,d/2:}\mathbf{W}h_j\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i + \mathbf{a}_{:,d/2:}\mathbf{W}h_k\right)}\\
&= \frac{\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i\right)\cdot\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_j\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}_{:,:d/2}\mathbf{W}h_i\right)\cdot\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_k\right)}\\
&= \frac{\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_j\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathbf{a}_{:,d/2:}\mathbf{W}h_k\right)}
\end{aligned}$$

We can see that without the non-linearity, the attention term with h_i actually cancels itself out, resulting in the attention being independent of the node itself. Hence, we would have the same issue as the GCN of creating the same output features for nodes with the same neighbors. This is why the LeakyReLU is crucial and adds some dependency on h_i to the attention.

Once we obtain all attention factors, we can calculate the output features for each node by performing the weighted average:

$$h_i' = \sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}\mathbf{W}h_j\right)$$

σ is yet another non-linearity, as in the GCN layer. Visually, we can represent the full message passing in an attention layer as follows (figure credit - Velickovic et al.):



To increase the expressiveness of the graph attention network, Velickovic et al. proposed to extend it to multiple heads similar to the Multi-Head Attention block in Transformers. This results in N attention layers being applied in parallel. In the image above, it is visualized as three different colors of arrows (green, blue, and purple) that are afterward concatenated. The average is only applied for the very final prediction layer in a network.

After having discussed the graph attention layer in detail, we can implement it below:

[6]:
```
class GATLayer(nn.Module):
    c_out : int  # Dimensionality of output features
    num_heads : int  # Number of heads, i.e. attention mechanisms to apply in parallel.
    concat_heads : bool = True  # If True, the output of the different heads is␣
↪concatenated instead of averaged.
    alpha : float = 0.2  # Negative slope of the LeakyReLU activation.

    def setup(self):
        if self.concat_heads:
            assert self.c_out % self.num_heads == 0, "Number of output features must be␣
↪a multiple of the count of heads."
            c_out_per_head = self.c_out // self.num_heads
        else:
            c_out_per_head = self.c_out

        # Sub-modules and parameters needed in the layer
        self.projection = nn.Dense(c_out_per_head * self.num_heads,
                                   kernel_init=nn.initializers.glorot_uniform())
        self.a = self.param('a',
                            nn.initializers.glorot_uniform(),
                            (self.num_heads, 2 * c_out_per_head))  # One per head


    def __call__(self, node_feats, adj_matrix, print_attn_probs=False):
        """
        Inputs:
            node_feats - Input features of the node. Shape: [batch_size, c_in]
            adj_matrix - Adjacency matrix including self-connections. Shape: [batch_size,
↪ num_nodes, num_nodes]
            print_attn_probs - If True, the attention weights are printed during the␣
↪forward pass (for debugging purposes)
```

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```
        """
        batch_size, num_nodes = node_feats.shape[0], node_feats.shape[1]

        # Apply linear layer and sort nodes by head
        node_feats = self.projection(node_feats)
        node_feats = node_feats.reshape((batch_size, num_nodes, self.num_heads, -1))

        # We need to calculate the attention logits for every edge in the adjacency␣
↪matrix
        # In order to take advantage of JAX's just-in-time compilation, we should not use
        # arrays with shapes that depend on e.g. the number of edges. Hence, we calculate
        # the logit for every possible combination of nodes. For efficiency, we can split
        # a[Wh_i||Wh_j] = a_:d/2 * Wh_i + a_d/2: * Wh_j.
        logit_parent = (node_feats * self.a[None,None,:,:self.a.shape[1]//2]).sum(axis=-
↪1)
        logit_child = (node_feats * self.a[None,None,:,self.a.shape[1]//2:]).sum(axis=-1)
        attn_logits = logit_parent[:,:,None,:] + logit_child[:,None,:,:]
        attn_logits = nn.leaky_relu(attn_logits, self.alpha)

        # Mask out nodes that do not have an edge between them
        attn_logits = jnp.where(adj_matrix[...,None] == 1.,
                                attn_logits,
                                jnp.ones_like(attn_logits) * (-9e15))

        # Weighted average of attention
        attn_probs = nn.softmax(attn_logits, axis=2)
        if print_attn_probs:
            print("Attention probs\n", attn_probs.transpose(0, 3, 1, 2))
        node_feats = jnp.einsum('bijh,bjhc->bihc', attn_probs, node_feats)

        # If heads should be concatenated, we can do this by reshaping. Otherwise, take␣
↪mean
        if self.concat_heads:
            node_feats = node_feats.reshape(batch_size, num_nodes, -1)
        else:
            node_feats = node_feats.mean(axis=2)

        return node_feats
```

Again, we can apply the graph attention layer on our example graph above to understand the dynamics better. As before, the input layer is initialized as an identity matrix, but we set $\mathbf{a}$ to be a vector of arbitrary numbers to obtain different attention values. We use two heads to show the parallel, independent attention mechanisms working in the layer.

[7]:
```
layer = GATLayer(2, num_heads=2)
params = {
    'projection': {
        'kernel': jnp.array([[1., 0.], [0., 1.]]),
        'bias': jnp.array([0., 0.])
    },
    'a': jnp.array([[-0.2, 0.3], [0.1, -0.1]])
}
out_feats = layer.apply({'params': params}, node_feats, adj_matrix, print_attn_
↪probs=True)
```

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```
print("Adjacency matrix", adj_matrix)
print("Input features", node_feats)
print("Output features", out_feats)
```

```
Attention probs
 [[[[0.35434368 0.6456563  0.         0.        ]
   [0.10956533 0.14496915 0.26415104 0.48131457]
   [0.         0.18580717 0.2885041  0.52568877]
   [0.         0.23912403 0.2696116  0.49126437]]

  [[0.5099987  0.49000138 0.         0.        ]
   [0.2975179  0.24358706 0.23403588 0.2248592 ]
   [0.         0.38382432 0.31424877 0.3019269 ]
   [0.         0.40175956 0.3289329  0.26930752]]]]
Adjacency matrix [[[1. 1. 0. 0.]
  [1. 1. 1. 1.]
  [0. 1. 1. 1.]
  [0. 1. 1. 1.]]]
Input features [[[0. 1.]
  [2. 3.]
  [4. 5.]
  [6. 7.]]]
Output features [[[1.2913126 1.9800028]
  [4.23443   3.7724729]
  [4.6797633 4.8362055]
  [4.504281  4.735096 ]]]
```

We recommend that you try to calculate the attention matrix at least for one head and one node for yourself. The entries are 0 where there does not exist an edge between i and j. For the others, we see a diverse set of attention probabilities. Moreover, the output features of node 3 and 4 are now different although they have the same neighbors.

4.35.2 Conclusion

In this tutorial, we have seen the application of neural networks to graph structures. We looked at how a graph can be represented (adjacency matrix or edge list), and discussed the implementation of common graph layers: GCN and GAT. The implementations showed the practical side of the layers, which is often easier than the theory. For implementing full GNNs in JAX, we recommend taking a look at Jraph. There are a lot of applications that benefit from GNNs, and the importance of these networks will likely increase over the next years.

If you found this tutorial helpful, consider -ing our repository.

For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.36 Tutorial 9 (JAX): Deep Autoencoders

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We note the training times for all models in the PyTorch and the JAX implementation below (PyTorch v1.11, JAX v0.3.13). The models were trained on the same hardware (NVIDIA RTX3090, 24 core CPU) and we slightly adjusted the tutorials to use the exact same training settings (same data loading parameters, evaluation schedule, etc.). Overall, the JAX implementation is about *1.8x faster* than PyTorch!

Models	PyTorch	JAX
AE - 64 latents	13min 10sec	7min 10sec
AE - 128 latents	13min 11sec	7min 10sec
AE - 256 latents	13min 11sec	7min 11sec
AE - 384 latents	13min 12sec	7min 14sec

In this tutorial, we will take a closer look at autoencoders (AE). Autoencoders are trained on encoding input data such as images into a smaller feature vector, and afterward, reconstruct it by a second neural network, called a decoder. The feature vector is called the "bottleneck" of the network as we aim to compress the input data into a smaller amount of features. This property is useful in many applications, in particular in compressing data or comparing images on a metric beyond pixel-level comparisons. Besides learning about the autoencoder framework, we will also see the "deconvolution" (or transposed convolution) operator in action for scaling up feature maps in height and width. Such deconvolution networks are necessary wherever we start from a small feature vector and need to output an image of full size (e.g. in VAE, GANs, or super-resolution applications).

First of all, we import most of our standard libraries. We use JAX as acceleration backend, Flax for implementing neural networks, and Optax to optimize the models.

[1]:
```
## Standard libraries
import os
import json
import math
import numpy as np
from scipy import spatial

## Imports for plotting
import matplotlib.pyplot as plt
```

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```
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()
sns.set()

## Progress bar
from tqdm.auto import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch Data Loading
import torch
import torch.utils.data as data
import torchvision
from torchvision.datasets import CIFAR10

# Tensorboard extension (for visualization purposes later)
from torch.utils.tensorboard import SummaryWriter
%load_ext tensorboard

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../../data"
```

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```
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial9_jax"

print("Device:", jax.devices()[0])
```

```
Device: gpu:0
```

We have 4 pretrained models that we have to download. Remember the adjust the variables DATASET_PATH and CHECKPOINT_PATH if needed.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial9/"
# Files to download
pretrained_files = ["cifar10_64.ckpt", "cifar10_128.ckpt", "cifar10_256.ckpt", "cifar10_
↪384.ckpt"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please contact the author with the full output␣
↪including the following error:\n", e)
```

In this tutorial, we work with the CIFAR10 dataset. In CIFAR10, each image has 3 color channels and is 32x32 pixels large. As autoencoders do not have the constrain of modeling images probabilistic, we can work on more complex image data (i.e. 3 color channels instead of black-and-white) much easier than for VAEs. In case you have downloaded CIFAR10 already in a different directory, make sure to set DATASET_PATH accordingly to prevent another download.

In contrast to previous tutorials on CIFAR10 like Tutorial 5 (CNN classification), we do not normalize the data explicitly with a mean of 0 and std of 1, but roughly estimate it scaling the data between -1 and 1. This is because limiting the range will make our task of predicting/reconstructing images easier.

[3]:
```
# Transformations applied on each image => bring them into a numpy array
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    if img.max() > 1:
        img = img / 255. * 2. - 1.
    return img

# For visualization, we might want to map JAX or numpy tensors back to PyTorch
def jax_to_torch(imgs):
    imgs = jax.device_get(imgs)
    imgs = torch.from_numpy(imgs.astype(np.float32))
    imgs = imgs.permute(0, 3, 1, 2)
```

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```
    return imgs

# We need to stack the batch elements
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=image_to_numpy,␣
↪download=True)
train_set, val_set = data.random_split(train_dataset, [45000, 5000], generator=torch.
↪Generator().manual_seed(42))

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=image_to_numpy,␣
↪download=True)

# We define a set of data loaders that we can use for various purposes later.
train_loader = data.DataLoader(train_set, batch_size=256, shuffle=True, drop_last=True,␣
↪pin_memory=True, num_workers=4, collate_fn=numpy_collate, persistent_workers=True)
val_loader = data.DataLoader(val_set, batch_size=256, shuffle=False, drop_last=False,␣
↪num_workers=4, collate_fn=numpy_collate)
test_loader = data.DataLoader(test_set, batch_size=256, shuffle=False, drop_last=False,␣
↪num_workers=4, collate_fn=numpy_collate)
```

```
Files already downloaded and verified
Files already downloaded and verified
```

4.36.1 Building the autoencoder

In general, an autoencoder consists of an **encoder** that maps the input x to a lower-dimensional feature vector z, and a **decoder** that reconstructs the input $\hat{x}$ from z. We train the model by comparing x to $\hat{x}$ and optimizing the parameters to increase the similarity between x and $\hat{x}$. See below for a small illustration of the autoencoder framework.

We first start by implementing the encoder. The encoder effectively consists of a deep convolutional network, where we scale down the image layer-by-layer using strided convolutions. After downscaling the image three times, we flatten the features and apply linear layers. The latent representation z is therefore a vector of size d which can be flexibly selected.

[4]:
```
class Encoder(nn.Module):
    c_hid : int
    latent_dim : int

    @nn.compact
    def __call__(self, x):
```

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```
        x = nn.Conv(features=self.c_hid, kernel_size=(3, 3), strides=2)(x)  # 32x32 =>␣
↪16x16
        x = nn.gelu(x)
        x = nn.Conv(features=self.c_hid, kernel_size=(3, 3))(x)
        x = nn.gelu(x)
        x = nn.Conv(features=2*self.c_hid, kernel_size=(3, 3), strides=2)(x)  # 16x16 =>␣
↪8x8
        x = nn.gelu(x)
        x = nn.Conv(features=2*self.c_hid, kernel_size=(3, 3))(x)
        x = nn.gelu(x)
        x = nn.Conv(features=2*self.c_hid, kernel_size=(3, 3), strides=2)(x)  # 8x8 =>␣
↪4x4
        x = nn.gelu(x)
        x = x.reshape(x.shape[0], -1)  # Image grid to single feature vector
        x = nn.Dense(features=self.latent_dim)(x)
        return x
```

[5]:
```
## Test encoder implementation
# Random key for initialization
rng = random.PRNGKey(0)
# Example images as input
imgs = next(iter(train_loader))[0]
# Create encoder
encoder = Encoder(c_hid=32, latent_dim=128)
# Initialize parameters of encoder with random key and images
params = encoder.init(rng, imgs)['params']
# Apply encoder with parameters on the images
out = encoder.apply({'params': params}, imgs)
out.shape

del out, encoder, params
```

Note that we do not apply Batch Normalization here. This is because we want the encoding of each image to be independent of all the other images. Otherwise, we might introduce correlations into the encoding or decoding that we do not want to have. In some implementations, you still can see Batch Normalization being used, because it can also serve as a form of regularization. Nevertheless, the better practice is to go with other normalization techniques if necessary like Instance Normalization or Layer Normalization. Given the small size of the model, we can neglect normalization for now.

The decoder is a mirrored, flipped version of the encoder. The only difference is that we replace strided convolutions by transposed convolutions (i.e. deconvolutions) to upscale the features. Transposed convolutions can be imagined as adding the stride to the input instead of the output, and can thus upscale the input. For an illustration of a `nn.ConvTranspose` layer with kernel size 3, stride 2, and padding 1, see below (figure credit - Vincent Dumoulin and Francesco Visin):

You see that for an input of size 3×3, we obtain an output of 5×5. However, to truly have a reverse operation of the convolution, we need to ensure that the layer scales the input shape by a factor of 2 (e.g. $4 \times 4 \rightarrow 8 \times 8$). Flax already has this as a default setting for the padding, so we do not need to adjust anything here.

Overall, the decoder can be implemented as follows:

[6]:
```
class Decoder(nn.Module):
    c_out : int
    c_hid : int
    latent_dim : int

    @nn.compact
    def __call__(self, x):
        x = nn.Dense(features=2*16*self.c_hid)(x)
        x = nn.gelu(x)
        x = x.reshape(x.shape[0], 4, 4, -1)
        x = nn.ConvTranspose(features=2*self.c_hid, kernel_size=(3, 3), strides=(2,␣
↪2))(x)
        x = nn.gelu(x)
        x = nn.Conv(features=2*self.c_hid, kernel_size=(3, 3))(x)
        x = nn.gelu(x)
        x = nn.ConvTranspose(features=self.c_hid, kernel_size=(3, 3), strides=(2, 2))(x)
        x = nn.gelu(x)
        x = nn.Conv(features=self.c_hid, kernel_size=(3, 3))(x)
        x = nn.gelu(x)
        x = nn.ConvTranspose(features=self.c_out, kernel_size=(3, 3), strides=(2, 2))(x)
        x = nn.tanh(x)
        return x
```

[7]:
```
## Test decoder implementation
# Random key for initialization
rng = random.PRNGKey(0)
# Example latents as input
rng, lat_rng = random.split(rng)
latents = random.normal(lat_rng, (16, 128))
# Create decoder
decoder = Decoder(c_hid=32, latent_dim=128, c_out=3)
# Initialize parameters of decoder with random key and latents
rng, init_rng = random.split(rng)
params = decoder.init(init_rng, latents)['params']
# Apply decoder with parameters on the images
out = decoder.apply({'params': params}, latents)
out.shape

del out, decoder, params
```

The encoder and decoder networks we chose here are relatively simple. Usually, more complex networks are applied, especially when using a ResNet-based architecture. For example, see VQ-VAE and NVAE (although the papers discuss architectures for VAEs, they can equally be applied to standard autoencoders).

In a final step, we add the encoder and decoder together into the autoencoder architecture.

[8]:
```
class Autoencoder(nn.Module):
    c_hid: int
    latent_dim : int

    def setup(self):
        # Alternative to @nn.compact -> explicitly define modules
        # Better for later when we want to access the encoder and decoder explicitly
```

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```
        self.encoder = Encoder(c_hid=self.c_hid, latent_dim=self.latent_dim)
        self.decoder = Decoder(c_hid=self.c_hid, latent_dim=self.latent_dim, c_out=3)

    def __call__(self, x):
        z = self.encoder(x)
        x_hat = self.decoder(z)
        return x_hat
```

[9]:
```
## Test Autoencoder implementation
# Random key for initialization
rng = random.PRNGKey(0)
# Example images as input
imgs = next(iter(train_loader))[0]
# Create encoder
autoencoder = Autoencoder(c_hid=32, latent_dim=128)
# Initialize parameters of encoder with random key and images
params = autoencoder.init(rng, imgs)['params']
# Apply encoder with parameters on the images
out = autoencoder.apply({'params': params}, imgs)
out.shape

del out, autoencoder, params
```

For the loss function, we use the mean squared error (MSE), which we implement below:

[10]:
```
def mse_recon_loss(model, params, batch):
    imgs, _ = batch
    recon_imgs = model.apply({'params': params}, imgs)
    loss = ((recon_imgs - imgs) ** 2).mean(axis=0).sum()  # Mean over batch, sum over␣
↪pixels
    return loss
```

The mean squared error pushes the network to pay special attention to those pixel values its estimate is far away. Predicting 127 instead of 128 is not important when reconstructing, but confusing 0 with 128 is much worse. Note that in contrast to VAEs, we do not predict the probability per pixel value, but instead use a distance measure. This saves a lot of parameters and simplifies training. To get a better intuition per pixel, we report the summed squared error averaged over the batch dimension (any other mean/sum leads to the same result/parameters).

However, MSE has also some considerable disadvantages. Usually, MSE leads to blurry images where small noise/high-frequent patterns are removed as those cause a very low error. To ensure realistic images to be reconstructed, one could combine Generative Adversarial Networks (lecture 10) with autoencoders as done in several works (e.g. see here, here or these slides). Additionally, comparing two images using MSE does not necessarily reflect their visual similarity. For instance, suppose the autoencoder reconstructs an image shifted by one pixel to the right and bottom. Although the images are almost identical, we can get a higher loss than predicting a constant pixel value for half of the image (see code below). An example solution for this issue includes using a separate, pre-trained CNN, and use a distance of visual features in lower layers as a distance measure instead of the original pixel-level comparison.

[11]:
```
def compare_imgs(img1, img2, title_prefix=""):
    # Calculate MSE loss between both images
    loss = ((img1 - img2) ** 2).sum()
    # Plot images for visual comparison
    imgs = jax_to_torch(np.stack([img1, img2], axis=0))
    grid = torchvision.utils.make_grid(imgs, nrow=2, normalize=True, value_range=(-1,1))
```

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```
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(4,2))
    plt.title(f"{title_prefix} Loss: {loss.item():4.2f}")
    plt.imshow(grid)
    plt.axis('off')
    plt.show()

for i in range(2):
    # Load example image
    img, _ = train_dataset[i]
    img_mean = img.mean(axis=(0,1), keepdims=True)

    # Shift image by one pixel
    SHIFT = 1
    img_shifted = np.roll(img, shift=SHIFT, axis=0)
    img_shifted = np.roll(img_shifted, shift=SHIFT, axis=1)
    img_shifted[:1,:,:] = img_mean
    img_shifted[:,:1,:] = img_mean
    compare_imgs(img, img_shifted, "Shifted -")

    # Set half of the image to zero
    img_masked = np.copy(img)
    img_masked[:img_masked.shape[1]//2,:,:] = img_mean
    compare_imgs(img, img_masked, "Masked -")
```

Training the model

During the training, we want to keep track of the learning progress by seeing reconstructions made by our model. For this, we implement a callback object which will add reconstructions every N epochs to our tensorboard. To align it with the PyTorch tutorial version, we implement it similar to how we would do it in PyTorch Lightning:

[12]:
```
class GenerateCallback:

    def __init__(self, input_imgs, every_n_epochs=1):
        super().__init__()
        self.input_imgs = input_imgs  # Images to reconstruct during training
        self.every_n_epochs = every_n_epochs  # Only save those images every N epochs␣
↪(otherwise tensorboard gets quite large)

    def log_generations(self, model, state, logger, epoch):
        if epoch % self.every_n_epochs == 0:
            reconst_imgs = model.apply({'params': state.params}, self.input_imgs)
            reconst_imgs = jax.device_get(reconst_imgs)

            # Plot and add to tensorboard
            imgs = np.stack([self.input_imgs, reconst_imgs], axis=1).reshape(-1, *self.
↪input_imgs.shape[1:])
            imgs = jax_to_torch(imgs)
            grid = torchvision.utils.make_grid(imgs, nrow=2, normalize=True, value_
↪range=(-1,1))
            logger.add_image("Reconstructions", grid, global_step=epoch)
```

Further, to train multiple models with different hyperparameters, we summarize all training functionalities in a trainer

object below:

[13]:
```
class TrainerModule:

    def __init__(self, c_hid, latent_dim, lr=1e-3, seed=42):
        super().__init__()
        self.c_hid = c_hid
        self.latent_dim = latent_dim
        self.lr = lr
        self.seed = seed
        # Create empty model. Note: no parameters yet
        self.model = Autoencoder(c_hid=self.c_hid, latent_dim=self.latent_dim)
        # Prepare logging
        self.exmp_imgs = next(iter(val_loader))[0][:8]
        self.log_dir = os.path.join(CHECKPOINT_PATH, f'cifar10_{self.latent_dim}')
        self.generate_callback = GenerateCallback(self.exmp_imgs, every_n_epochs=50)
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model()

    def create_functions(self):
        # Training function
        def train_step(state, batch):
            loss_fn = lambda params: mse_recon_loss(self.model, params, batch)
            loss, grads = jax.value_and_grad(loss_fn)(state.params)  # Get loss and␣
↪gradients for loss
            state = state.apply_gradients(grads=grads)  # Optimizer update step
            return state, loss
        self.train_step = jax.jit(train_step)
        # Eval function
        def eval_step(state, batch):
            return mse_recon_loss(self.model, state.params, batch)
        self.eval_step = jax.jit(eval_step)

    def init_model(self):
        # Initialize model
        rng = jax.random.PRNGKey(self.seed)
        rng, init_rng = jax.random.split(rng)
        params = self.model.init(init_rng, self.exmp_imgs)['params']
        # Initialize learning rate schedule and optimizer
        lr_schedule = optax.warmup_cosine_decay_schedule(
            init_value=0.0,
            peak_value=1e-3,
            warmup_steps=100,
            decay_steps=500*len(train_loader),
            end_value=1e-5
        )
        optimizer = optax.chain(
            optax.clip(1.0),  # Clip gradients at 1
            optax.adam(lr_schedule)
        )
```

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```
        # Initialize training state
        self.state = train_state.TrainState.create(apply_fn=self.model.apply,␣
↪params=params, tx=optimizer)

    def train_model(self, num_epochs=500):
        # Train model for defined number of epochs
        best_eval = 1e6
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(epoch=epoch_idx)
            if epoch_idx % 10 == 0:
                eval_loss = self.eval_model(val_loader)
                self.logger.add_scalar('val/loss', eval_loss, global_step=epoch_idx)
                if eval_loss < best_eval:
                    best_eval = eval_loss
                    self.save_model(step=epoch_idx)
                self.generate_callback.log_generations(self.model, self.state,␣
↪logger=self.logger, epoch=epoch_idx)
                self.logger.flush()

    def train_epoch(self, epoch):
        # Train model for one epoch, and log avg loss
        losses = []
        for batch in train_loader:
            self.state, loss = self.train_step(self.state, batch)
            losses.append(loss)
        losses_np = np.stack(jax.device_get(losses))
        avg_loss = losses_np.mean()
        self.logger.add_scalar('train/loss', avg_loss, global_step=epoch)

    def eval_model(self, data_loader):
        # Test model on all images of a data loader and return avg loss
        losses = []
        batch_sizes = []
        for batch in data_loader:
            loss = self.eval_step(self.state, batch)
            losses.append(loss)
            batch_sizes.append(batch[0].shape[0])
        losses_np = np.stack(jax.device_get(losses))
        batch_sizes_np = np.stack(batch_sizes)
        avg_loss = (losses_np * batch_sizes_np).sum() / batch_sizes_np.sum()
        return avg_loss

    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir, target=self.state.params,␣
↪prefix=f'cifar10_{self.latent_dim}_', step=step)

    def load_model(self, pretrained=False):
        # Load model. We use different checkpoint for pretrained models
        if not pretrained:
            params = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir, target=self.
↪state.params, prefix=f'cifar10_{self.latent_dim}_')
```

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```
        else:
            params = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'cifar10_{self.latent_dim}.ckpt'), target=self.state.params)
        self.state = train_state.TrainState.create(apply_fn=self.model.apply,␣
↪params=params, tx=self.state.tx)

    def checkpoint_exists(self):
        # Check whether a pretrained model exist for this autoencoder
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'cifar10_{self.latent_dim}.
↪ckpt'))
```

We will now write a training function that allows us to train the autoencoder with different latent dimensionality and returns the test score. We provide pre-trained models and recommend you using those, especially when you work on a computer without GPU. Of course, feel free to train your own models.

[14]:
```
def train_cifar(latent_dim):
    # Create a trainer module with specified hyperparameters
    trainer = TrainerModule(c_hid=32, latent_dim=latent_dim)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(num_epochs=500)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    test_loss = trainer.eval_model(test_loader)
    # Bind parameters to model for easier inference
    trainer.model_bd = trainer.model.bind({'params': trainer.state.params})
    return trainer, test_loss
```

Comparing latent dimensionality

When training an autoencoder, we need to choose a dimensionality for the latent representation z. The higher the latent dimensionality, the better we expect the reconstruction to be. However, the idea of autoencoders is to *compress* data. Hence, we are also interested in keeping the dimensionality low. To find the best tradeoff, we can train multiple models with different latent dimensionalities. The original input has $32 \times 32 \times 3 = 3072$ pixels. Keeping this in mind, a reasonable choice for the latent dimensionality might be between 64 and 384:

[15]:
```
model_dict = {}
for latent_dim in [64, 128, 256, 384]:
    trainer_ld, test_loss_ld = train_cifar(latent_dim)
    model_dict[latent_dim] = {"trainer": trainer_ld, "result": test_loss_ld}
```

After training the models, we can plot the reconstruction loss over the latent dimensionality to get an intuition how these two properties are correlated:

[16]:
```
latent_dims = sorted([k for k in model_dict])
val_scores = [model_dict[k]["result"] for k in latent_dims]

fig = plt.figure(figsize=(6,4))
plt.plot(latent_dims, val_scores, '--', color="#000", marker="*", markeredgecolor="#000",
↪ markerfacecolor="y", markersize=16)
plt.xscale("log")
```

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```
plt.xticks(latent_dims, labels=latent_dims)
plt.title("Reconstruction error over latent dimensionality", fontsize=14)
plt.xlabel("Latent dimensionality")
plt.ylabel("Reconstruction error")
plt.minorticks_off()
plt.ylim(0,100)
plt.show()
```

As we initially expected, the reconstruction loss goes down with increasing latent dimensionality. For our model and setup, the two properties seem to be exponentially (or double exponentially) correlated. To understand what these differences in reconstruction error mean, we can visualize example reconstructions of the four models. For simplicity, we visualize four training images of CIFAR10 we have seen already before. For larger models that may overfit, it is recommended to use images from the validation set.

[17]:
```
def visualize_reconstructions(trainer, input_imgs):
    # Reconstruct images
    reconst_imgs = trainer.model_bd(input_imgs)
    imgs = np.stack([input_imgs, reconst_imgs], axis=1).reshape(-1, *reconst_imgs.
↪shape[1:])

    # Plotting
    imgs = jax_to_torch(imgs)
    grid = torchvision.utils.make_grid(imgs, nrow=4, normalize=True, value_range=(-1,1))
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(7,4.5))
    plt.title(f"Reconstructed from {trainer.latent_dim} latents")
    plt.imshow(grid)
    plt.axis('off')
```

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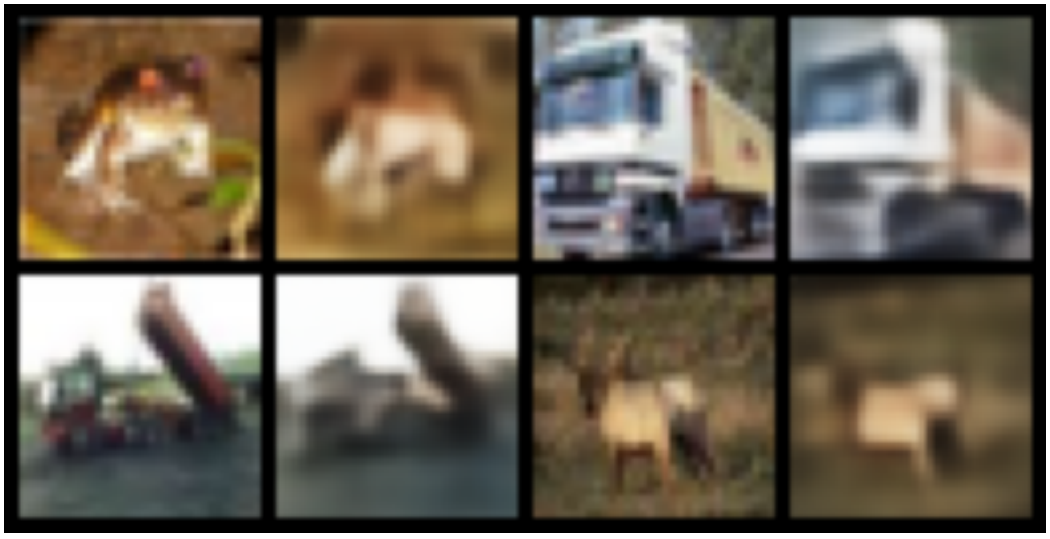
```
    plt.show()
```

[18]:
```
input_imgs = np.stack([image_to_numpy(train_dataset[i][0]) for i in range(4)], axis=0)
for latent_dim in model_dict:
    visualize_reconstructions(model_dict[latent_dim]["trainer"], input_imgs)
```



Clearly, the smallest latent dimensionality can only save information about the rough shape and color of the object, but the reconstructed image is extremely blurry and it is hard to recognize the original object in the reconstruction. With 128 features, we can recognize some shapes again although the picture remains blurry. The models with the highest two dimensionalities reconstruct the images quite well. The difference between 256 and 384 is marginal at first sight but can be noticed when comparing, for instance, the backgrounds of the first image (the 384 features model more of the pattern than 256).

Out-of-distribution images

Before continuing with the applications of autoencoder, we can actually explore some limitations of our autoencoder. For example, what happens if we try to reconstruct an image that is clearly out of the distribution of our dataset? We expect the decoder to have learned some common patterns in the dataset, and thus might in particular fail to reconstruct images that do not follow these patterns.

The first experiment we can try is to reconstruct noise. We, therefore, create two images whose pixels are randomly sampled from a uniform distribution over pixel values, and visualize the reconstruction of the model (feel free to test different latent dimensionalities):

[19]:
```
rng = jax.random.PRNGKey(123)
rgn, noise_rgn = jax.random.split(rng)
rand_imgs = jax.random.uniform(rng, (2, 32, 32, 3)) * 2 - 1
visualize_reconstructions(model_dict[256]["trainer"], rand_imgs)
```

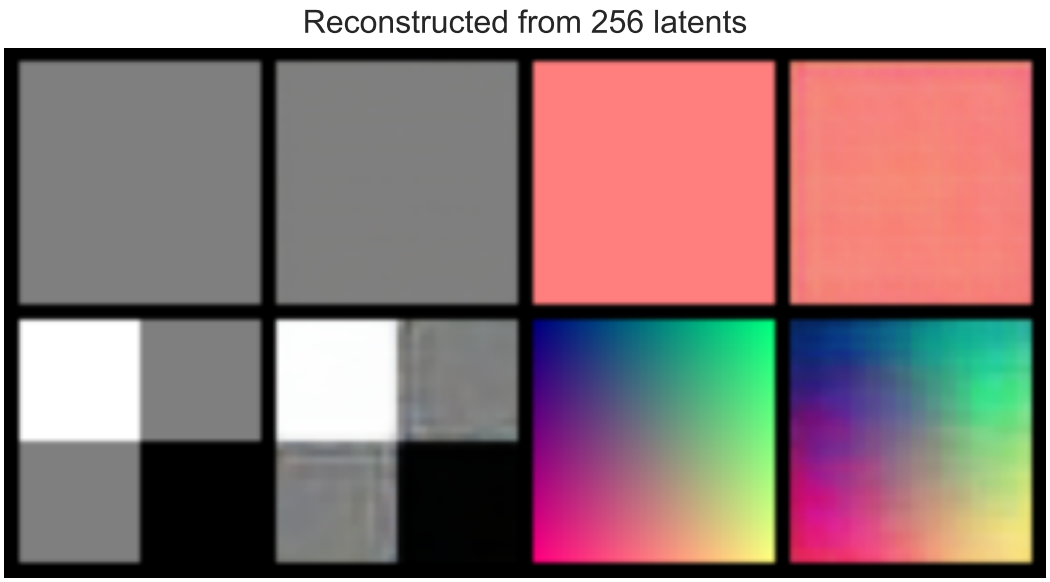
The reconstruction of the noise is quite poor, and seems to introduce some rough patterns. As the input does not follow the patterns of the CIFAR dataset, the model has issues reconstructing it accurately.

We can also check how well the model can reconstruct other manually-coded patterns:

[20]:
```
# JAX arrays are natively immutable. This is why we first create the images in numpy,␣
↪and push them to JAX afterwards
plain_imgs = np.zeros((4, 32, 32, 3))

# Single color channel
plain_imgs[1,:,:,0] = 1
# Checkboard pattern
plain_imgs[2,:16,:16] = 1
plain_imgs[2,16:,16:] = -1
# Color progression
xx, yy = np.meshgrid(np.linspace(-1,1,32), np.linspace(-1,1,32), indexing='ij')
plain_imgs[3,:,:,0] = xx
plain_imgs[3,:,:,1] = yy

visualize_reconstructions(model_dict[256]["trainer"], plain_imgs)
```



The plain, constant images are reconstructed relatively good although the single color channel contains some noticeable noise. The hard borders of the checkboard pattern are not as sharp as intended, as well as the color progression, both because such patterns never occur in the real-world pictures of CIFAR.

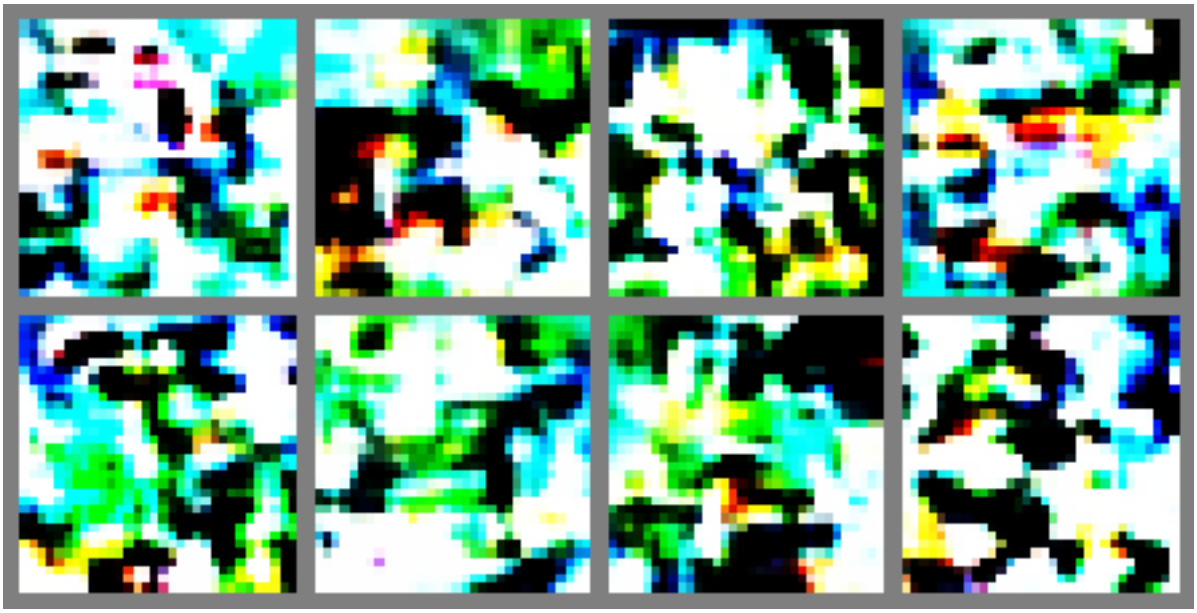
In general, autoencoders tend to fail reconstructing high-frequent noise (i.e. sudden, big changes across few pixels) due to the choice of MSE as loss function (see our previous discussion about loss functions in autoencoders). Small misalignments in the decoder can lead to huge losses so that the model settles for the expected value/mean in these regions. For low-frequent noise, a misalignment of a few pixels does not result in a big difference to the original image. However, the larger the latent dimensionality becomes, the more of this high-frequent noise can be accurately reconstructed.

Generating new images

Variational autoencoders are a generative version of the autoencoders because we regularize the latent space to follow a Gaussian distribution. However, in vanilla autoencoders, we do not have any restrictions on the latent vector. So what happens if we would actually input a randomly sampled latent vector into the decoder? Let's find it out below:

[21]:
```
trainer = model_dict[256]["trainer"]
rgn, latent_noise = jax.random.split(rng)
latent_vectors = jax.random.normal(latent_noise, (8, trainer.latent_dim))
# Decode images -> Run model.decode method of the trainer's model with given parameters
imgs = trainer.model_bd.decoder(latent_vectors) # nn.apply(lambda model: model.
↪decode(latent_vectors), trainer.model)({'params': trainer.state.params})

imgs = jax_to_torch(imgs)
grid = torchvision.utils.make_grid(imgs, nrow=4, normalize=True, value_range=(-1,1), pad_
↪value=0.5)
grid = grid.permute(1, 2, 0)
plt.figure(figsize=(8,5))
plt.imshow(grid)
plt.axis('off')
plt.show()
```



As we can see, the generated images more look like art than realistic images. As the autoencoder was allowed to structure the latent space in whichever way it suits the reconstruction best, there is no incentive to map every possible latent vector to realistic images. Furthermore, the distribution in latent space is unknown to us and doesn't necessarily follow a multivariate normal distribution. Thus, we can conclude that vanilla autoencoders are indeed not generative.

4.36.2 Finding visually similar images

One application of autoencoders is to build an image-based search engine to retrieve visually similar images. This can be done by representing all images as their latent dimensionality, and find the closest K images in this domain. The first step to such a search engine is to encode all images into z. In the following, we will use the training set as a search corpus, and the test set as queries to the system.

Warning: the following cells can be computationally heavy for a weak CPU-only system. If you do not have a strong computer and are not on Google Colab, you might want to skip the execution of the following cells and rely on the results shown in the filled notebook.

[22]:
```
# We use the following model throughout this section.
# If you want to try a different latent dimensionality, change it here!
trainer = model_dict[128]["trainer"]
```

[23]:
```
def embed_imgs(trainer, data_loader):
    # Encode all images in the data_laoder using model, and return both images and␣
↪encodings
    img_list, embed_list = [], []

    @jax.jit
    def encode(imgs):
        return trainer.model.bind({'params': trainer.state.params}).encoder(imgs)
```

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```
    for imgs, _ in tqdm(data_loader, desc="Encoding images", leave=False):
        z = encode(imgs)
        z = jax.device_get(z)
        imgs = jax.device_get(imgs)
        img_list.append(imgs)
        embed_list.append(z)
    return (np.concatenate(img_list, axis=0), np.concatenate(embed_list, axis=0))

train_img_embeds = embed_imgs(trainer, train_loader)
test_img_embeds = embed_imgs(trainer, test_loader)
```

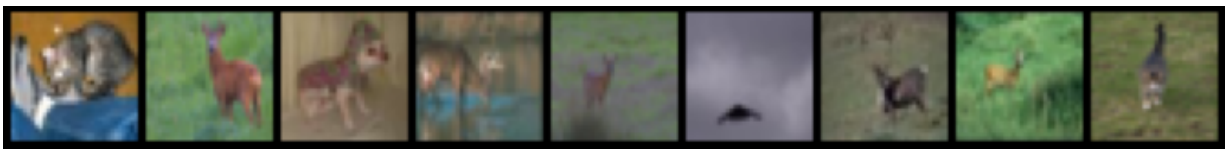
```
Encoding images:   0%|          | 0/175 [00:00<?, ?it/s]
```

```
Encoding images:   0%|          | 0/40 [00:00<?, ?it/s]
```

After encoding all images, we just need to write a function that finds the closest K images and returns (or plots) those:

[24]:
```
def find_similar_images(query_img, query_z, key_embeds, K=8):
    # Find closest K images. We use the euclidean distance here but other like cosine␣
↪distance can also be used.
    dist = np.linalg.norm(query_z[None,:] - key_embeds[1], axis=-1)
    indices = np.argsort(dist)
    dist = dist[indices]
    # Plot K closest images
    imgs_to_display = np.concatenate([query_img[None], key_embeds[0][indices[:K]]],␣
↪axis=0)
    imgs_to_display = torch.from_numpy(imgs_to_display)
    imgs_to_display = imgs_to_display.permute(0, 3, 1, 2)
    grid = torchvision.utils.make_grid(imgs_to_display, nrow=K+1, normalize=True, value_
↪range=(-1,1))
    grid = grid.permute(1, 2, 0)
    plt.figure(figsize=(12,3))
    plt.imshow(grid)
    plt.axis('off')
    plt.show()
```

[25]:
```
# Plot the closest images for the first N test images as example
for i in range(8):
    find_similar_images(test_img_embeds[0][i], test_img_embeds[1][i], key_embeds=train_
↪img_embeds)
```



Based on our autoencoder, we see that we are able to retrieve many similar images to the test input. In particular, in row 4, we can spot that some test images might not be that different from the training set as we thought (same poster, just different scaling/color scaling). We also see that although we haven't given the model any labels, it can cluster different classes in different parts of the latent space (airplane + ship, animals, etc.). This is why autoencoders can also be used as a pre-training strategy for deep networks, especially when we have a large set of unlabeled images (often the case). However, it should be noted that the background still plays a big role in autoencoders while it doesn't for classification. Hence, we don't get "perfect" clusters and need to finetune such models for classification.

Tensorboard clustering

Another way of exploring the similarity of images in the latent space is by dimensionality-reduction methods like PCA or T-SNE. Luckily, Tensorboard provides a nice interface for this and we can make use of it in the following:

[26]:
```
# We use the following model throughout this section.
# If you want to try a different latent dimensionality, change it here!
trainer = model_dict[128]["trainer"]
```

[27]:
```
# Create a summary writer
writer = SummaryWriter("tensorboard/")
```

The function `add_embedding` allows us to add high-dimensional feature vectors to TensorBoard on which we can perform clustering. What we have to provide in the function are the feature vectors, additional metadata such as the labels, and the original images so that we can identify a specific image in the clustering.

[28]:
```
## In case you obtain the following error in the next cell, execute the import␣
↪statements and last line in this cell
##   AttributeError: module 'tensorflow._api.v2.io.gfile' has no attribute 'get_filesystem'

import tensorflow as tf
import tensorboard as tb
tf.io.gfile = tb.compat.tensorflow_stub.io.gfile
```

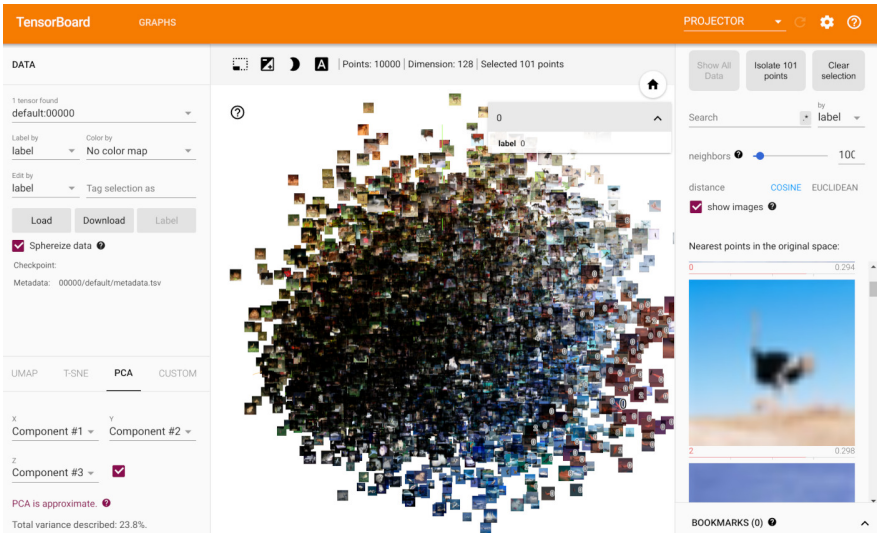
[29]:
```
# Note: the embedding projector in tensorboard is computationally heavy.
# Reduce the image amount below if your computer struggles with visualizing all 10k␣
↪points
NUM_IMGS = len(test_set)

writer.add_embedding(test_img_embeds[1][:NUM_IMGS], # Encodings per image
                     metadata=[test_set[i][1] for i in range(NUM_IMGS)], # Adding the␣
↪labels per image to the plot
                     label_img=torch.from_numpy(test_img_embeds[0][:NUM_IMGS]+1).
↪permute(0, 3, 1, 2)/2.0) # Adding the original images to the plot
```

Finally, we can run tensorboard to explore similarities among images:

[30]:
```
%tensorboard --logdir tensorboard/
```

You should be able to see something similar as in the following image. In case the projector stays empty, try to start the TensorBoard outside of the Jupyter notebook.



Overall, we can see that the model indeed clustered images together that are visually similar. Especially the background color seems to be a crucial factor in the encoding. This correlates to the chosen loss function, here Mean Squared Error on pixel-level because the background is responsible for more than half of the pixels in an average image. Hence, the model learns to focus on it. Nevertheless, we can see that the encodings also separate a couple of classes in the latent space although it hasn't seen any labels. This shows again that autoencoding can also be used as a "pre-training"/transfer learning task before classification.

[31]:
```
# Closing the summary writer
writer.close()
```

4.36.3 Conclusion

In this tutorial, we have implemented our own autoencoder on small RGB images and explored various properties of the model. In contrast to variational autoencoders, vanilla AEs are not generative and can work on MSE loss functions. This makes them often easier to train. Both versions of AE can be used for dimensionality reduction, as we have seen for finding visually similar images beyond pixel distances. Despite autoencoders gaining less interest in the research community due to their more "theoretically" challenging counterpart of VAEs, autoencoders still find usage in a lot of applications like denoising and compression. Hence, AEs are an essential tool that every Deep Learning engineer/researcher should be familiar with.

If you found this tutorial helpful, consider -ing our repository.

For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.37 Tutorial 11 (JAX): Normalizing Flows for image modeling

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We note the training times for all models in the PyTorch and the JAX implementation below (PyTorch v1.11, JAX v0.3.13). The models were trained on the same hardware (NVIDIA RTX3090, 24 core CPU) and we slightly adjusted the tutorials to use the exact same training settings (200 epochs, data loading parameters, evaluation schedule, etc.). Overall, the JAX implementation is *2.0-2.5x faster* than PyTorch! Different network architectures may have different speedups.

Models	PyTorch	JAX
MNIST Flow - Simple	2hrs 37min 29sec	1hrs 17min 59sec
MNIST Flow - VarDeq	3hrs 25min 10sec	1hrs 36min 56sec
MNIST Flow - Multiscale	2hrs 17min 10sec	57min 57sec

In this tutorial, we will take a closer look at complex, deep normalizing flows. The most popular, current application of deep normalizing flows is to model datasets of images. As for other generative models, images are a good domain to start working on because (1) CNNs are widely studied and strong models exist, (2) images are high-dimensional and complex, and (3) images are discrete integers. In this tutorial, we will review current advances in normalizing flows for image modeling, and get hands-on experience on coding normalizing flows. Note that normalizing flows are commonly parameter heavy and therefore computationally expensive. We will use relatively simple and shallow flows to save computational cost and allow you to run the notebook on CPU, but keep in mind that a simple way to improve the scores of the flows we study here is to make them deeper. The first cell imports our usual libraries.

[1]:
```
## Standard libraries
import os
import math
import time
import json
import numpy as np
from typing import Sequence

## Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
```

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```
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## Progress bar
from tqdm.notebook import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch Data Loading
import torch
import torch.utils.data as data
from torch.utils.tensorboard import SummaryWriter
import torchvision
from torchvision.datasets import MNIST

# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial11_jax"

print("Device:", jax.devices()[0])
```

```
/home/phillip/anaconda3/envs/dl2020/lib/python3.7/site-packages/chex/_src/pytypes.py:37:␣
↪FutureWarning: jax.tree_structure is deprecated, and will be removed in a future␣
↪release. Use jax.tree_util.tree_structure instead.
  PyTreeDef = type(jax.tree_structure(None))
WARNING:absl:GlobalAsyncCheckpointManager is not imported correctly. Checkpointing of␣
↪GlobalDeviceArrays will not be available.To use the feature, install tensorstore.
```

```
Device: gpu:0
```

Again, we have a few pretrained models. We download them below to the specified path above.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial11/"
# Files to download
pretrained_files = ["MNISTFlow_simple.ckpt", "MNISTFlow_vardeq.ckpt", "MNISTFlow_
↪multiscale.ckpt",
                    "MNISTFlow_simple_results.json", "MNISTFlow_vardeq_results.json",
↪"MNISTFlow_multiscale_results.json"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please contact the author with the full output␣
↪including the following error:\n", e)
```

We will use the MNIST dataset in this notebook. MNIST constitutes, despite its simplicity, a challenge for small generative models as it requires the global understanding of an image. At the same time, we can easily judge whether generated images come from the same distribution as the dataset (i.e. represent real digits), or not.

To deal better with the discrete nature of the images, we transform them from a range of 0-1 to a range of 0-255 as integers.

[3]:
```
# Transformations applied on each image => bring them into a numpy array
# Note that we keep them in the range 0-255 (integers)
def image_to_numpy(img):
    img = np.array(img, dtype=np.int32)
    img = img[...,None]  # Make image [28, 28, 1]
    return img

# We need to stack the batch elements
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
```

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```
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = MNIST(root=DATASET_PATH, train=True, transform=image_to_numpy,␣
↪download=True)
train_set, val_set = torch.utils.data.random_split(train_dataset, [50000, 10000],
                                                   generator=torch.Generator().manual_
↪seed(42))

# Loading the test set
test_set = MNIST(root=DATASET_PATH, train=False, transform=image_to_numpy, download=True)

# We define a set of data loaders that we can use for various purposes
# Data loader for loading examples throughout the notebook
train_exmp_loader = data.DataLoader(train_set, batch_size=256, shuffle=False, drop_
↪last=False, collate_fn=numpy_collate)
# Actual data loaders for training, validation, and testing
train_data_loader = data.DataLoader(train_set,
                                    batch_size=128,
                                    shuffle=True,
                                    drop_last=True,
                                    collate_fn=numpy_collate,
                                    num_workers=8,
                                    persistent_workers=True)
val_loader = data.DataLoader(val_set, batch_size=64, shuffle=False, drop_last=False, num_
↪workers=4, collate_fn=numpy_collate)
test_loader = data.DataLoader(test_set, batch_size=64, shuffle=False, drop_last=False,␣
↪num_workers=4, collate_fn=numpy_collate)
```

In addition, we will define below a function to simplify the visualization of images/samples. Some training examples of the MNIST dataset is shown below.

[4]:
```
def show_imgs(imgs, title=None, row_size=4):
    # Form a grid of pictures (we use max. 8 columns)
    imgs = np.copy(jax.device_get(imgs))
    num_imgs = imgs.shape[0]
    is_int = (imgs.dtype==np.int32)
    nrow = min(num_imgs, row_size)
    ncol = int(math.ceil(num_imgs/nrow))
    imgs_torch = torch.from_numpy(imgs).permute(0, 3, 1, 2)
    imgs = torchvision.utils.make_grid(imgs_torch, nrow=nrow, pad_value=128 if is_int␣
↪else 0.5)
    np_imgs = imgs.cpu().numpy()
    # Plot the grid
    plt.figure(figsize=(1.5*nrow, 1.5*ncol))
    plt.imshow(np.transpose(np_imgs, (1,2,0)), interpolation='nearest')
    plt.axis('off')
    if title is not None:
        plt.title(title)
```

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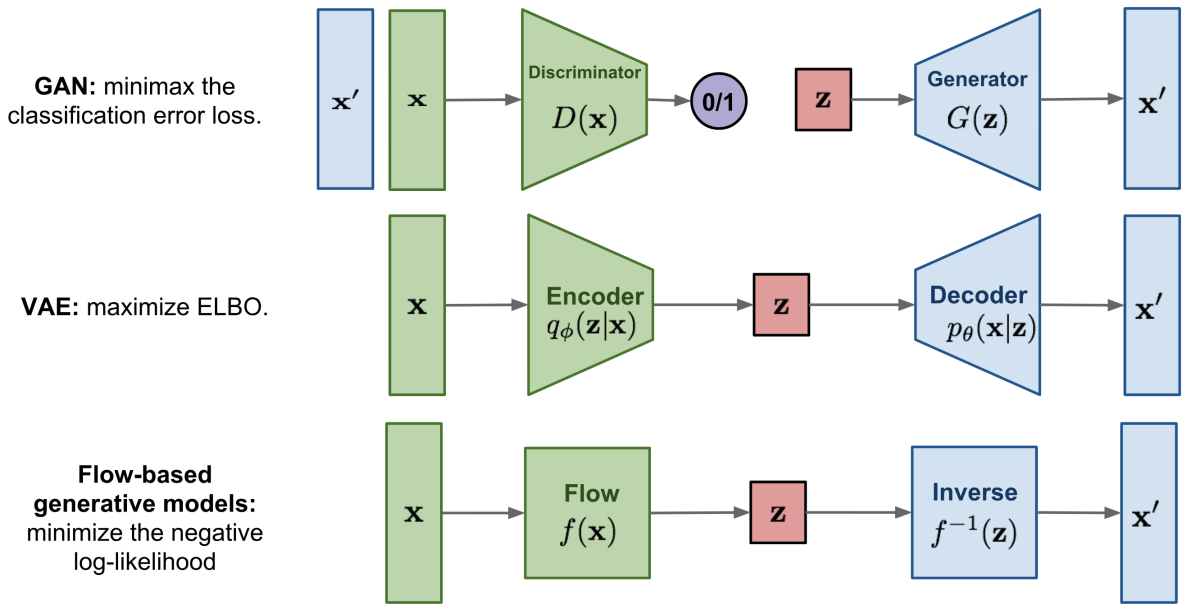
```
    plt.show()
    plt.close()

show_imgs(np.stack([train_set[i][0] for i in range(8)], axis=0))
```

4.37.1 Normalizing Flows as generative model

In the previous lectures, we have seen Energy-based models, Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) as example of generative models. However, none of them explicitly learn the probability density function $p(x)$ of the real input data. While VAEs model a lower bound, energy-based models only implicitly learn the probability density. GANs on the other hand provide us a sampling mechanism for generating new data, without offering a likelihood estimate. The generative model we will look at here, called Normalizing Flows, actually models the true data distribution $p(x)$ and provides us with an exact likelihood estimate. Below, we can visually compare VAEs, GANs and Flows (figure credit - Lilian Weng):



The major difference compared to VAEs is that flows use *invertible* functions f to map the input data x to a latent

representation z. To realize this, z must be of the same shape as x. This is in contrast to VAEs where z is usually much lower dimensional than the original input data. However, an invertible mapping also means that for every data point x, we have a corresponding latent representation z which allows us to perform lossless reconstruction (z to x). In the visualization above, this means that $x = x'$ for flows, no matter what invertible function f and input x we choose.

Nonetheless, how are normalizing flows modeling a probability density with an invertible function? The answer to this question is the rule for change of variables. Specifically, given a prior density $p_z(z)$ (e.g. Gaussian) and an invertible function f, we can determine $p_x(x)$ as follows:

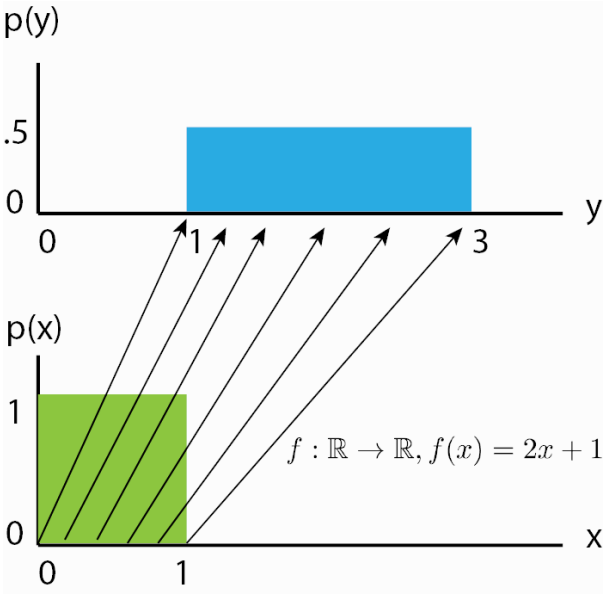
$$\int p_x(x)dx = \int p_z(z)dz = 1 \qquad \text{(by definition of a probability distribution)}$$

$$\Leftrightarrow p_x(x) = p_z(z)\left|\frac{dz}{dx}\right| = p_z(f(x))\left|\frac{df(x)}{dx}\right|$$

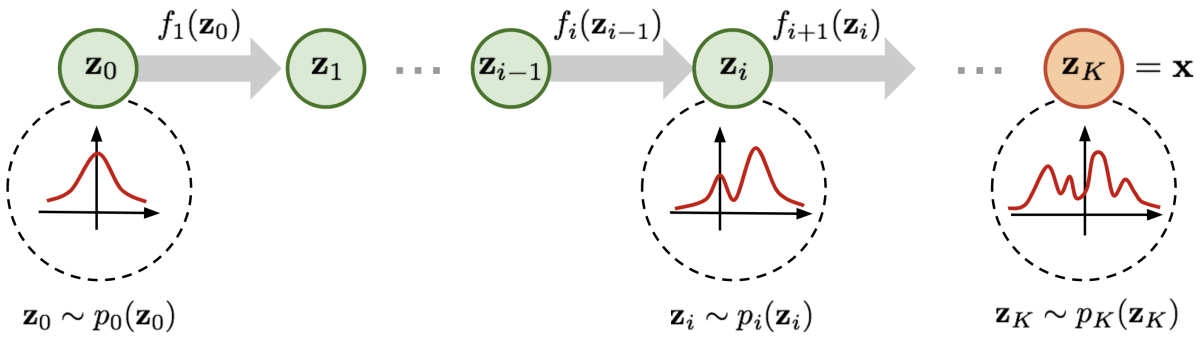
Hence, in order to determine the probability of x, we only need to determine its probability in latent space, and get the derivate of f. Note that this is for a univariate distribution, and f is required to be invertible and smooth. For a multivariate case, the derivative becomes a Jacobian of which we need to take the determinant. As we usually use the log-likelihood as objective, we write the multivariate term with logarithms below:

$$\log p_x(\mathbf{x}) = \log p_z(f(\mathbf{x})) + \log\left|\det\frac{df(\mathbf{x})}{d\mathbf{x}}\right|$$

Although we now know how a normalizing flow obtains its likelihood, it might not be clear what a normalizing flow does intuitively. For this, we should look from the inverse perspective of the flow starting with the prior probability density $p_z(z)$. If we apply an invertible function on it, we effectively "transform" its probability density. For instance, if $f^{-1}(z) = z + 1$, we shift the density by one while still remaining a valid probability distribution, and being invertible. We can also apply more complex transformations, like scaling: $f^{-1}(z) = 2z + 1$, but there you might see a difference. When you scale, you also change the volume of the probability density, as for example on uniform distributions (figure credit - Eric Jang):



You can see that the height of $p(y)$ should be lower than $p(x)$ after scaling. This change in volume represents $\left|\frac{df(x)}{dx}\right|$ in our equation above, and ensures that even after scaling, we still have a valid probability distribution. We can go on with making our function f more complex. However, the more complex f becomes, the harder it will be to find the inverse f^{-1} of it, and to calculate the log-determinant of the Jacobian $\log\left|\det\frac{df(\mathbf{x})}{d\mathbf{x}}\right|$ (often abbreviated as *LDJ*). An easier trick to stack multiple invertible functions $f_{1,\dots,K}$ after each other, as all together, they still represent a single, invertible function. Using multiple, learnable invertible functions, a normalizing flow attempts to transform $p_z(z)$ slowly into a more complex distribution which should finally be $p_x(x)$. We visualize the idea below (figure credit - Lilian Weng):



Starting from z_0, which follows the prior Gaussian distribution, we sequentially apply the invertible functions $f_1, f_2, ..., f_K$, until z_K represents x. Note that in the figure above, the functions f represent the inverted function from f we had above (here: $f : Z \to X$, above: $f : X \to Z$). This is just a different notation and has no impact on the actual flow design because all f need to be invertible anyways. When we estimate the log likelihood of a data point x as in the equations above, we run the flows in the opposite direction than visualized above. Multiple flow layers have been proposed that use a neural network as learnable parameters, such as the planar and radial flow. However, we will focus here on flows that are commonly used in image modeling, and will discuss them in the rest of the notebook along with the details of how to train a normalizing flow.

4.37.2 Normalizing Flows on images

To become familiar with normalizing flows, especially for the application of image modeling, it is best to discuss the different elements in a flow along with the implementation. As a general concept, we want to build a normalizing flow that maps an input image (here MNIST) to an equally sized latent space:

As a first step, we will implement a template of a normalizing flow. During training and validation, a normalizing flow performs density estimation in the forward direction. For this, we apply a series of flow transformations on the input x and estimate the probability of the input by determining the probability of the transformed point z given a prior, and the change of volume caused by the transformations. During inference, we can do both density estimation and sampling new points by inverting the flow transformations. Therefore, we define a function `_get_likelihood` which performs density estimation, and `sample` to generate new examples.

The standard metric used in generative models, and in particular normalizing flows, is bits per dimensions (bpd). Bpd is motivated from an information theory perspective and describes how many bits we would need to encode a particular example in our modeled distribution. The less bits we need, the more likely the example in our distribution. When we test for the bits per dimension of our test dataset, we can judge whether our model generalizes to new samples of the dataset and didn't memorize the training dataset. In order to calculate the bits per dimension score, we can rely on the negative log-likelihood and change the log base (as bits are binary while NLL is usually exponential):

$$\text{bpd} = \text{nll} \cdot \log_2\left(\exp(1)\right) \cdot \left(\prod d_i\right)^{-1}$$

where $d_1, ..., d_K$ are the dimensions of the input. For images, this would be the height, width and channel number. We divide the log likelihood by these extra dimensions to have a metric which we can compare for different image resolutions. In the original image space, MNIST examples have a bits per dimension score of 8 (we need 8 bits to encode each pixel as there are 256 possible values).

[5]:
```
class ImageFlow(nn.Module):
    flows : Sequence[nn.Module]  # A list of flows (each a nn.Module) that should be␣
↪applied on the images.
    import_samples : int = 8  # Number of importance samples to use during testing (see␣
↪explanation below).
```

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```
    def __call__(self, x, rng, testing=False):
        if not testing:
            bpd, rng = self._get_likelihood(x, rng)
        else:
            # Perform importance sampling during testing => estimate likelihood M times␣
↪for each image
            img_ll, rng = self._get_likelihood(x.repeat(self.import_samples, 0),
                                               rng,
                                               return_ll=True)
            img_ll = img_ll.reshape(-1, self.import_samples)

            # To average the probabilities, we need to go from log-space to exp, and␣
↪back to log.
            # Logsumexp provides us a stable implementation for this
            img_ll = jax.nn.logsumexp(img_ll, axis=-1) - np.log(self.import_samples)

            # Calculate final bpd
            bpd = -img_ll * np.log2(np.exp(1)) / np.prod(x.shape[1:])
            bpd = bpd.mean()
        return bpd, rng

    def encode(self, imgs, rng):
        # Given a batch of images, return the latent representation z and
        # log-determinant jacobian (ldj) of the transformations
        z, ldj = imgs, jnp.zeros(imgs.shape[0])
        for flow in self.flows:
            z, ldj, rng = flow(z, ldj, rng, reverse=False)
        return z, ldj, rng

    def _get_likelihood(self, imgs, rng, return_ll=False):
        """
        Given a batch of images, return the likelihood of those.
        If return_ll is True, this function returns the log likelihood of the input.
        Otherwise, the ouptut metric is bits per dimension (scaled negative log␣
↪likelihood)
        """
        z, ldj, rng = self.encode(imgs, rng)
        log_pz = jax.scipy.stats.norm.logpdf(z).sum(axis=(1,2,3))
        log_px = ldj + log_pz
        nll = -log_px
        # Calculating bits per dimension
        bpd = nll * np.log2(np.exp(1)) / np.prod(imgs.shape[1:])
        return (bpd.mean() if not return_ll else log_px), rng

    def sample(self, img_shape, rng, z_init=None):
        """
        Sample a batch of images from the flow.
        """
        # Sample latent representation from prior
        if z_init is None:
            rng, normal_rng = random.split(rng)
```

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```
            z = random.normal(normal_rng, shape=img_shape)
        else:
            z = z_init

        # Transform z to x by inverting the flows
        # The log-determinant jacobian (ldj) is usually not of interest during sampling
        ldj = jnp.zeros(img_shape[0])
        for flow in reversed(self.flows):
            z, ldj, rng = flow(z, ldj, rng, reverse=True)
        return z, rng
```

The test step differs from the training and validation step in that it makes use of importance sampling. We will discuss the motivation and details behind this after understanding how flows model discrete images in continuous space.

Dequantization

Normalizing flows rely on the rule of change of variables, which is naturally defined in continuous space. Applying flows directly on discrete data leads to undesired density models where arbitrarily high likelihood are placed on a few, particular values. See the illustration below:

The black points represent the discrete points, and the green volume the density modeled by a normalizing flow in continuous space. The flow would continue to increase the likelihood for $x = 0, 1, 2, 3$ while having no volume on any other point. Remember that in continuous space, we have the constraint that the overall volume of the probability density must be 1 ($\int p(x)dx = 1$). Otherwise, we don't model a probability distribution anymore. However, the discrete points $x = 0, 1, 2, 3$ represent delta peaks with no width in continuous space. This is why the flow can place an infinite high likelihood on these few points while still representing a distribution in continuous space. Nonetheless, the learned density does not tell us anything about the distribution among the discrete points, as in discrete space, the likelihoods of those four points would have to sum to 1, not to infinity.

To prevent such degenerated solutions, a common solution is to add a small amount of noise to each discrete value, which is also referred to as dequantization. Considering x as an integer (as it is the case for images), the dequantized representation v can be formulated as $v = x + u$ where $u \in [0, 1)^D$. Thus, the discrete value 1 is modeled by a distribution over the interval $[1.0, 2.0)$, the value 2 by an volume over $[2.0, 3.0)$, etc. Our objective of modeling $p(x)$ becomes:

$$p(x) = \int p(x+u)du = \int \frac{q(u|x)}{q(u|x)} p(x+u)du = \mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right]$$

with $q(u|x)$ being the noise distribution. For now, we assume it to be uniform, which can also be written as $p(x) = \mathbb{E}_{u \sim U(0,1)^D} [p(x+u)]$.

In the following, we will implement Dequantization as a flow transformation itself. After adding noise to the discrete values, we additionally transform the volume into a Gaussian-like shape. This is done by scaling $x + u$ between 0 and 1, and applying the invert of the sigmoid function $\sigma(z)^{-1} = \log z - \log 1 - z$. If we would not do this, we would face two problems:

1. The input is scaled between 0 and 256 while the prior distribution is a Gaussian with mean 0 and standard deviation 1. In the first iterations after initializing the parameters of the flow, we would have extremely low likelihoods for large values like 256. This would cause the training to diverge instantaneously.
2. As the output distribution is a Gaussian, it is beneficial for the flow to have a similarly shaped input distribution. This will reduce the modeling complexity that is required by the flow.

Overall, we can implement dequantization as follows:

[6]:
```
class Dequantization(nn.Module):
    alpha : float = 1e-5  # Small constant that is used to scale the original input for␣
↪numerical stability.
    quants : int = 256    # Number of possible discrete values (usually 256 for 8-bit␣
↪image)

    def __call__(self, z, ldj, rng, reverse=False):
        if not reverse:
            z, ldj, rng = self.dequant(z, ldj, rng)
            z, ldj = self.sigmoid(z, ldj, reverse=True)
        else:
            z, ldj = self.sigmoid(z, ldj, reverse=False)
            z = z * self.quants
            ldj += np.log(self.quants) * np.prod(z.shape[1:])
            z = jnp.floor(z)
            z = jax.lax.clamp(min=0., x=z, max=self.quants-1.).astype(jnp.int32)
        return z, ldj, rng

    def sigmoid(self, z, ldj, reverse=False):
        # Applies an invertible sigmoid transformation
        if not reverse:
            ldj += (-z-2*jax.nn.softplus(-z)).sum(axis=[1,2,3])
            z = nn.sigmoid(z)
            # Reversing scaling for numerical stability
            ldj -= np.log(1 - self.alpha) * np.prod(z.shape[1:])
            z = (z - 0.5 * self.alpha) / (1 - self.alpha)
        else:
            z = z * (1 - self.alpha) + 0.5 * self.alpha  # Scale to prevent boundaries 0␣
↪and 1
            ldj += np.log(1 - self.alpha) * np.prod(z.shape[1:])
            ldj += (-jnp.log(z) - jnp.log(1-z)).sum(axis=[1,2,3])
            z = jnp.log(z) - jnp.log(1-z)
        return z, ldj

    def dequant(self, z, ldj, rng):
        # Transform discrete values to continuous volumes
        z = z.astype(jnp.float32)
        rng, uniform_rng = random.split(rng)
        z = z + random.uniform(uniform_rng, z.shape)
        z = z / self.quants
        ldj -= np.log(self.quants) * np.prod(z.shape[1:])
        return z, ldj, rng
```

A good check whether a flow is correctly implemented or not, is to verify that it is invertible. Hence, we will dequantize a randomly chosen training image, and then quantize it again. We would expect that we would get the exact same image out:

[7]:
```
## Testing invertibility of dequantization layer
orig_img = train_set[0][0][None]  # Example image
ldj = jnp.zeros(1,)
dequant_module = Dequantization()
dequant_rng = random.PRNGKey(5)
deq_img, ldj, dequant_rng = dequant_module(orig_img, ldj, dequant_rng, reverse=False)
```

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```
reconst_img, ldj, dequant_rng = dequant_module(deq_img, ldj, dequant_rng, reverse=True)

d1, d2 = jnp.where(orig_img.squeeze() != reconst_img.squeeze())
if len(d1) != 0:
    print("Dequantization was not invertible.")
    for i in range(d1.shape[0]):
        print("Original value:", orig_img[0,d1[i],d2[i],0].item())
        print("Reconstructed value:", reconst_img[0,d1[i],d2[i],0].item())
else:
    print("Successfully inverted dequantization")

# Layer is not strictly invertible due to float precision constraints
# assert (orig_img == reconst_img).all().item()
```

```
Successfully inverted dequantization
```

The test succeeds as we would expect. However, there is a chance that the test fails due to numerical inaccuracies in the sigmoid invert. While the input space to the inverted sigmoid is scaled between 0 and 1, the output space is between $-\infty$ and ∞. And as we use 32 bits to represent the numbers (in addition to applying logs over and over again), such inaccuries can occur and should not be worrisome. Nevertheless, it is good to be aware of them, and can be improved by using a double tensor (float64).

Finally, we can take our dequantization and actually visualize the distribution it transforms the discrete values into:

[8]:
```
def visualize_dequantization(quants, prior=None):
    """
    Function for visualizing the dequantization values of discrete values in continuous␣
↪space
    """
    # Prior over discrete values. If not given, a uniform is assumed
    if prior is None:
        prior = np.ones(quants, dtype=np.float32) / quants
    prior = prior / prior.sum()  # Ensure proper categorical distribution

    inp = jnp.arange(-4, 4, 0.01).reshape(-1, 1, 1, 1)  # Possible continuous values we␣
↪want to consider
    ldj = jnp.zeros(inp.shape[0])
    dequant_module = Dequantization(quants=quants)
    # Invert dequantization on continuous values to find corresponding discrete value
    out, ldj, _ = dequant_module(inp, ldj, rng=None, reverse=True)
    inp, out, prob = inp.squeeze(), out.squeeze(), jnp.exp(ldj)
    prob = prob * prior[out] # Probability scaled by categorical prior

    # Plot volumes and continuous distribution
    sns.set_style("white")
    fig = plt.figure(figsize=(6,3))
    x_ticks = []
    for v in np.unique(out):
        indices = np.where(out==v)
        color = to_rgb(f"C{v}")
        plt.fill_between(inp[indices], prob[indices], np.zeros(indices[0].shape[0]),␣
↪color=color+(0.5,), label=str(v))
        plt.plot([inp[indices[0][0]]]*2,  [0, prob[indices[0][0]]],  color=color)
```

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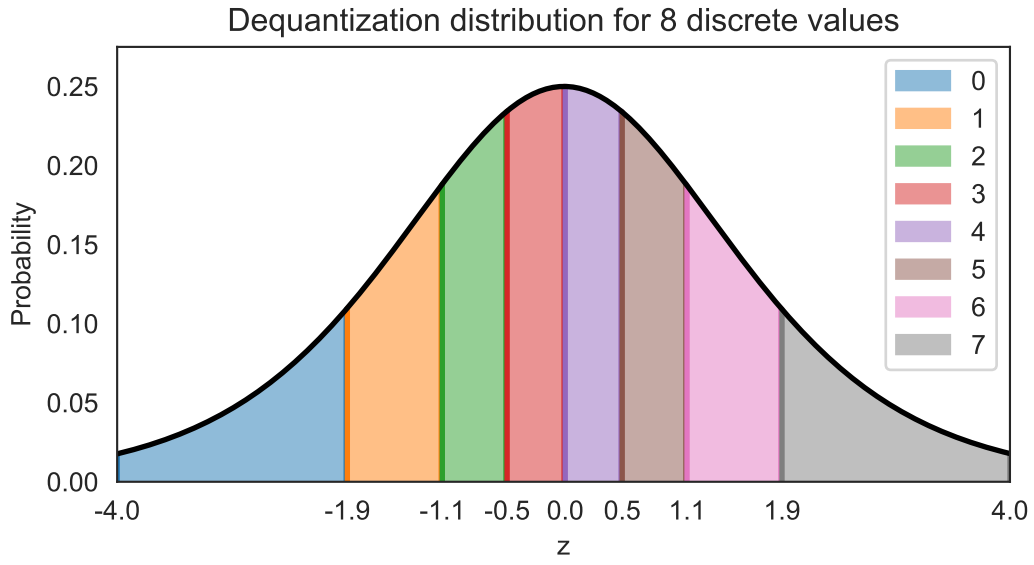
```
            plt.plot([inp[indices[0][-1]]]*2, [0, prob[indices[0][-1]]], color=color)
            x_ticks.append(inp[indices[0][0]])
        x_ticks.append(inp.max())
        plt.xticks(x_ticks, [f"{x:.1f}" for x in x_ticks])
        plt.plot(inp,prob, color=(0.0,0.0,0.0))
        # Set final plot properties
        plt.ylim(0, prob.max()*1.1)
        plt.xlim(inp.min(), inp.max())
        plt.xlabel("z")
        plt.ylabel("Probability")
        plt.title(f"Dequantization distribution for {quants} discrete values")
        plt.legend()
        plt.show()
        plt.close()

visualize_dequantization(quants=8)
```



The visualized distribution show the sub-volumes that are assigned to the different discrete values. The value 0 has its volume between $[-\infty, -1.9)$, the value 1 is represented by the interval $[-1.9, -1.1)$, etc. The volume for each discrete value has the same probability mass. That's why the volumes close to the center (e.g. 3 and 4) have a smaller area on the z-axis as others (z is being used to denote the output of the whole dequantization flow).

Effectively, the consecutive normalizing flow models discrete images by the following objective:

$$\log p(x) = \log \mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right] \geq \mathbb{E}_u \left[\log \frac{p(x+u)}{q(u|x)} \right]$$

Although normalizing flows are exact in likelihood, we have a lower bound. Specifically, this is an example of the Jensen inequality because we need to move the log into the expectation so we can use Monte-carlo estimates. In general, this bound is considerably smaller than the ELBO in variational autoencoders. Actually, we can reduce the bound ourselves by estimating the expectation not by one, but by M samples. In other words, we can apply importance sampling which leads to the following inequality:

$$\log p(x) = \log \mathbb{E}_{u \sim q(u|x)} \left[\frac{p(x+u)}{q(u|x)} \right] \geq \mathbb{E}_u \left[\log \frac{1}{M} \sum_{m=1}^{M} \frac{p(x+u_m)}{q(u_m|x)} \right] \geq \mathbb{E}_u \left[\log \frac{p(x+u)}{q(u|x)} \right]$$

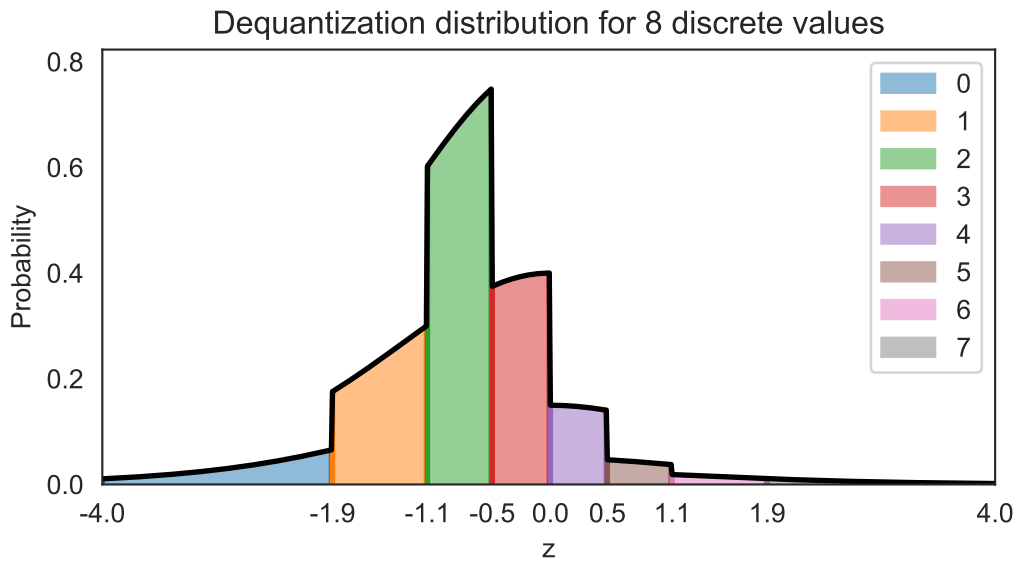
The importance sampling $\frac{1}{M}\sum_{m=1}^{M}\frac{p(x+u_m)}{q(u_m|x)}$ becomes $\mathbb{E}_{u\sim q(u|x)}\left[\frac{p(x+u)}{q(u|x)}\right]$ if $M\to\infty$, so that the more samples we use, the tighter the bound is. During testing, we can make use of this property and have it implemented in `test_step` in `ImageFlow`. In theory, we could also use this tighter bound during training. However, related work has shown that this does not necessarily lead to an improvement given the additional computational cost, and it is more efficient to stick with a single estimate [5].

Variational Dequantization

Dequantization uses a uniform distribution for the noise u which effectively leads to images being represented as hypercubes (cube in high dimensions) with sharp borders. However, modeling such sharp borders is not easy for a flow as it uses smooth transformations to convert it into a Gaussian distribution.

Another way of looking at it is if we change the prior distribution in the previous visualization. Imagine we have independent Gaussian noise on pixels which is commonly the case for any real-world taken picture. Therefore, the flow would have to model a distribution as above, but with the individual volumes scaled as follows:

[9]:
```
visualize_dequantization(quants=8, prior=np.array([0.075, 0.2, 0.4, 0.2, 0.075, 0.025, 0.
↪0125, 0.0125]))
```



Transforming such a probability into a Gaussian is a difficult task, especially with such hard borders. Dequantization has therefore been extended to more sophisticated, learnable distributions beyond uniform in a variational framework. In particular, if we remember the learning objective $\log p(x) = \log \mathbb{E}_u\left[\frac{p(x+u)}{q(u|x)}\right]$, the uniform distribution can be replaced by a learned distribution $q_\theta(u|x)$ with support over $u\in[0,1)^D$. This approach is called Variational Dequantization and has been proposed by Ho et al. [3]. How can we learn such a distribution? We can use a second normalizing flow that takes x as external input and learns a flexible distribution over u. To ensure a support over $[0,1)^D$, we can apply a sigmoid activation function as final flow transformation.

Inheriting the original dequantization class, we can implement variational dequantization as follows:

[10]:
```
class VariationalDequantization(Dequantization):
    var_flows : Sequence[nn.Module] = None  # A list of flow transformations to use for␣
↪modeling q(u|x)

    def dequant(self, z, ldj, rng):
```

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```
        z = z.astype(jnp.float32)
        img = (z / 255.0) * 2 - 1 # We condition the flows on x, i.e. the original image

        # Prior of u is a uniform distribution as before
        # As most flow transformations are defined on [-infinity,+infinity], we apply an␣
↪inverse sigmoid first.
        rng, uniform_rng = random.split(rng)
        deq_noise = random.uniform(uniform_rng, z.shape)
        deq_noise, ldj = self.sigmoid(deq_noise, ldj, reverse=True)
        if self.var_flows is not None:
            for flow in self.var_flows:
                deq_noise, ldj, rng = flow(deq_noise, ldj, rng, reverse=False, orig_
↪img=img)
        deq_noise, ldj = self.sigmoid(deq_noise, ldj, reverse=False)

        # After the flows, apply u as in standard dequantization
        z = (z + deq_noise) / 256.0
        ldj -= np.log(256.0) * np.prod(z.shape[1:])
        return z, ldj, rng
```

Variational dequantization can be used as a substitute for dequantization. We will compare dequantization and variational dequantization in later experiments.

Coupling layers

Next, we look at possible transformations to apply inside the flow. A recent popular flow layer, which works well in combination with deep neural networks, is the coupling layer introduced by Dinh et al. [1]. The input z is arbitrarily split into two parts, $z_{1:j}$ and $z_{j+1:d}$, of which the first remains unchanged by the flow. Yet, $z_{1:j}$ is used to parameterize the transformation for the second part, $z_{j+1:d}$. Various transformations have been proposed in recent time [3,4], but here we will settle for the simplest and most efficient one: affine coupling. In this coupling layer, we apply an affine transformation by shifting the input by a bias μ and scale it by σ. In other words, our transformation looks as follows:

$$z'_{j+1:d} = \mu_\theta(z_{1:j}) + \sigma_\theta(z_{1:j}) \odot z_{j+1:d}$$

The functions μ and σ are implemented as a shared neural network, and the sum and multiplication are performed element-wise. The log-determinant Jacobian (LDJ) is thereby the sum of the logs of the scaling factors: $\sum_i \left[\log \sigma_\theta(z_{1:j})\right]_i$. Inverting the layer can as simply be done as subtracting the bias and dividing by the scale:

$$z_{j+1:d} = \left(z'_{j+1:d} - \mu_\theta(z_{1:j})\right) / \sigma_\theta(z_{1:j})$$

We can also visualize the coupling layer in form of a computation graph, where z_1 represents $z_{1:j}$, and z_2 represents $z_{j+1:d}$:

In our implementation, we will realize the splitting of variables as masking. The variables to be transformed, $z_{j+1:d}$, are masked when passing z to the shared network to predict the transformation parameters. When applying the transformation, we mask the parameters for $z_{1:j}$ so that we have an identity operation for those variables:

[11]:
```
class CouplingLayer(nn.Module):
    network : nn.Module  # NN to use in the flow for predicting mu and sigma
    mask : np.ndarray  # Binary mask where 0 denotes that the element should be␣
↪transformed, and 1 not.
```

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```
    c_in : int  # Number of input channels

    def setup(self):
        self.scaling_factor = self.param('scaling_factor',
                                         nn.initializers.zeros,
                                         (self.c_in,))

    def __call__(self, z, ldj, rng, reverse=False, orig_img=None):
        """
        Inputs:
            z - Latent input to the flow
            ldj - The current ldj of the previous flows.
                  The ldj of this layer will be added to this tensor.
            rng - PRNG state
            reverse - If True, we apply the inverse of the layer.
            orig_img (optional) - Only needed in VarDeq. Allows external
                                  input to condition the flow on (e.g. original image)
        """
        # Apply network to masked input
        z_in = z * self.mask
        if orig_img is None:
            nn_out = self.network(z_in)
        else:
            nn_out = self.network(jnp.concatenate([z_in, orig_img], axis=-1))
        s, t = nn_out.split(2, axis=-1)

        # Stabilize scaling output
        s_fac = jnp.exp(self.scaling_factor).reshape(1, 1, 1, -1)
        s = nn.tanh(s / s_fac) * s_fac

        # Mask outputs (only transform the second part)
        s = s * (1 - self.mask)
        t = t * (1 - self.mask)

        # Affine transformation
        if not reverse:
            # Whether we first shift and then scale, or the other way round,
            # is a design choice, and usually does not have a big impact
            z = (z + t) * jnp.exp(s)
            ldj += s.sum(axis=[1,2,3])
        else:
            z = (z * jnp.exp(-s)) - t
            ldj -= s.sum(axis=[1,2,3])

        return z, ldj, rng
```

For stabilization purposes, we apply a $\tanh$ activation function on the scaling output. This prevents sudden large output values for the scaling that can destabilize training. To still allow scaling factors smaller or larger than -1 and 1 respectively, we have a learnable parameter per dimension, called `scaling_factor`. This scales the tanh to different limits. Below, we visualize the effect of the scaling factor on the output activation of the scaling terms:

[12]:
```
x = jnp.arange(-5,5,0.01)
```

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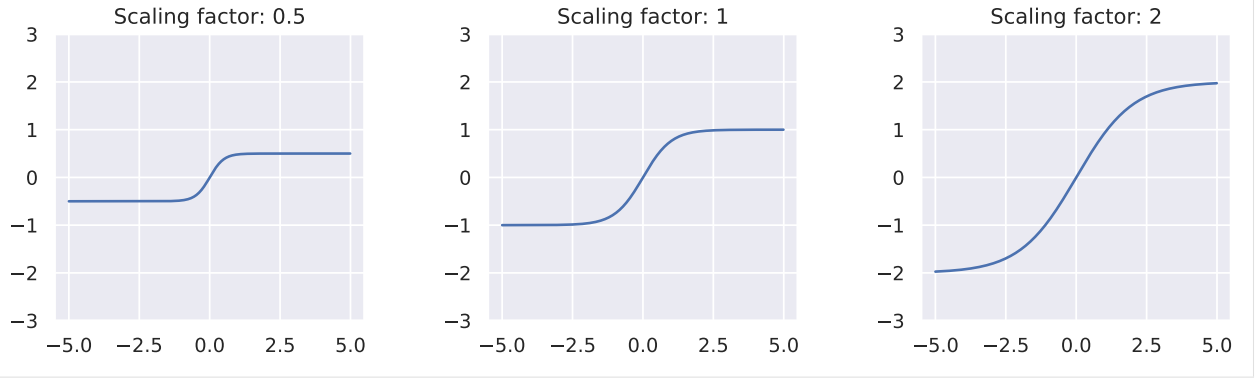
```
scaling_factors = [0.5, 1, 2]
sns.set()
fig, ax = plt.subplots(1, 3, figsize=(12,3))
for i, scale in enumerate(scaling_factors):
    y = nn.tanh(x / scale) * scale
    ax[i].plot(x, y)
    ax[i].set_title("Scaling factor: " + str(scale))
    ax[i].set_ylim(-3, 3)
plt.subplots_adjust(wspace=0.4)
sns.reset_orig()
plt.show()
```



Coupling layers generalize to any masking technique we could think of. However, the most common approach for images is to split the input z in half, using a checkerboard mask or channel mask. A checkerboard mask splits the variables across the height and width dimensions and assigns each other pixel to $z_{j+1:d}$. Thereby, the mask is shared across channels. In contrast, the channel mask assigns half of the channels to $z_{j+1:d}$, and the other half to $z_{1:j+1}$. Note that when we apply multiple coupling layers, we invert the masking for each other layer so that each variable is transformed a similar amount of times.

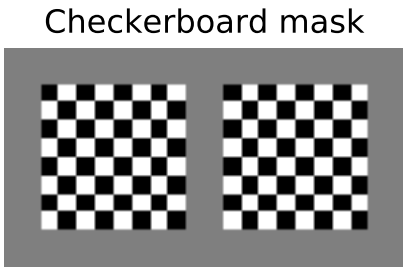
Let's implement a function that creates a checkerboard mask and a channel mask for us:

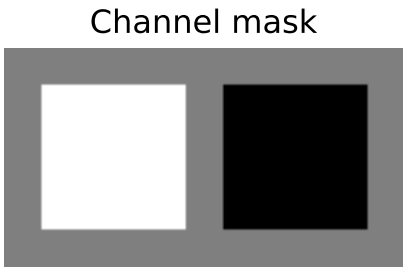
[13]:
```
def create_checkerboard_mask(h, w, invert=False):
    x, y = jnp.arange(h, dtype=jnp.int32), jnp.arange(w, dtype=jnp.int32)
    xx, yy = jnp.meshgrid(x, y, indexing='ij')
    mask = jnp.fmod(xx + yy, 2)
    mask = mask.astype(jnp.float32).reshape(1, h, w, 1)
    if invert:
        mask = 1 - mask
    return mask

def create_channel_mask(c_in, invert=False):
    mask = jnp.concatenate([
                jnp.ones((c_in//2,), dtype=jnp.float32),
                jnp.zeros((c_in-c_in//2,), dtype=jnp.float32)
            ])
    mask = mask.reshape(1, 1, 1, c_in)
    if invert:
        mask = 1 - mask
    return mask
```

We can also visualize the corresponding masks for an image of size $8 \times 8 \times 2$ (2 channels):

[14]:
```
checkerboard_mask = create_checkerboard_mask(h=8, w=8).repeat(2, -1)
channel_mask = jnp.resize(create_channel_mask(c_in=2), (1,8,8,2))
show_imgs(checkerboard_mask.swapaxes(0, 3), "Checkerboard mask")
show_imgs(channel_mask.swapaxes(0, 3), "Channel mask")
```





As a last aspect of coupling layers, we need to decide for the deep neural network we want to apply in the coupling layers. The input to the layers is an image, and hence we stick with a CNN. Because the input to a transformation depends on all transformations before, it is crucial to ensure a good gradient flow through the CNN back to the input, which can be optimally achieved by a ResNet-like architecture. Specifically, we use a Gated ResNet that adds a σ-gate to the skip connection, similarly to the input gate in LSTMs. The details are not necessarily important here, and the network is strongly inspired from Flow++ [3] in case you are interested in building even stronger models.

[15]:
```
class ConcatELU(nn.Module):
    """
    Activation function that applies ELU in both direction (inverted and plain).
    Allows non-linearity while providing strong gradients for any input (important for␣
↪final convolution)
    """

    def __call__(self, x):
        return jnp.concatenate([nn.elu(x), nn.elu(-x)], axis=-1)


class GatedConv(nn.Module):
    """ This module applies a two-layer convolutional ResNet block with input gate """
    c_in : int  # Number of input channels
    c_hidden : int  # Number of hidden dimensions

    @nn.compact
    def __call__(self, x):
        out = nn.Sequential([
            ConcatELU(),
            nn.Conv(self.c_hidden, kernel_size=(3, 3)),
```

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```
            ConcatELU(),
            nn.Conv(2*self.c_in, kernel_size=(1, 1))
        ])(x)
        val, gate = out.split(2, axis=-1)
        return x + val * nn.sigmoid(gate)


class GatedConvNet(nn.Module):
    c_hidden : int  # Number of hidden dimensions to use within the network
    c_out : int  # Number of output channels
    num_layers : int = 3 # Number of gated ResNet blocks to apply

    def setup(self):
        layers = []
        layers += [nn.Conv(self.c_hidden, kernel_size=(3, 3))]
        for layer_index in range(self.num_layers):
            layers += [GatedConv(self.c_hidden, self.c_hidden),
                       nn.LayerNorm()]
        layers += [ConcatELU(),
                   nn.Conv(self.c_out, kernel_size=(3, 3),
                           kernel_init=nn.initializers.zeros)]
        self.nn = nn.Sequential(layers)

    def __call__(self, x):
        return self.nn(x)
```

Training loop

Finally, we can add Dequantization, Variational Dequantization and Coupling Layers together to build our full normalizing flow on MNIST images. We apply 8 coupling layers in the main flow, and 4 for variational dequantization if applied. We apply a checkerboard mask throughout the network as with a single channel (black-white images), we cannot apply channel mask. The overall architecture is visualized below.

[17]:
```
def create_simple_flow(use_vardeq=True):
    flow_layers = []
    if use_vardeq:
        vardeq_layers = [CouplingLayer(network=GatedConvNet(c_out=2, c_hidden=16),
                                       mask=create_checkerboard_mask(h=28, w=28,␣
↪invert=(i%2==1)),
                                       c_in=1) for i in range(4)]
        flow_layers += [VariationalDequantization(var_flows=vardeq_layers)]
    else:
        flow_layers += [Dequantization()]

    for i in range(8):
        flow_layers += [CouplingLayer(network=GatedConvNet(c_out=2, c_hidden=32),
                                      mask=create_checkerboard_mask(h=28, w=28, invert=(i
↪%2==1)),
                                      c_in=1)]
```

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```
    flow_model = ImageFlow(flow_layers)
    return flow_model
```

For implementing the training loop, we use a similar trainer module as we have done in several tutorials before. Note that we again provide pre-trained models (see later on in the notebook) as normalizing flows are particularly expensive to train. We have also run validation and testing as this can take some time as well with the added importance sampling.

[18]:
```
class TrainerModule:

    def __init__(self, model_name, flow, lr=1e-3, seed=42):
        super().__init__()
        self.model_name = model_name
        self.lr = lr
        self.seed = seed
        # Create empty model. Note: no parameters yet
        self.model = flow
        # Prepare logging
        self.exmp_imgs = next(iter(train_exmp_loader))[0]
        self.log_dir = os.path.join(CHECKPOINT_PATH, self.model_name)
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model()

    def create_functions(self):
        # Training function
        def train_step(state, rng, batch):
            imgs, _ = batch
            loss_fn = lambda params: self.model.apply({'params': params}, imgs, rng,␣
↪testing=False)
            (loss, rng), grads = jax.value_and_grad(loss_fn, has_aux=True)(state.params)␣
↪ # Get loss and gradients for loss
            state = state.apply_gradients(grads=grads)  # Optimizer update step
            return state, rng, loss
        self.train_step = jax.jit(train_step)
        # Eval function, which is separately jitted for validation and testing
        def eval_step(state, rng, batch, testing):
            return self.model.apply({'params': state.params}, batch[0], rng,␣
↪testing=testing)
        self.eval_step = jax.jit(eval_step, static_argnums=(3,))

    def init_model(self):
        # Initialize model
        self.rng = jax.random.PRNGKey(self.seed)
        self.rng, init_rng, flow_rng = jax.random.split(self.rng, 3)
        params = self.model.init(init_rng, self.exmp_imgs, flow_rng)['params']
        # Initialize learning rate schedule and optimizer
        lr_schedule = optax.exponential_decay(
            init_value=self.lr,
            transition_steps=len(train_data_loader),
```

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```
            decay_rate=0.99,
            end_value=0.01*self.lr
        )
        optimizer = optax.chain(
            optax.clip_by_global_norm(1.0),  # Clip gradients at 1
            optax.adam(lr_schedule)
        )
        # Initialize training state
        self.state = train_state.TrainState.create(apply_fn=self.model.apply,␣
↪params=params, tx=optimizer)

    def train_model(self, train_loader, val_loader, num_epochs=500):
        # Train model for defined number of epochs
        best_eval = 1e6
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(train_loader, epoch=epoch_idx)
            if epoch_idx % 5 == 0:
                eval_bpd = self.eval_model(val_loader, testing=False)
                self.logger.add_scalar('val/bpd', eval_bpd, global_step=epoch_idx)
                if eval_bpd < best_eval:
                    best_eval = eval_bpd
                    self.save_model(step=epoch_idx)
                self.logger.flush()

    def train_epoch(self, data_loader, epoch):
        # Train model for one epoch, and log avg loss
        avg_loss = 0.
        for batch in tqdm(data_loader, leave=False):
            self.state, self.rng, loss = self.train_step(self.state, self.rng, batch)
            avg_loss += loss
        avg_loss /= len(data_loader)
        self.logger.add_scalar('train/bpd', avg_loss.item(), global_step=epoch)

    def eval_model(self, data_loader, testing=False):
        # Test model on all images of a data loader and return avg loss
        losses = []
        batch_sizes = []
        for batch in data_loader:
            loss, self.rng = self.eval_step(self.state, self.rng, batch, testing=testing)
            losses.append(loss)
            batch_sizes.append(batch[0].shape[0])
        losses_np = np.stack(jax.device_get(losses))
        batch_sizes_np = np.stack(batch_sizes)
        avg_loss = (losses_np * batch_sizes_np).sum() / batch_sizes_np.sum()
        return avg_loss

    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir, target=self.state.params,␣
↪step=step)

    def load_model(self, pretrained=False):
```

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```
        # Load model. We use different checkpoint for pretrained models
        if not pretrained:
            params = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir, target=self.
↪state.params)
        else:
            params = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'{self.model_name}.ckpt'),
                                                    target=self.state.params)
        self.state = train_state.TrainState.create(apply_fn=self.model.apply,␣
↪params=params, tx=self.state.tx)

    def checkpoint_exists(self):
        # Check whether a pretrained model exist for this autoencoder
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'{self.model_name}.ckpt'))
```

[19]:
```
def train_flow(flow, model_name="MNISTFlow"):
    # Create a trainer module with specified hyperparameters
    trainer = TrainerModule(model_name, flow)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(train_data_loader,
                            val_loader,
                            num_epochs=200)
        trainer.load_model()
        val_bpd = trainer.eval_model(val_loader, testing=True)
        start_time = time.time()
        test_bpd = trainer.eval_model(test_loader, testing=True)
        duration = time.time() - start_time
        results = {'val': val_bpd, 'test': test_bpd, 'time': duration / len(test_loader)␣
↪/ trainer.model.import_samples}
    else:
        trainer.load_model(pretrained=True)
        with open(os.path.join(CHECKPOINT_PATH, f'{trainer.model_name}_results.json'), 'r
↪') as f:
            results = json.load(f)

    # Bind parameters to model for easier inference
    trainer.model_bd = trainer.model.bind({'params': trainer.state.params})
    return trainer, results
```

4.37.3 Multi-scale architecture

One disadvantage of normalizing flows is that they operate on the exact same dimensions as the input. If the input is high-dimensional, so is the latent space, which requires larger computational cost to learn suitable transformations. However, particularly in the image domain, many pixels contain less information in the sense that we could remove them without loosing the semantical information of the image.

Based on this intuition, deep normalizing flows on images commonly apply a multi-scale architecture [1]. After the first N flow transformations, we split off half of the latent dimensions and directly evaluate them on the prior. The other half is run through N more flow transformations, and depending on the size of the input, we split it again in half or stop overall at this position. The two operations involved in this setup is `Squeeze` and `Split` which we will review more closely and implement below.

Squeeze and Split

When we want to remove half of the pixels in an image, we have the problem of deciding which variables to cut, and how to rearrange the image. Thus, the squeezing operation is commonly used before split, which divides the image into subsquares of shape $2 \times 2 \times C$, and reshapes them into $1 \times 1 \times 4C$ blocks. Effectively, we reduce the height and width of the image by a factor of 2 while scaling the number of channels by 4. Afterwards, we can perform the split operation over channels without the need of rearranging the pixels. The smaller scale also makes the overall architecture more efficient. Visually, the squeeze operation should transform the input as follows:

The input of $4 \times 4 \times 1$ is scaled to $2 \times 2 \times 4$ following the idea of grouping the pixels in $2 \times 2 \times 1$ subsquares. Next, let's try to implement this layer:

[20]:
```
class SqueezeFlow(nn.Module):

    def __call__(self, z, ldj, rng, reverse=False):
        B, H, W, C = z.shape
        if not reverse:
            # Forward direction: H x W x C => H/2 x W/2 x 4C
            z = z.reshape(B, H//2, 2, W//2, 2, C)
            z = z.transpose((0, 1, 3, 2, 4, 5))
            z = z.reshape(B, H//2, W//2, 4*C)
        else:
            # Reverse direction: H/2 x W/2 x 4C => H x W x C
            z = z.reshape(B, H, W, 2, 2, C//4)
            z = z.transpose((0, 1, 3, 2, 4, 5))
            z = z.reshape(B, H*2, W*2, C//4)
        return z, ldj, rng
```

Before moving on, we can verify our implementation by comparing our output with the example figure above:

[21]:
```
sq_flow = SqueezeFlow()
rand_img = jnp.arange(1,17).reshape(1, 4, 4, 1)
print("Image (before)\n", rand_img.transpose(0, 3, 1, 2)) # Permute for readability
forward_img, _, _ = sq_flow(rand_img, ldj=None, rng=None, reverse=False)
print("\nImage (forward)\n", forward_img)
reconst_img, _, _ = sq_flow(forward_img, ldj=None, rng=None, reverse=True)
print("\nImage (reverse)\n", reconst_img.transpose(0, 3, 1, 2))
```

```
Image (before)
 [[[[ 1  2  3  4]
    [ 5  6  7  8]
    [ 9 10 11 12]
    [13 14 15 16]]]]

Image (forward)
 [[[[ 1  2  5  6]
    [ 3  4  7  8]]

   [[ 9 10 13 14]
    [11 12 15 16]]]]

Image (reverse)
 [[[[ 1  2  3  4]
```

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```
   [ 5  6  7  8]
   [ 9 10 11 12]
   [13 14 15 16]]]]
```

The split operation divides the input into two parts, and evaluates one part directly on the prior. So that our flow operation fits to the implementation of the previous layers, we will return the prior probability of the first part as the log determinant jacobian of the layer. It has the same effect as if we would combine all variable splits at the end of the flow, and evaluate them together on the prior.

[22]:
```
class SplitFlow(nn.Module):

    def __call__(self, z, ldj, rng, reverse=False):
        if not reverse:
            z, z_split = z.split(2, axis=-1)
            ldj += jax.scipy.stats.norm.logpdf(z_split).sum(axis=[1,2,3])
        else:
            z_split = random.normal(rng, z.shape)
            z = jnp.concatenate([z, z_split], axis=-1)
            ldj -= jax.scipy.stats.norm.logpdf(z_split).sum(axis=[1,2,3])
        return z, ldj, rng
```

Building a multi-scale flow

After defining the squeeze and split operation, we are finally able to build our own multi-scale flow. Deep normalizing flows such as Glow and Flow++ [2,3] often apply a split operation directly after squeezing. However, with shallow flows, we need to be more thoughtful about where to place the split operation as we need at least a minimum amount of transformations on each variable. Our setup is inspired by the original RealNVP architecture [1] which is shallower than other, more recent state-of-the-art architectures.

Hence, for the MNIST dataset, we will apply the first squeeze operation after two coupling layers, but don't apply a split operation yet. Because we have only used two coupling layers and each the variable has been only transformed once, a split operation would be too early. We apply two more coupling layers before finally applying a split flow and squeeze again. The last four coupling layers operate on a scale of $7 \times 7 \times 8$. The full flow architecture is shown below.

Note that while the feature maps inside the coupling layers reduce with the height and width of the input, the increased number of channels is not directly considered. To counteract this, we increase the hidden dimensions for the coupling layers on the squeezed input. The dimensions are often scaled by 2 as this approximately increases the computation cost by 4 canceling with the squeezing operation. However, we will choose the hidden dimensionalities $32, 48, 64$ for the three scales respectively to keep the number of parameters reasonable and show the efficiency of multi-scale architectures.

[23]:
```
def create_multiscale_flow():
    flow_layers = []

    vardeq_layers = [CouplingLayer(network=GatedConvNet(c_out=2, c_hidden=16),
                                   mask=create_checkerboard_mask(h=28, w=28, invert=(i
↪%2==1)),
                                   c_in=1) for i in range(4)]
    flow_layers += [VariationalDequantization(var_flows=vardeq_layers)]

    flow_layers += [CouplingLayer(network=GatedConvNet(c_out=2, c_hidden=32),
```

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```
                                    mask=create_checkerboard_mask(h=28, w=28, invert=(i
↪%2==1)),
                                    c_in=1) for i in range(2)]
    flow_layers += [SqueezeFlow()]
    for i in range(2):
        flow_layers += [CouplingLayer(network=GatedConvNet(c_out=8, c_hidden=48),
                                      mask=create_channel_mask(c_in=4, invert=(i%2==1)),
                                      c_in=4)]
    flow_layers += [SplitFlow(),
                    SqueezeFlow()]
    for i in range(4):
        flow_layers += [CouplingLayer(network=GatedConvNet(c_out=16, c_hidden=64),
                                      mask=create_channel_mask(c_in=8, invert=(i%2==1)),
                                      c_in=8)]

    flow_model = ImageFlow(flow_layers)
    return flow_model
```

4.37.4 Analysing the flows

In the last part of the notebook, we will train all the models we have implemented above, and try to analyze the effect of the multi-scale architecture and variational dequantization.

Training flow variants

Before we can analyse the flow models, we need to train them first. We provide pre-trained models that contain the validation and test performance, and run-time information. As flow models are computationally expensive, we advice you to rely on those pretrained models for a first run through the notebook.

[24]:
```
flow_dict = {"simple": {}, "vardeq": {}, "multiscale": {}}
flow_dict["simple"]["model"], flow_dict["simple"]["result"] = train_flow(create_simple_
↪flow(use_vardeq=False), model_name="MNISTFlow_simple")
flow_dict["vardeq"]["model"], flow_dict["vardeq"]["result"] = train_flow(create_simple_
↪flow(use_vardeq=True), model_name="MNISTFlow_vardeq")
flow_dict["multiscale"]["model"], flow_dict["multiscale"]["result"] = train_flow(create_
↪multiscale_flow(), model_name="MNISTFlow_multiscale")
```

We can show the difference in number of parameters below:

[25]:
```
def print_num_params(model):
    num_params = sum([np.prod(p.shape) for p in jax.tree_util.tree_leaves(model.state.
↪params)])
    print("Number of parameters: {:,}".format(num_params))

print_num_params(flow_dict["simple"]["model"])
print_num_params(flow_dict["vardeq"]["model"])
print_num_params(flow_dict["multiscale"]["model"])
```

```
Number of parameters: 556,312
Number of parameters: 628,388
Number of parameters: 1,711,818
```

Although the multi-scale flow has almost 3 times the parameters of the single scale flow, it is not necessarily more computationally expensive than its counterpart. We will compare the runtime in the following experiments as well.

Density modeling and sampling

Firstly, we can compare the models on their quantitative results. The following table shows all important statistics. The inference time specifies the time needed to determine the probability for a batch of 64 images for each model, and the sampling time the duration it took to sample a batch of 64 images.

[26]:
```
%%html
<!-- Some HTML code to increase font size in the following table -->
<style>
th {font-size: 120%;}
td {font-size: 120%;}
</style>
```

```
<IPython.core.display.HTML object>
```

[27]:
```
import tabulate
from IPython.display import display, HTML

table = [[key,
          "%4.3f bpd" % flow_dict[key]["result"]["val"],
          "%4.3f bpd" % flow_dict[key]["result"]["test"],
          "%2.1f ms" % (1000 * flow_dict[key]["result"]["time"]),
          "%2.1f ms" % (1000 * flow_dict[key]["result"].get("samp_time", 0)),
          "{:,}".format(sum([np.prod(p.shape) for p in jax.tree_util.tree_leaves(flow_
↪dict[key]["model"].state.params)]))]
         for key in flow_dict]
display(HTML(tabulate.tabulate(table, tablefmt='html', headers=["Model", "Validation Bpd
↪", "Test Bpd", "Inference time", "Sampling time", "Num Parameters"])))
```

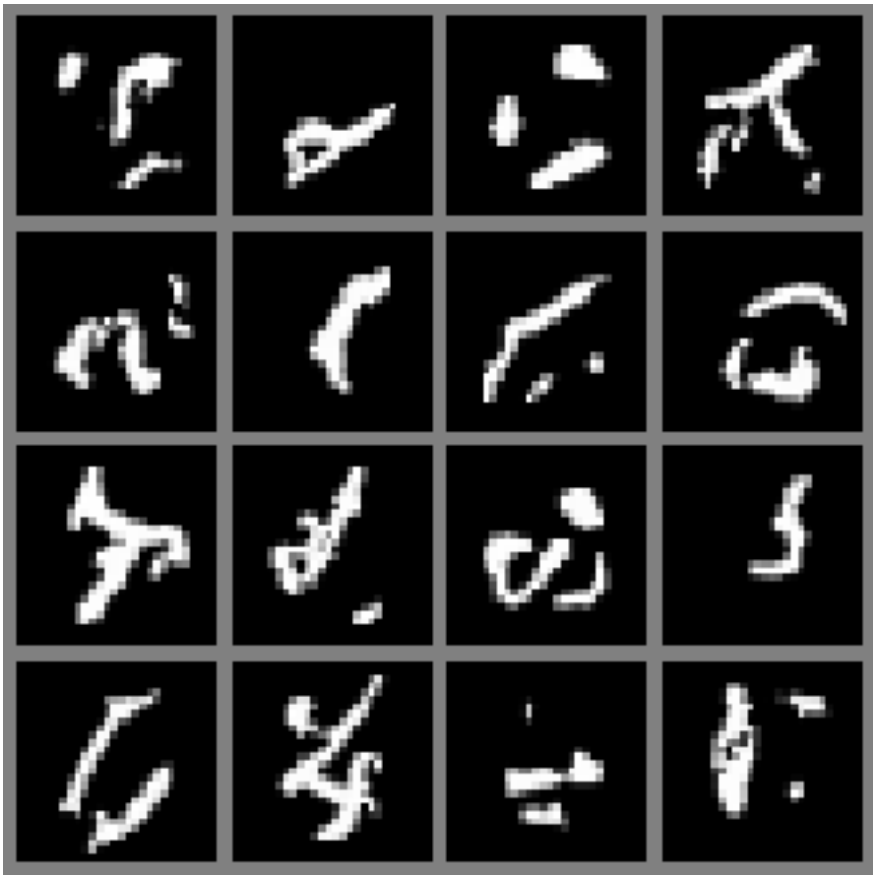
```
<IPython.core.display.HTML object>
```

As we have intially expected, using variational dequantization improves upon standard dequantization in terms of bits per dimension. Although the difference with 0.04bpd doesn't seem impressive first, it is a considerably step for generative models (most state-of-the-art models improve upon previous models in a range of 0.02-0.1bpd on CIFAR with three times as high bpd). While it takes longer to evaluate the probability of an image due to the variational dequantization, which also leads to a longer training time, it does not have an effect on the sampling time. This is because inverting variational dequantization is the same as dequantization: finding the next lower integer.

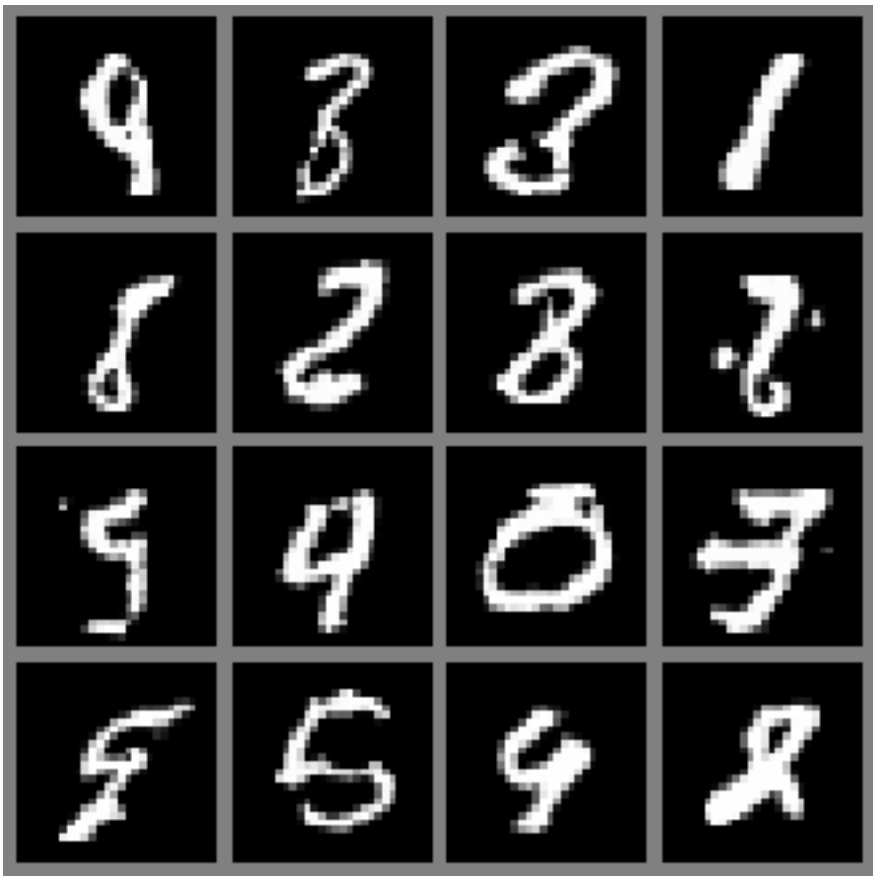
When we compare the two models to multi-scale architecture, we can see that the bits per dimension score again dropped by about 0.02bpd. Additionally, the inference time and sampling time improved notably despite having more parameters. Thus, we see that the multi-scale flow is not only stronger for density modeling, but also more efficient.

Next, we can test the sampling quality of the models. We should note that the samples for variational dequantization and standard dequantization are very similar, and hence we visualize here only the ones for variational dequantization and the multi-scale model. However, feel free to also test out the `"simple"` model. The seeds are set to obtain reproducable generations and are not cherry picked.

[28]:
```
sample_rng = random.PRNGKey(44)
samples, _ = flow_dict["vardeq"]["model"].model_bd.sample(img_shape=[16,28,28,1],␣
↪rng=sample_rng)
show_imgs(samples)
```



[29]:
```
sample_rng = random.PRNGKey(44)
samples, _ = flow_dict["multiscale"]["model"].model_bd.sample(img_shape=[16,7,7,8],␣
↪rng=sample_rng)
show_imgs(samples)
```



From the few samples, we can see a clear difference between the simple and the multi-scale model. The single-scale model has only learned local, small correlations while the multi-scale model was able to learn full, global relations that form digits. This show-cases another benefit of the multi-scale model. In contrast to VAEs, the outputs are sharp as normalizing flows can naturally model complex, multi-modal distributions while VAEs have the independent decoder output noise. Nevertheless, the samples from this flow are far from perfect as not all samples show true digits.

Interpolation in latent space

Another popular test for the smoothness of the latent space of generative models is to interpolate between two training examples. As normalizing flows are strictly invertible, we can guarantee that any image is represented in the latent space. We again compare the variational dequantization model with the multi-scale model below.

[30]:
```
def interpolate(model, rng, img1, img2, num_steps=8):
    """
    Inputs:
        model - object of ImageFlow class that represents the (trained) flow model
        img1, img2 - Image tensors of shape [1, 28, 28]. Images between which should be␣
↪interpolated.
        num_steps - Number of interpolation steps. 8 interpolation steps mean 6␣
↪intermediate pictures besides img1 and img2
    """
    imgs = np.stack([img1, img2], axis=0)
    z, _, rng = model.encode(imgs, rng)
```

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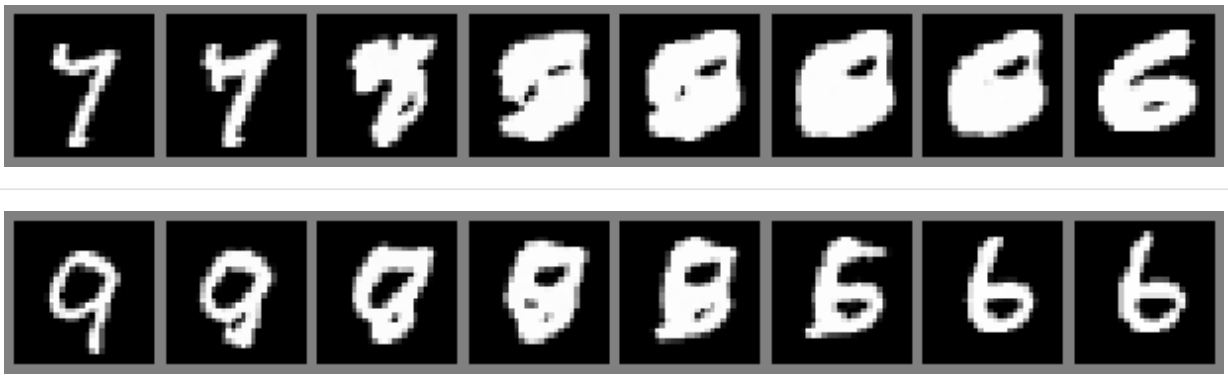
```
    alpha = jnp.linspace(0, 1, num=num_steps).reshape(-1, 1, 1, 1)
    interpolations = z[0:1] * alpha + z[1:2] * (1 - alpha)
    interp_imgs, _ = model.sample(interpolations.shape[:1] + imgs.shape[1:], rng=rng, z_
↪init=interpolations)
    show_imgs(interp_imgs, row_size=8)

exmp_imgs, _ = next(iter(train_exmp_loader))
```

[31]:
```
sample_rng = random.PRNGKey(42)
for i in range(2):
    interpolate(flow_dict["vardeq"]["model"].model_bd, sample_rng, exmp_imgs[2*i], exmp_
↪imgs[2*i+1])
```



[32]:
```
sample_rng = random.PRNGKey(42)
for i in range(2):
    interpolate(flow_dict["multiscale"]["model"].model_bd, sample_rng, exmp_imgs[2*i],␣
↪exmp_imgs[2*i+1])
```

The interpolations of the multi-scale model result in more realistic digits (first row $7 \leftrightarrow 8 \leftrightarrow 6$, second row $9 \leftrightarrow 6$), while the variational dequantization model focuses on local patterns that globally do not form a digit. For the multi-scale model, we actually did not do the "true" interpolation between the two images as we did not consider the variables that were split along the flow (they have been sampled randomly for all samples). However, as we will see in the next experiment, the early variables do not effect the overall image much.

Visualization of latents in different levels of multi-scale

In the following we will focus more on the multi-scale flow. We want to analyse what information is being stored in the variables split at early layers, and what information for the final variables. For this, we sample 8 images where each of them share the same final latent variables, but differ in the other part of the latent variables. Below we visualize three examples of this:

[33]:
```
sample_rng = random.PRNGKey(46)
for _ in range(3):
    sample_rng, iter_rng = random.split(sample_rng)
    z_init = random.normal(sample_rng, [1,7,7,8])
    z_init = z_init.repeat(8, 0)
    samples, sample_rng = flow_dict["multiscale"]["model"].model_bd.sample(img_shape=z_
↪init.shape, rng=sample_rng, z_init=z_init)
    show_imgs(samples)
```

We see that the early split variables indeed have a smaller effect on the image. Still, small differences can be spot when we look carefully at the borders of the digits. For instance, the hole at the left of the 0 changes for different samples although all of them represent the same coarse structure. This shows that the flow indeed learns to separate the higher-level information in the final variables, while the early split ones contain local noise patterns.

Visualizing Dequantization

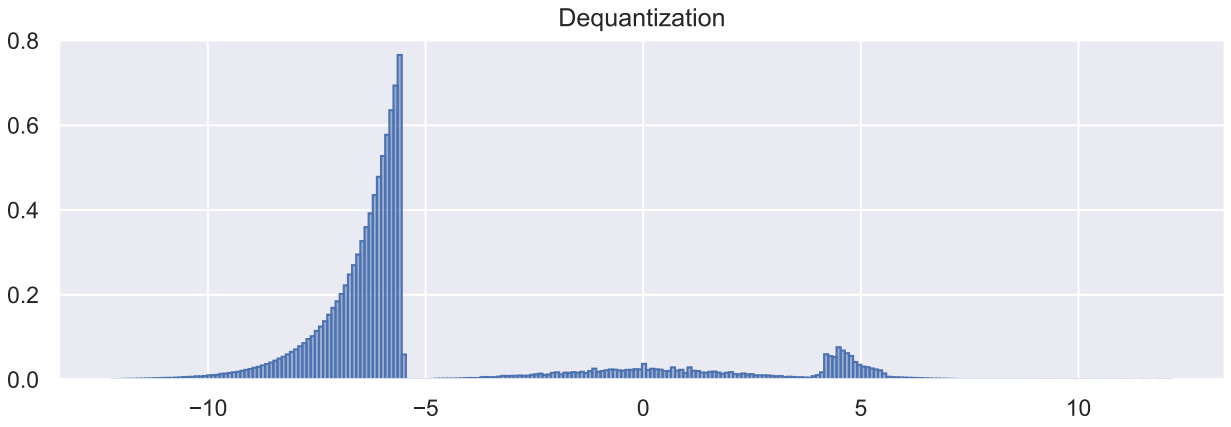
As a final part of this notebook, we will look at the effect of variational dequantization. We have motivated variational dequantization by the issue of sharp edges/boarders being difficult to model, and a flow would rather prefer smooth, prior-like distributions. To check how what noise distribution $q(u|x)$ the flows in the variational dequantization module have learned, we can plot a histogram of output values from the dequantization and variational dequantization module.

[34]:
```
def visualize_dequant_distribution(model, rng, imgs, title):
    """
    Inputs:
        model - The flow of which we want to visualize the dequantization distribution
        imgs - Example training images of which we want to visualize the dequantization␣
↪distribution
    """
    ldj = jnp.zeros(imgs.shape[0], dtype=jnp.float32)
    dequant_vals = []
    for _ in tqdm(range(8), leave=False):
        d, _, rng = model.flows[0](imgs, ldj, rng, reverse=False)
        dequant_vals.append(d)
    dequant_vals = jnp.concatenate(dequant_vals, axis=0)
    dequant_vals = jax.device_get(dequant_vals.reshape(-1))
    sns.set()
    plt.figure(figsize=(10,3))
    plt.hist(dequant_vals, bins=256, color=to_rgb("C0")+(0.5,), edgecolor="C0",␣
↪density=True)
    if title is not None:
        plt.title(title)
    plt.show()
    plt.close()

sample_imgs, _ = next(iter(train_exmp_loader))
```

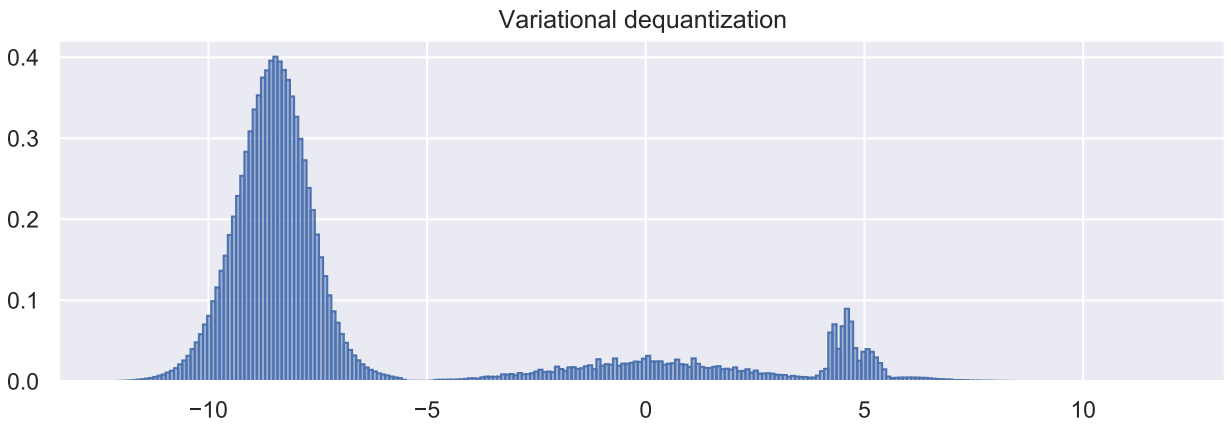
[35]:
```
sample_rng = random.PRNGKey(42)
visualize_dequant_distribution(flow_dict["simple"]["model"].model_bd, sample_rng, sample_
↪imgs, title="Dequantization")
```

```
  0%|          | 0/8 [00:00<?, ?it/s]
```



[36]:
```
sample_rng = random.PRNGKey(42)
visualize_dequant_distribution(flow_dict["vardeq"]["model"].model_bd, sample_rng, sample_
↪imgs, title="Variational dequantization")
```

```
  0%|          | 0/8 [00:00<?, ?it/s]
```



The dequantization distribution in the first plot shows that the MNIST images have a strong bias towards 0 (black), and the distribution of them have a sharp border as mentioned before. The variational dequantization module has indeed learned a much smoother distribution with a Gaussian-like curve which can be modeled much better. For the other values, we would need to visualize the distribution $q(u|x)$ on a deeper level, depending on x. However, as all u's interact and depend on each other, we would need to visualize a distribution in 784 dimensions, which is not that intuitive anymore.

4.37.5 Conclusion

In conclusion, we have seen how to implement our own normalizing flow, and what difficulties arise if we want to apply them on images. Dequantization is a crucial step in mapping the discrete images into continuous space to prevent underisable delta-peak solutions. While dequantization creates hypercubes with hard border, variational dequantization allows us to fit a flow much better on the data. This allows us to obtain a lower bits per dimension score, while not affecting the sampling speed. The most common flow element, the coupling layer, is simple to implement, and yet effective. Furthermore, multi-scale architectures help to capture the global image context while allowing us to efficiently scale up the flow. Normalizing flows are an interesting alternative to VAEs as they allow an exact likelihood estimate in continuous space, and we have the guarantee that every possible input x has a corresponding latent vector z. However, even beyond continuous inputs and images, flows can be applied and allow us to exploit the data structure in latent space, as e.g. on graphs for the task of molecule generation [6]. Recent advances in Neural ODEs allow a flow with infinite number of layers, called Continuous Normalizing Flows, whose potential is yet to fully explore. Overall, normalizing flows are an exciting research area which will continue over the next couple of years.

4.37.6 References

[1] Dinh, L., Sohl-Dickstein, J., and Bengio, S. (2017). "Density estimation using Real NVP," In: 5th International Conference on Learning Representations, ICLR 2017. Link

[2] Kingma, D. P., and Dhariwal, P. (2018). "Glow: Generative Flow with Invertible 1x1 Convolutions," In: Advances in Neural Information Processing Systems, vol. 31, pp. 10215–10224. Link

[3] Ho, J., Chen, X., Srinivas, A., Duan, Y., and Abbeel, P. (2019). "Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design," in Proceedings of the 36th International Conference on Machine Learning, vol. 97, pp. 2722–2730. Link

[4] Durkan, C., Bekasov, A., Murray, I., and Papamakarios, G. (2019). "Neural Spline Flows," In: Advances in Neural Information Processing Systems, pp. 7509–7520. Link

[5] Hoogeboom, E., Cohen, T. S., and Tomczak, J. M. (2020). "Learning Discrete Distributions by Dequantization," arXiv preprint arXiv2001.11235v1. Link

[6] Lippe, P., and Gavves, E. (2021). "Categorical Normalizing Flows via Continuous Transformations," In: International Conference on Learning Representations, ICLR 2021. Link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.38 Tutorial 12 (JAX): Autoregressive Image Modeling

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We will report a speed comparison between the PyTorch and JAX/Flax implementation here soon.

Models	PyTorch	JAX
PixelCNN	-min -sec	-min -sec

In this tutorial, we implement an autoregressive likelihood model for the task of image modeling. Autoregressive models are naturally strong generative models that constitute one of the current state-of-the-art architectures on likelihood-based image modeling, and are also the basis for large language generation models such as GPT3. Similar to the language generation you have seen in assignment 2, autoregressive models work on images by modeling the likelihood of a pixel given all previous ones. For instance, in the picture below, we model the pixel x_i as a conditional probability distribution based on all previous (here blue) pixels (figure credit - Aaron van den Oord et al.):

Generally, autoregressive model over high-dimensional data $\mathbf{x}$ factor the joint distribution as the following product of conditionals:

$$p(\mathbf{x}) = p(x_1, ..., x_n) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

Learning these conditionals is often much simpler than learning the joint distribution $p(\mathbf{x})$ all together. However, disadvantages of autoregressive models include slow sampling, especially for large images, as we need height-times-width forward passes through the model. In addition, for some applications, we require a latent space as modeled in VAEs and Normalizing Flows. For instance, in autoregressive models, we cannot interpolate between two images because of the lack of a latent representation. We will explore and discuss these benefits and drawbacks alongside with our implementation.

Our implementation will focus on the PixelCNN [2] model which has been discussed in detail in the lecture. Most current SOTA models use PixelCNN as their fundamental architecture, and various additions have been proposed to improve the performance (e.g. PixelCNN++ and PixelSNAIL). Hence, implementing PixelCNN is a good starting point for our short tutorial.

First of all, we need to import our standard libraries. Similarly as in the last couple of tutorials, we will use JAX with Flax and Optax here as well.

[1]:
```
## Standard libraries
import os
import math
import numpy as np
from typing import Any

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
```

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```
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import seaborn as sns

## tqdm for progress bars
from tqdm.auto import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch Data Loading
import torch
import torch.utils.data as data
from torch.utils.tensorboard import SummaryWriter
# Torchvision
from torchvision.datasets import MNIST
from torchvision import transforms

# Path to the folder where the datasets are/should be downloaded (e.g. MNIST)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial12_jax"

print("Device:", jax.devices()[0])
```

```
Device: gpu:0
```

We again provide a pretrained model, which is downloaded below:

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial12/"
# Files to download
pretrained_files = ["PixelCNN.ckpt"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

Similar to the Normalizing Flows in Tutorial 11, we will work on the MNIST dataset and use 8-bits per pixel (values between 0 and 255). The dataset is loaded below:

[3]:
```
# Transformations applied on each image => bring them into a numpy array
# Note that we keep them in the range 0-255 (integers)
def image_to_numpy(img):
    img = np.array(img, dtype=np.int32)
    img = img[..., None]  # Make image [28, 28, 1]
    return img

# We need to stack the batch elements
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple, list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

# Loading the training dataset. We need to split it into a training and validation part
train_dataset = MNIST(root=DATASET_PATH, train=True,
                      transform=image_to_numpy, download=True)
train_set, val_set = torch.utils.data.random_split(train_dataset, [50000, 10000],
                                                   generator=torch.Generator().manual_
↪seed(42))
# Loading the test set
test_set = MNIST(root=DATASET_PATH, train=False,
                 transform=image_to_numpy, download=True)

# We define a set of data loaders that we can use for various purposes
```

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```
train_loader = data.DataLoader(train_set,
                               batch_size=128,
                               shuffle=True,
                               drop_last=True,
                               collate_fn=numpy_collate,
                               num_workers=8,
                               persistent_workers=True)
val_loader = data.DataLoader(val_set, batch_size=128, shuffle=False,
                             drop_last=False, num_workers=4, collate_fn=numpy_collate)
test_loader = data.DataLoader(test_set, batch_size=128, shuffle=False,
                              drop_last=False, num_workers=4, collate_fn=numpy_collate)
```

A good practice is to always visualize some data examples to get an intuition of the data:

[4]:
```
def show_imgs(imgs):
    imgs = jax.device_get(imgs)
    if isinstance(imgs, (list, tuple)):
        imgs = np.stack(imgs, axis=0)
    num_imgs = imgs.shape[0]
    if num_imgs < 4 or num_imgs % 4 == 0:
        nrow = min(num_imgs, 4)
        ncol = int(math.ceil(num_imgs/nrow))
    else:
        nrow = num_imgs
        ncol = 1
    imgs = np.pad(imgs, pad_width=[(0,0), (1,1), (1,1), (0,0)], constant_values=128)
    imgs = np.reshape(imgs, (nrow, ncol, *imgs.shape[1:]))
    imgs = np.transpose(imgs, (1, 2, 0, 3, 4))
    imgs = np.reshape(imgs, (imgs.shape[0]*imgs.shape[1], imgs.shape[2]*imgs.shape[3], -
↪1))
    imgs = np.pad(imgs, pad_width=[(1,1), (1,1), (0,0)], constant_values=128)
    imgs = np.squeeze(imgs, axis=-1)
    plt.figure(figsize=(1.5*nrow, 1.5*ncol))
    plt.imshow(imgs, interpolation='nearest', cmap='gray')
    plt.axis('off')
    plt.show()
    plt.close()

show_imgs([train_set[i][0] for i in range(8)])
```

4.38.1 Masked autoregressive convolutions

The core module of PixelCNN is its masked convolutions. In contrast to language models, we don't apply an LSTM on each pixel one-by-one. This would be inefficient because images are grids instead of sequences. Thus, it is better to rely on convolutions that have shown great success in deep CNN classification models.

Nevertheless, we cannot just apply standard convolutions without any changes. Remember that during training of autoregressive models, we want to use teacher forcing which both helps the model training, and significantly reduces the time needed for training. For image modeling, teacher forcing is implemented by using a training image as input to the model, and we want to obtain as output the prediction for each pixel based on *only* its predecessors. Thus, we need to ensure that the prediction for a specific pixel can only be influenced by its predecessors and not by its own value or any "future" pixels. For this, we apply convolutions with a mask.

Which mask we use depends on the ordering of pixels we decide on, i.e. which is the first pixel we predict, which is the second one, etc. The most commonly used ordering is to denote the upper left pixel as the start pixel, and sort the pixels row by row, as shown in the visualization at the top of the tutorial. Thus, the second pixel is on the right of the first one (first row, second column), and once we reach the end of the row, we start in the second row, first column. If we now want to apply this to our convolutions, we need to ensure that the prediction of pixel 1 is not influenced by its own "true" input, and all pixels on its right and in any lower row. In convolutions, this means that we want to set those entries of the weight matrix to zero that take pixels on the right and below into account. As an example for a 5x5 kernel, see a mask below (figure credit - Aaron van den Oord):

Before looking into the application of masked convolutions in PixelCNN in detail, let's first implement a module that allows us to apply an arbitrary mask to a convolution:

[5]:
```
class MaskedConvolution(nn.Module):
    c_out : int
    mask : np.ndarray
    dilation : int = 1

    @nn.compact
    def __call__(self, x):
        # Flax's convolution module already supports masking
        # The mask must be the same size as kernel
        # => extend over input and output feature channels
        if len(self.mask.shape) == 2:
```

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```
            mask_ext = self.mask[...,None,None]
            mask_ext = jnp.tile(mask_ext, (1, 1, x.shape[-1], self.c_out))
        else:
            mask_ext = self.mask
        # Convolution with masking
        x = nn.Conv(features=self.c_out,
                    kernel_size=self.mask.shape[:2],
                    kernel_dilation=self.dilation,
                    mask=mask_ext)(x)
        return x
```

Vertical and horizontal convolution stacks

To build our own autoregressive image model, we could simply stack a few masked convolutions on top of each other. This was actually the case for the original PixelCNN model, discussed in the paper Pixel Recurrent Neural Networks, but this leads to a considerable issue. When sequentially applying a couple of masked convolutions, the receptive field of a pixel show to have a "blind spot" on the right upper side, as shown in the figure below (figure credit - Aaron van den Oord et al.):

Although a pixel should be able to take into account all other pixels above and left of it, a stack of masked convolutions does not allow us to look to the upper pixels on the right. This is because the features of the pixels above, which we use for convolution, do not contain any information of the pixels on the right of the same row. If they would, we would be "cheating" and actually looking into the future. To overcome this issue, van den Oord et. al [2] proposed to split the convolutions into a vertical and a horizontal stack. The vertical stack looks at all pixels above the current one, while the horizontal takes into account all on the left. While keeping both of them separate, we can actually look at the pixels on the right with the vertical stack without breaking any of our assumptions. The two convolutions are also shown in the figure above.

Let us implement them here as follows:

[6]:
```
class VerticalStackConvolution(nn.Module):
    c_out : int
    kernel_size : int
    mask_center : bool = False
    dilation : int = 1

    def setup(self):
        # Mask out all pixels below. For efficiency, we could also reduce the kernel
        # size in height, but for simplicity, we stick with masking here.
        mask = np.ones((self.kernel_size, self.kernel_size), dtype=np.float32)
        mask[self.kernel_size//2+1:,:] = 0
        # For the very first convolution, we will also mask the center row
        if self.mask_center:
            mask[self.kernel_size//2,:] = 0
        # Our convolution module
        self.conv = MaskedConvolution(c_out=self.c_out,
                                      mask=mask,
                                      dilation=self.dilation)

    def __call__(self, x):
```

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```
        return self.conv(x)


class HorizontalStackConvolution(nn.Module):
    c_out : int
    kernel_size : int
    mask_center : bool = False
    dilation : int = 1

    def setup(self):
        # Mask out all pixels on the left. Note that our kernel has a size of 1
        # in height because we only look at the pixel in the same row.
        mask = np.ones((1, self.kernel_size), dtype=np.float32)
        mask[0,self.kernel_size//2+1:] = 0
        # For the very first convolution, we will also mask the center pixel
        if self.mask_center:
            mask[0,self.kernel_size//2] = 0
        # Our convolution module
        self.conv = MaskedConvolution(c_out=self.c_out,
                                      mask=mask,
                                      dilation=self.dilation)

    def __call__(self, x):
        return self.conv(x)
```

Note that we have an input argument called `mask_center`. Remember that the input to the model is the actual input image. Hence, the very first convolution we apply cannot use the center pixel as input, but must be masked. All consecutive convolutions, however, should use the center pixel as we otherwise lose the features of the previous layer. Hence, the input argument `mask_center` is True for the very first convolutions, and False for all others.

Visualizing the receptive field

To validate our implementation of masked convolutions, we can visualize the receptive field we obtain with such convolutions. We should see that with increasing number of convolutional layers, the receptive field grows in both vertical and horizontal direction, without the issue of a blind spot. The receptive field can be empirically measured by back-propagating an arbitrary loss for the output features of a speicifc pixel with respect to the input. We implement this idea below, and visualize the receptive field below.

[7]:
```
inp_img = np.zeros((1, 11, 11, 1), dtype=np.float32)

def show_center_recep_field(img, apply_fn):
    """
    Calculates the gradients of the input with respect to the output center pixel,
    and visualizes the overall receptive field.
    Inputs:
        img - Input image for which we want to calculate the receptive field on.
        out - Output features/loss which is used for backpropagation, and should be
              the output of the network/computation graph.
    """
    # Determine gradients
    grad_fn = jax.grad(lambda inp: apply_fn(inp)[0,inp.shape[1]//2,inp.shape[2]//2].
↪sum()) # L1 loss for simplicity
```

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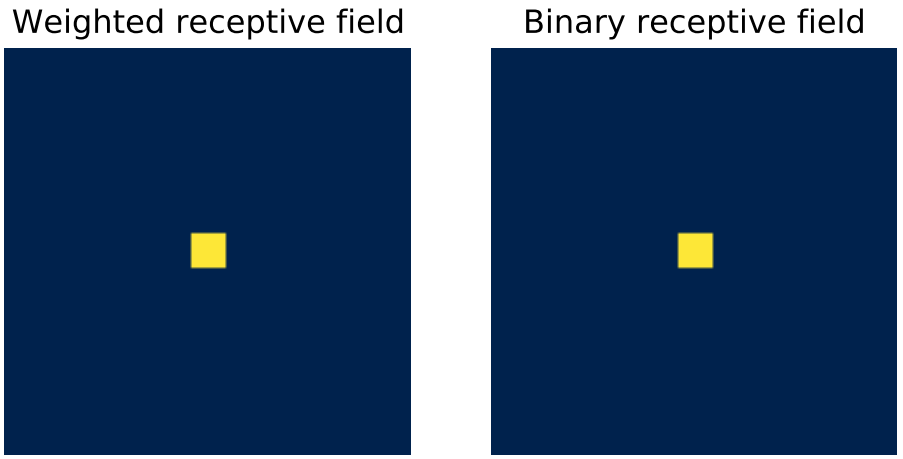
```
    img_grads = jnp.abs(grad_fn(img))
    img_grads = jax.device_get(img_grads)

    # Plot receptive field
    img = img_grads[0,...,0]
    fig, ax = plt.subplots(1,2)
    pos = ax[0].imshow(img)
    ax[1].imshow(img>0)
    # Mark the center pixel in red if it doesn't have any gradients (should be the case␣
↪for standard autoregressive models)
    show_center = (img[img.shape[0]//2,img.shape[1]//2] == 0)
    if show_center:
        center_pixel = np.zeros(img.shape + (4,))
        center_pixel[center_pixel.shape[0]//2,center_pixel.shape[1]//2,:] = np.array([1.
↪0, 0.0, 0.0, 1.0])
    for i in range(2):
        ax[i].axis('off')
        if show_center:
            ax[i].imshow(center_pixel)
    ax[0].set_title("Weighted receptive field")
    ax[1].set_title("Binary receptive field")
    plt.show()
    plt.close()

show_center_recep_field(inp_img, lambda x: x)
```



Let's first visualize the receptive field of a horizontal convolution without the center pixel. We use a small, arbitrary input image (11×11 pixels), and calculate the loss for the center pixel. For simplicity, we initialize all weights with 1 and the bias with 0, and use a single channel. This is sufficient for our visualization purposes.

[8]:
```
horiz_conv = HorizontalStackConvolution(c_out=1, kernel_size=3, mask_center=True)
# Create parameters with kernel filled with 1, and bias filled with zeros.
# As alternative, one could overwrite kernel init of
init_params = lambda params: jax.tree_map(lambda x: jnp.full(x.shape, (0 if len(x.shape)␣
↪== 1 else 1), dtype=x.dtype), params)
horiz_params = horiz_conv.init(random.PRNGKey(0), inp_img)
```

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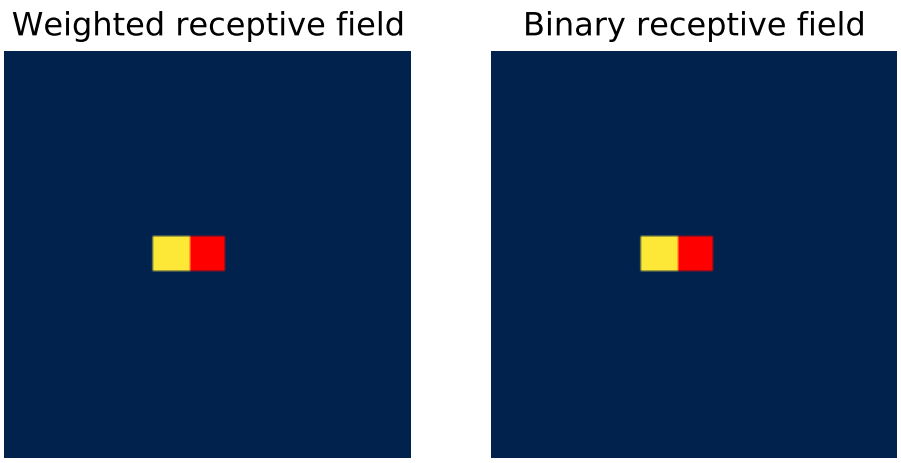
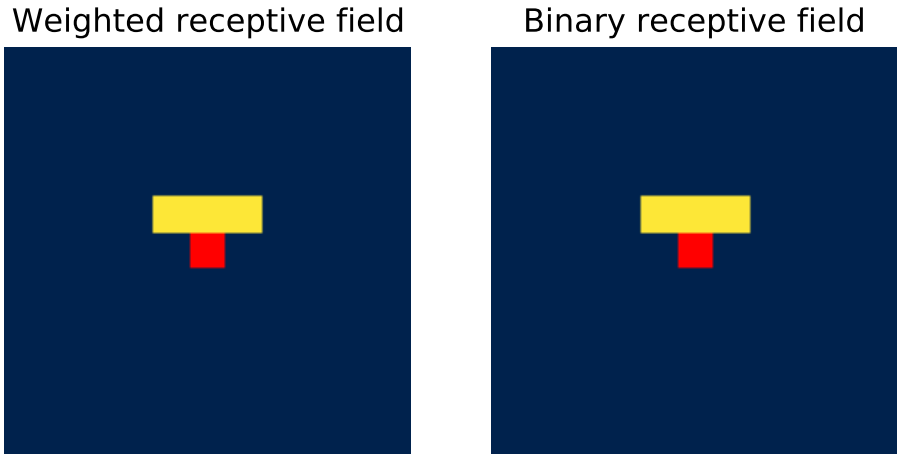
```
horiz_params = init_params(horiz_params)
# Apply horizontal convolution
horiz_conv = horiz_conv.bind(horiz_params)
show_center_recep_field(inp_img, lambda inp: horiz_conv(inp))
```



The receptive field is shown in yellow, the center pixel in red, and all other pixels outside of the receptive field are dark blue. As expected, the receptive field of a single horizontal convolution with the center pixel masked and a 3×3 kernel is only the pixel on the left. If we use a larger kernel size, more pixels would be taken into account on the left.

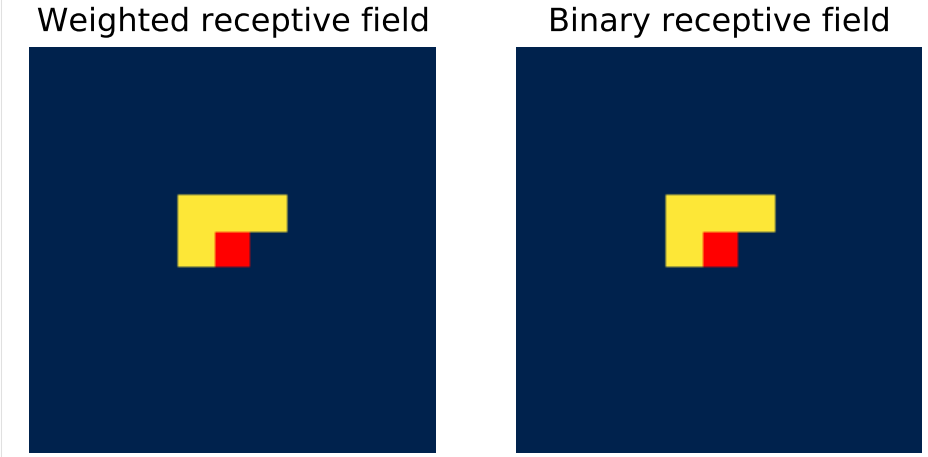
Next, let's take a look at the vertical convolution:

[9]:
```
vert_conv = VerticalStackConvolution(c_out=1, kernel_size=3, mask_center=True)
vert_params = vert_conv.init(random.PRNGKey(0), inp_img)
vert_params = init_params(vert_params)
vert_conv = vert_conv.bind(vert_params)
show_center_recep_field(inp_img, lambda inp: vert_conv(inp))
```



The vertical convolution takes all pixels above into account. Combining these two, we get the L-shaped receptive field of the original masked convolution:

[10]:
```
show_center_recep_field(inp_img, lambda inp: vert_conv(inp) + horiz_conv(inp))
```



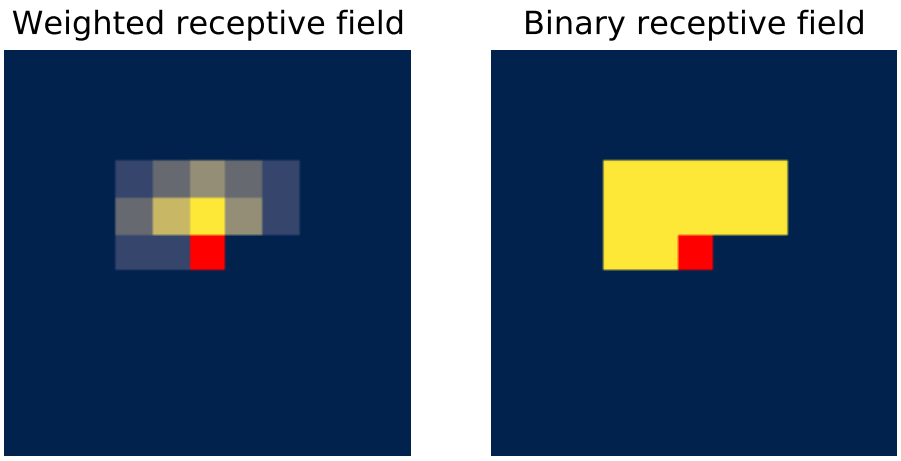
If we stack multiple horizontal and vertical convolutions, we need to take two aspects into account:

1. The center should not be masked anymore for the following convolutions as the features at the pixel's position are already independent of its actual value. If it is hard to imagine why we can do this, just change the value below to `mask_center=True` and see what happens.
2. The vertical convolution is not allowed to work on features from the horizontal convolution. In the feature map of the horizontal convolutions, a pixel contains information about all of the "true" pixels on the left. If we apply a vertical convolution which also uses features from the right, we effectively expand our receptive field to the true input which we want to prevent. Thus, the feature maps can only be merged for the horizontal convolution.

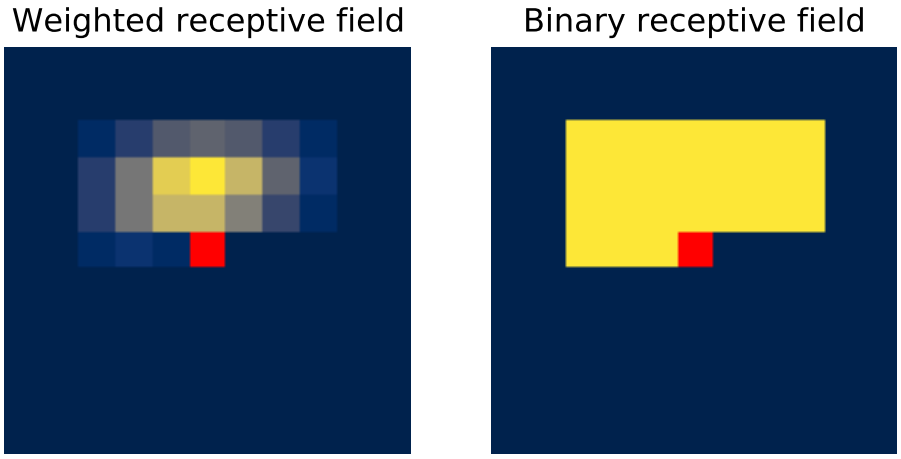
Using this, we can stack the convolutions in the following way. We have two feature streams: one for the vertical stack, and one for the horizontal stack. The horizontal convolutions can operate on the joint features of the previous horizontals and vertical convolutions, while the vertical stack only takes its own previous features as input. For a quick implementation, we can therefore sum the horizontal and vertical output features at each layer, and use those as final output features to calculate the loss on. An implementation of up to 4 consecutive layers is shown below. Note that we reuse the features from the other convolutions with `mask_center=True` from above.

[11]:
```
# Convolutions with mask_center=False, no need for new parameters since
horiz_noc_conv = HorizontalStackConvolution(c_out=1, kernel_size=3, mask_center=False)
vert_noc_conv = VerticalStackConvolution(c_out=1, kernel_size=3, mask_center=False)
horiz_noc_conv = horiz_noc_conv.bind(horiz_params)
vert_noc_conv = vert_noc_conv.bind(vert_params)

# We reuse our convolutions for the several layers with same parameters just for␣
↪visualization.
def num_layer_network(inp, num_layers):
    vert_img = vert_conv(inp)
    horiz_img = horiz_conv(inp) + vert_img
    for _ in range(num_layers-1):
        vert_img = vert_noc_conv(vert_img)
        horiz_img = horiz_noc_conv(horiz_img) + vert_img
    return horiz_img, vert_img

for layer_count in range(2, 6):
    print(f"Layer {layer_count}")
    show_center_recep_field(inp_img, lambda inp: num_layer_network(inp, layer_count)[0])
```

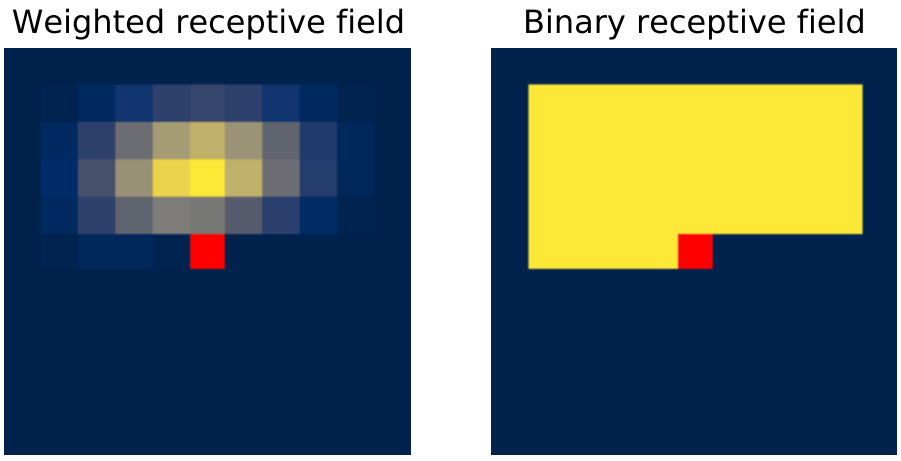
```
Layer 2
```



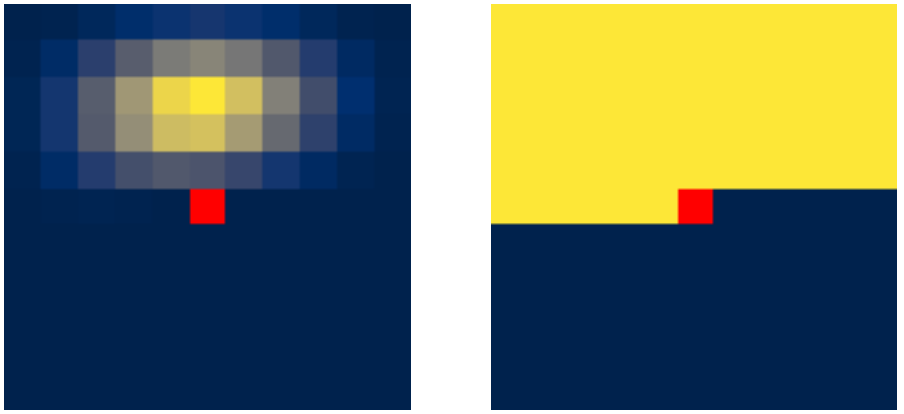

```
Layer 3
```




```
Layer 4
```



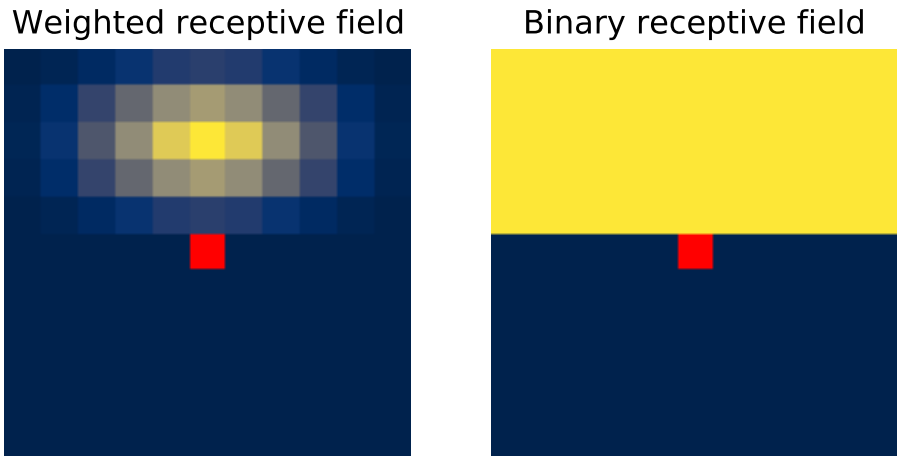

```
Layer 5
```



The receptive field above it visualized for the horizontal stack, which includes the features of the vertical convolutions. It grows over layers without any blind spot as we had before. The difference between "weighted" and "binary" receptive field is that for the latter, we check whether there are any gradients flowing back to this pixel. This indicates that the center pixel indeed can use information from this pixel. Nevertheless, due to the convolution weights, some pixels have a stronger effect on the prediction than others. This is visualized in the weighted receptive field by plotting the gradient magnitude for each pixel instead of a binary yes/no.

Another receptive field we can check is the one for the vertical stack as the one above is for the horizontal stack. Let's visualize it below:

[12]:
```
show_center_recep_field(inp_img, lambda inp: num_layer_network(inp, 5)[1])
```



As we have discussed before, the vertical stack only looks at pixels above the one we want to predict. Hence, we can validate that our implementation works as we initially expected it to.

4.38.2 Gated PixelCNN

In the next step, we will use the masked convolutions to build a full autoregressive model, called Gated PixelCNN. The difference between the original PixelCNN and Gated PixelCNN is the use of separate horizontal and vertical stacks. However, in literature, you often see that people refer to the Gated PixelCNN simply as "PixelCNN". Hence, in the following, if we say "PixelCNN", we usually mean the gated version. What "Gated" refers to in the model name is explained next.

Gated Convolutions

For visualizing the receptive field, we assumed a very simplified stack of vertical and horizontal convolutions. Obviously, there are more sophisticated ways of doing it, and PixelCNN uses gated convolutions for this. Specifically, the Gated Convolution block in PixelCNN looks as follows (figure credit - Aaron van den Oord et al.):

The left path is the vertical stack (the $N \times N$ convolution is masked correspondingly), and the right path is the horizontal stack. Gated convolutions are implemented by having a twice as large output channel size, and combine them by a element-wise multiplication of $\tanh$ and a sigmoid. For a linear layer, we can express a gated activation unit as follows:

$$\mathbf{y} = \tanh\left(\mathbf{W}_f \mathbf{x}\right) \odot \sigma\left(\mathbf{W}_g \mathbf{x}\right)$$

For simplicity, biases have been neglected and the linear layer split into two part, $\mathbf{W}_f$ and $\mathbf{W}_g$. This concept resembles the input and modulation gate in an LSTM, and has been used in many other architectures as well. The main motivation behind this gated activation is that it might allow to model more complex interactions and simplifies learning. But as in any other architecture, this is mostly a design choice and can be considered a hyperparameters.

Besides the gated convolutions, we also see that the horizontal stack uses a residual connection while the vertical stack does not. This is because we use the output of the horizontal stack for prediction. Each convolution in the vertical stack also receives a strong gradient signal as it is only two 1×1 convolutions away from the residual connection, and does not require another residual connection to all its earleri layers.

The implementation in Flax is fairly straight forward for this block, because the visualization above gives us a computation graph to follow:

[13]:
```
class GatedMaskedConv(nn.Module):
    dilation : int = 1

    @nn.compact
    def __call__(self, v_stack, h_stack):
        c_in = v_stack.shape[-1]

        # Layers (depend on input shape)
        conv_vert = VerticalStackConvolution(c_out=2*c_in,
                                             kernel_size=3,
                                             mask_center=False,
                                             dilation=self.dilation)
        conv_horiz = HorizontalStackConvolution(c_out=2*c_in,
                                                kernel_size=3,
                                                mask_center=False,
                                                dilation=self.dilation)
        conv_vert_to_horiz = nn.Conv(2*c_in,
                                     kernel_size=(1, 1))
        conv_horiz_1x1 = nn.Conv(c_in,
```

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```
                                    kernel_size=(1, 1))

        # Vertical stack (left)
        v_stack_feat = conv_vert(v_stack)
        v_val, v_gate = v_stack_feat.split(2, axis=-1)
        v_stack_out = nn.tanh(v_val) * nn.sigmoid(v_gate)

        # Horizontal stack (right)
        h_stack_feat = conv_horiz(h_stack)
        h_stack_feat = h_stack_feat + conv_vert_to_horiz(v_stack_feat)
        h_val, h_gate = h_stack_feat.split(2, axis=-1)
        h_stack_feat = nn.tanh(h_val) * nn.sigmoid(h_gate)
        h_stack_out = conv_horiz_1x1(h_stack_feat)
        h_stack_out = h_stack_out + h_stack

        return v_stack_out, h_stack_out
```

Building the model

Using the gated convolutions, we can now build our PixelCNN model. The architecture consists of multiple stacked GatedMaskedConv blocks, where we add an additional dilation factor to a few convolutions. This is used to increase the receptive field of the model and allows to take a larger context into accout during generation. As a reminder, dilation on a convolution works looks as follows (figure credit - Vincent Dumoulin and Francesco Visin):

Note that the smaller output size is only because the animation assumes no padding. In our implementation, we will pad the input image correspondingly. Alternatively to dilated convolutions, we could downsample the input and use a encoder-decoder architecture as in PixelCNN++ [3]. This is especially beneficial if we want to build a very deep autoregressive model. Nonetheless, as we seek to train a reasonably small model, dilated convolutions are the more efficient option to use here.

Below, we implement the PixelCNN model as a Flax module. Besides the stack of gated convolutions, we also have the initial horizontal and vertical convolutions which mask the center pixel, and a final 1×1 convolution which maps the output features to class predictions. To determine the likelihood of a batch of images, we first create our initial features using the masked horizontal and vertical input convolution. Next, we forward the features through the stack of gated convolutions. Finally, we take the output features of the horizontal stack, and apply the 1×1 convolution for classification. We use the bits per dimension metric for the likelihood, similarly to Tutorial 11.

[14]:
```
class PixelCNN(nn.Module):
    c_in : int
    c_hidden : int

    def setup(self):
        # Initial convolutions skipping the center pixel
        self.conv_vstack = VerticalStackConvolution(self.c_hidden, kernel_size=3, mask_
↪center=True)
        self.conv_hstack = HorizontalStackConvolution(self.c_hidden, kernel_size=3, mask_
↪center=True)
        # Convolution block of PixelCNN. We use dilation instead of downscaling
        self.conv_layers = [
            GatedMaskedConv(),
```

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```
            GatedMaskedConv(dilation=2),
            GatedMaskedConv(),
            GatedMaskedConv(dilation=4),
            GatedMaskedConv(),
            GatedMaskedConv(dilation=2),
            GatedMaskedConv()
        ]
        # Output classification convolution (1x1)
        self.conv_out = nn.Conv(self.c_in * 256, kernel_size=(1, 1))

    def __call__(self, x):
        # Forward pass with bpd likelihood calculation
        logits = self.pred_logits(x)
        labels = x.astype(jnp.int32)
        nll = optax.softmax_cross_entropy_with_integer_labels(logits, labels)
        bpd = nll.mean() * np.log2(np.exp(1))
        return bpd

    def pred_logits(self, x):
        """
        Forward image through model and return logits for each pixel.
        Inputs:
            x - Image tensor with integer values between 0 and 255.
        """
        # Scale input from 0 to 255 back to -1 to 1
        x = (x.astype(jnp.float32) / 255.0) * 2 - 1

        # Initial convolutions
        v_stack = self.conv_vstack(x)
        h_stack = self.conv_hstack(x)
        # Gated Convolutions
        for layer in self.conv_layers:
            v_stack, h_stack = layer(v_stack, h_stack)
        # 1x1 classification convolution
        # Apply ELU before 1x1 convolution for non-linearity on residual connection
        out = self.conv_out(nn.elu(h_stack))

        # Output dimensions: [Batch, Height, Width, Channels, Classes]
        out = out.reshape(out.shape[0], out.shape[1], out.shape[2], out.shape[3]//256,␣
↪256)
        return out

    def sample(self, img_shape, rng, img=None):
        """
        Sampling function for the autoregressive model.
        Inputs:
            img_shape - Shape of the image to generate (B,C,H,W)
            img (optional) - If given, this tensor will be used as
                             a starting image. The pixels to fill
                             should be -1 in the input tensor.
        """
        # Create empty image
```

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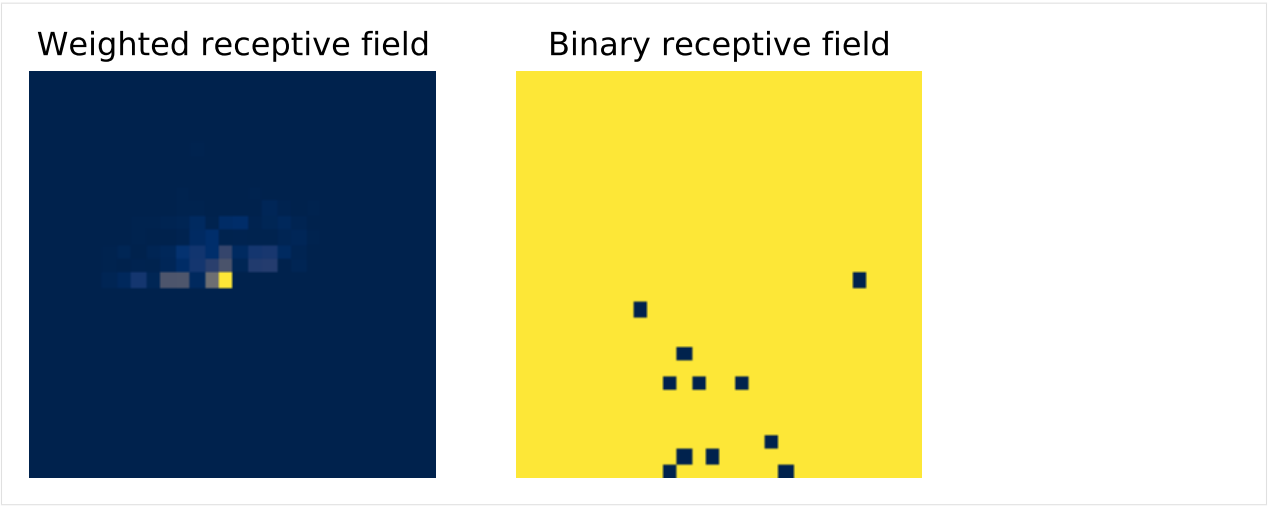
```
        if img is None:
            img = jnp.zeros(img_shape, dtype=jnp.int32) - 1
        # We jit a prediction step. One could jit the whole loop, but this
        # is expensive to compile and only worth for a lot of sampling calls.
        get_logits = jax.jit(lambda inp: self.pred_logits(inp))
        # Generation loop
        for h in tqdm(range(img_shape[1]), leave=False):
            for w in range(img_shape[2]):
                for c in range(img_shape[3]):
                    # Skip if not to be filled (-1)
                    if (img[:,h,w,c] != -1).all().item():
                        continue
                    # For efficiency, we only have to input the upper part of the image
                    # as all other parts will be skipped by the masked convolutions␣
↪anyways
                    logits = get_logits(img)
                    logits = logits[:,h,w,c,:]
                    rng, pix_rng = random.split(rng)
                    img = img.at[:,h,w,c].set(random.categorical(pix_rng, logits, axis=-
↪1))
        return img
```

To sample from the autoregressive model, we need to iterate over all dimensions of the input. We start with an empty image, and fill the pixels one by one, starting from the upper left corner. Note that as for predicting x_i, all pixels below it have no influence on the prediction. Hence, we can cut the image in height without changing the prediction while increasing efficiency. Nevertheless, all the loops in the sampling function already show that it will take us quite some time to sample. A lot of computation could be reused across loop iterations as those the features on the already predicted pixels will not change over iterations. Nevertheless, this takes quite some effort to implement, and is often not done in implementations because in the end, autoregressive sampling remains sequential and slow. Hence, we settle with the default implementation here.

Before training the model, we can check the full receptive field of the model on an MNIST image of size 28×28:

[15]:
```
model = PixelCNN(c_in=1, c_hidden=64)
# inp = random.randint(random.PRNGKey(1), (1,28,28,1), 0, 255).astype(jnp.float32)
inp = jnp.zeros((1,28,28,1))
params = model.init(random.PRNGKey(0), inp)
show_center_recep_field(inp, lambda x: model.bind(params).pred_logits(x)[...,0,0])
```



Wait, the receptive field for a single pixel is suddenly the whole image?! Did we make a mistake in our implementation? Unlikely. As it turns out, masked convolutions in Flax show a behavior that leaks gradients through the input mask for larger channel numbers. Note that these gradients for the masked elements is often smaller by a factor of 10^{-6}. What about the gradients for the parameters? Let's check:

[16]:
```
grads = jax.grad(lambda p: model.apply(p, inp))(params)
# Gradients of the weights in the first h-stack convolution
# for the first feature map:
grads['params']['conv_hstack']['conv']['Conv_0']['kernel'][:,:,:,0]
```

[16]:
```
DeviceArray([[[0.10623012],
              [0.        ],
              [0.        ]]], dtype=float32)
```

The last two entries indicate the gradients for the center and right pixel of the initial horizontal stack convolution. The gradients are zero, as we expected. So, the gradients for the weights are correct, only the gradients propagating through the feature layers has minor noise that we unintended. Nonetheless, this should be good enough for training.

Note: If you know the details behind why the gradients leak through the mask, I would appreciate any hint on the corresponding GitHub disccusion on Flax.

Despite a large receptive field, keep in mind that this is the "theoretical" receptive field and not necessarily the effective receptive field, which is usually much smaller. For a stronger model, we should therefore try to increase the receptive field even further. Especially, for the pixel on the bottom right, the very last pixel, we would be allowed to take into account the whole image. However, our current receptive field only spans across 1/4 of the image. An encoder-decoder architecture can help with this, but it also shows that we require a much deeper, more complex network in autoregressive models than in VAEs or energy-based models.

Training loop

To train the model, we again can rely on building ourselves a small trainer module that gives us a full training loop, including loading and saving the model.

[17]:
```
class TrainerModule:

    def __init__(self,
                 c_in : int,
                 c_hidden : int,
                 exmp_imgs : Any,
                 lr : float = 1e-3,
                 seed : int = 42):
        """
        Module for summarizing all training functionalities for the PixelCNN.
        """
        super().__init__()
        self.lr = lr
        self.seed = seed
        self.model_name = 'PixelCNN'
        # Create empty model. Note: no parameters yet
        self.model = PixelCNN(c_in=c_in, c_hidden=c_hidden)
        # Prepare logging
        self.log_dir = os.path.join(CHECKPOINT_PATH, self.model_name)
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model(exmp_imgs)

    def create_functions(self):
        # Training function
        def train_step(state, batch):
            imgs, _ = batch
            loss_fn = lambda params: state.apply_fn(params, imgs)
            loss, grads = jax.value_and_grad(loss_fn)(state.params)
            state = state.apply_gradients(grads=grads)
            return state, loss
        # Eval function
        def eval_step(state, batch):
            imgs, _ = batch
            loss = state.apply_fn(state.params, imgs)
            return loss
        # jit for efficiency
        self.train_step = jax.jit(train_step)
        self.eval_step = jax.jit(eval_step)

    def init_model(self, exmp_imgs):
        # Initialize model
        init_rng = random.PRNGKey(self.seed)
        params = self.model.init(init_rng, exmp_imgs)
        self.state = train_state.TrainState(step=0,
                                            apply_fn=self.model.apply,
```

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```
                                          params=params,
                                          tx=None,
                                          opt_state=None)

    def init_optimizer(self, num_epochs, num_steps_per_epoch):
        # Initialize learning rate schedule and optimizer
        lr_schedule = optax.exponential_decay(
            init_value=self.lr,
            transition_steps=num_steps_per_epoch,
            decay_rate=0.99
        )
        optimizer = optax.adam(lr_schedule)
        # Initialize training state
        self.state = train_state.TrainState.create(apply_fn=self.state.apply_fn,
                                                   params=self.state.params,
                                                   tx=optimizer)

    def train_model(self, train_loader, val_loader, num_epochs=200):
        # Train model for defined number of epochs
        # We first need to create optimizer and the scheduler for the given number of␣
↪epochs
        self.init_optimizer(num_epochs, len(train_loader))
        # Track best eval bpd score.
        best_eval = 1e6
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(train_loader, epoch=epoch_idx)
            if epoch_idx % 1 == 0:
                eval_bpd = self.eval_model(val_loader)
                self.logger.add_scalar('val/bpd', eval_bpd, global_step=epoch_idx)
                if eval_bpd <= best_eval:
                    best_eval = eval_bpd
                    self.save_model(step=epoch_idx)
            self.logger.flush()

    def train_epoch(self, train_loader, epoch):
        # Train model for one epoch, and log avg bpd
        avg_loss = 0
        for batch in tqdm(train_loader, desc='Training', leave=False):
            self.state, loss = self.train_step(self.state, batch)
            avg_loss += loss
        avg_loss /= len(train_loader)
        self.logger.add_scalar('train/bpd', avg_loss.item(), global_step=epoch)

    def eval_model(self, data_loader):
        # Test model on all images of a data loader and return avg bpd
        avg_bpd, count = 0, 0
        for batch in data_loader:
            bpd = self.eval_step(self.state, batch)
            avg_bpd += bpd * batch[0].shape[0]
            count += batch[0].shape[0]
        eval_bpd = (avg_bpd / count).item()
        return eval_bpd
```

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```
    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir,
                                    target=self.state.params,
                                    step=step,
                                    overwrite=True)

    def load_model(self, pretrained=False):
        # Load model. We use different checkpoint for pretrained models
        if not pretrained:
            state_dict = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir,␣
↪target=None)
        else:
            state_dict = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'{self.model_name}.ckpt'), target=None)
        self.state = train_state.TrainState.create(apply_fn=self.state.apply_fn,
                                                   params=state_dict,
                                                   tx=self.state.tx if self.state.tx␣
↪else optax.sgd(0.1)   # Default optimizer
                                                  )

    def checkpoint_exists(self):
        # Check whether a pretrained model exist for this autoencoder
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'{self.model_name}.ckpt'))
```

Finally, let's write a training function that loads the pretrained model if it exists.

[18]:
```
def train_model(max_epochs=150, **model_args):
    # Create a trainer module with specified hyperparameters
    trainer = TrainerModule(exmp_imgs=next(iter(train_loader))[0],
                            **model_args)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(train_loader, val_loader, num_epochs=max_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    val_bpd = trainer.eval_model(val_loader)
    test_bpd = trainer.eval_model(test_loader)
    # Bind parameters to model for easier inference
    trainer.model_bd = trainer.model.bind(trainer.state.params)
    return trainer, {'val_bpd': val_bpd, 'test_bpd': test_bpd}
```

Training the model is time consuming and we recommend using the provided pre-trained model for going through this notebook. However, feel free to play around with the hyperparameter like number of layers etc. if you want to get a feeling for those.

When calling the training function with a pre-trained model, we automatically load it and print its test performance:

[19]:
```
trainer, result = train_model(max_epochs=150, c_in=1, c_hidden=64)
print(f'Test bpd: {result["test_bpd"]:4.3f}')
```

```
Test bpd: 0.820
```

With a test performance of 0.820bpd, the PixelCNN significantly outperforms the normalizing flows we have seen in Tutorial 11. Considering image modeling as an autoregressive problem simplifies the learning process as predicting one pixel given the ground truth of all others is much easier than predicting all pixels at once. In addition, PixelCNN can explicitly predict the pixel values by a discrete softmax while Normalizing Flows have to learn transformations in continuous latent space. These two aspects allow the PixelCNN to achieve a notably better performance.

To fully compare the models, let's also measure the number of parameters of the PixelCNN:

[20]:
```
num_params = sum([np.prod(p.shape) for p in jax.tree_leaves(trainer.state.params)])
print("Number of parameters: {:,}".format(num_params))
```

```
Number of parameters: 852,160
```

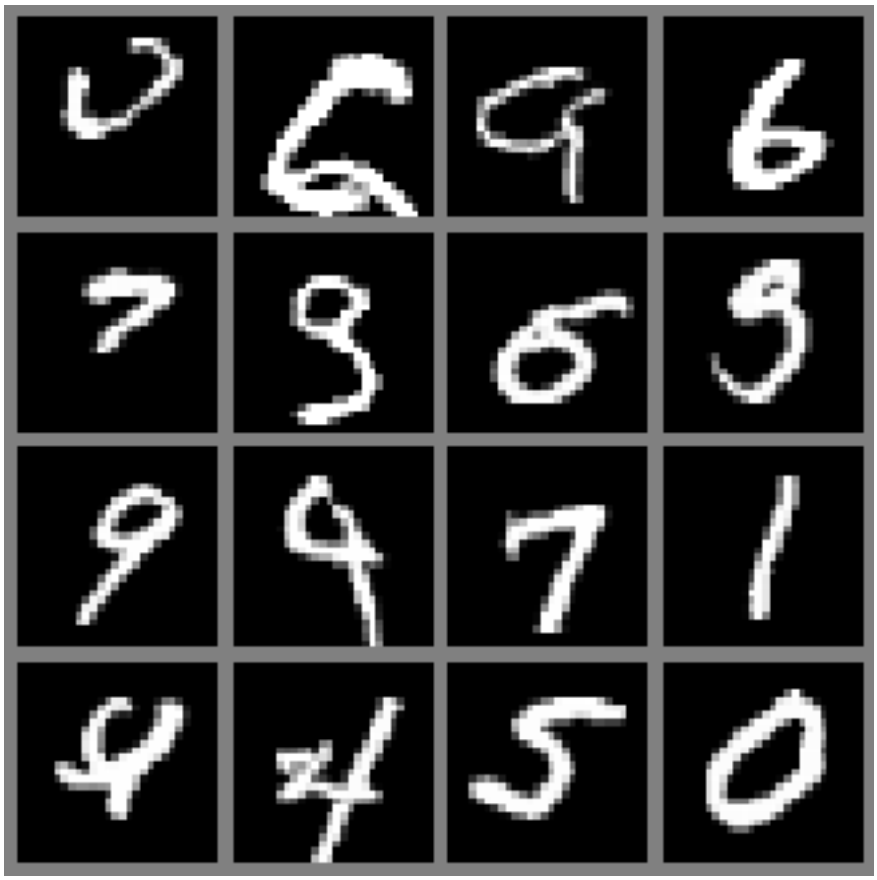
Compared to the multi-scale normalizing flows, the PixelCNN has considerably less parameters. Of course, the number of parameters depend on our hyperparameter choices. Nevertheless, in general, it can be said that autoregressive models require considerably less parameters than normalizing flows to reach good performance, based on the reasons stated above. Still, autoregressive models are much slower in sampling than normalizing flows, which limits their possible applications.

4.38.3 Sampling

One way of qualitatively analysing generative models is by looking at the actual samples. Let's therefore use our sampling function to generate a few digits:

[21]:
```
samples = trainer.model_bd.sample(img_shape=(16,28,28,1), rng=random.PRNGKey(0))
show_imgs(samples)
```

```
  0%|          | 0/28 [00:00<?, ?it/s]
```



Most of the samples can be identified as digits, and overall we achieve a better quality than we had in normalizing flows. This goes along with the lower likelihood we achieved with autoregressive models. Nevertheless, we also see that there is still place for improvement as a considerable amount of samples cannot be identified (for example the first row). Deeper autoregressive models are expected to achieve better quality, as they can take more context into account for generating the pixels.

The trained model itself is not restricted to any specific image size. However, what happens if we actually sample a larger image than we had seen in our training dataset? Let's try below to sample images of size 64×64 instead of 28×28:

[22]:
```
samples = trainer.model_bd.sample(img_shape=(8,64,64,1), rng=random.PRNGKey(0))
show_imgs(samples)
```

```
  0%|          | 0/64 [00:00<?, ?it/s]
```

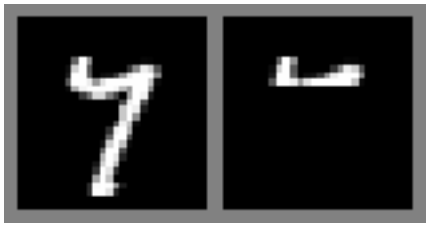
The larger images show that changing the size of the image during testing confuses the model and generates abstract figures (you can sometimes spot a digit in the upper left corner). In addition, sampling for images of 64x64 pixels take up to a minute on a GPU. Clearly, autoregressive models cannot be scaled to large images without changing the sampling procedure such as with forecasting. Our implementation is also not the most efficient as many computations can be stored and reused throughout the sampling process. Nevertheless, the sampling procedure stays sequential which is inherently slower than parallel generation like done in normalizing flows.

Autocompletion

One common application done with autoregressive models is auto-completing an image. As autoregressive models predict pixels one by one, we can set the first N pixels to predefined values and check how the model completes the image. For implementing this, we just need to skip the iterations in the sampling loop that already have a value unequals -1. See above in our Flax module for the specific implementation. In the cell below, we randomly take three images from the training set, mask about the lower half of the image, and let the model autocomplete it. To see the diversity of samples, we do this 12 times for each image:

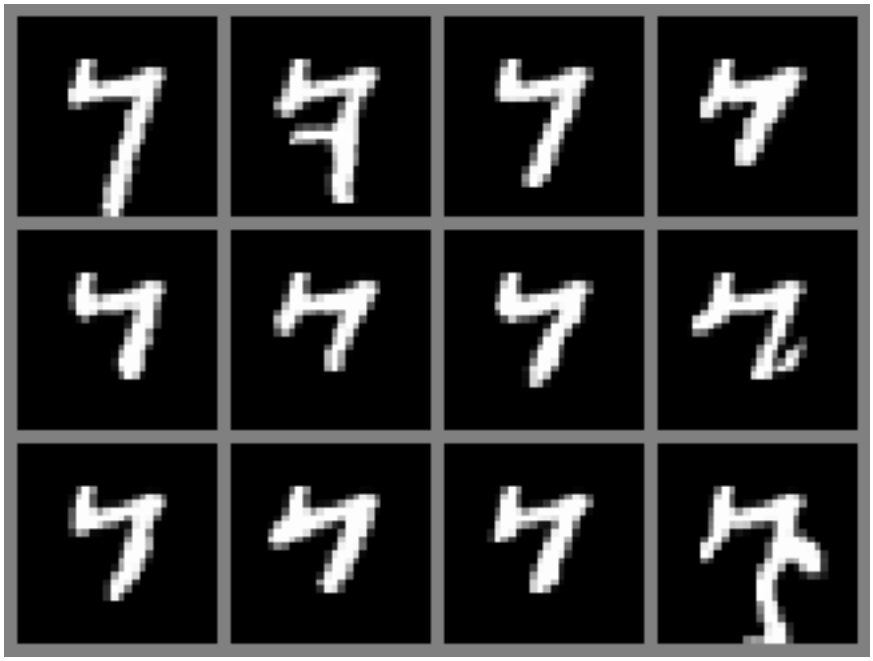
[23]:
```
def autocomplete_image(img):
    # Remove lower half of the image
    img_init = np.copy(img)
    img_init[10:] = -1
    print("Original image and input image to sampling:")
    show_imgs([img,img_init])
    # Generate 12 example completions
    img_init = np.repeat(img_init[None], 12, axis=0)
    img_init = jax.device_put(img_init)
    img_generated = trainer.model_bd.sample(img_init.shape,
                                            rng=random.PRNGKey(42),
                                            img=img_init)
    print("Autocompletion samples:")
    show_imgs(img_generated)

for i in range(1,4):
    img = train_set[i][0]
    autocomplete_image(img)
```

```
Original image and input image to sampling:
```



```
  0%|          | 0/28 [00:00<?, ?it/s]
```

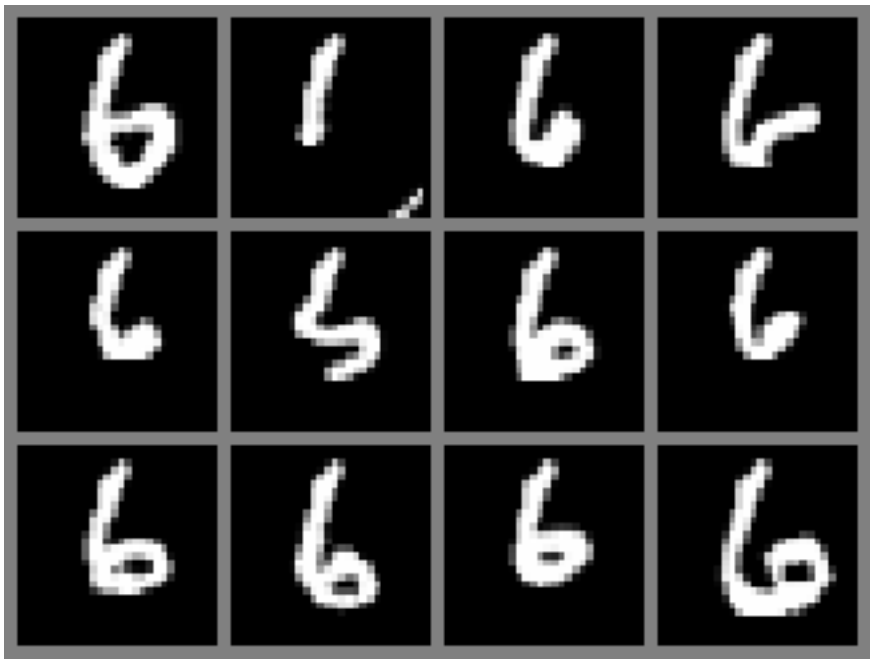
```
Autocompletion samples:
```



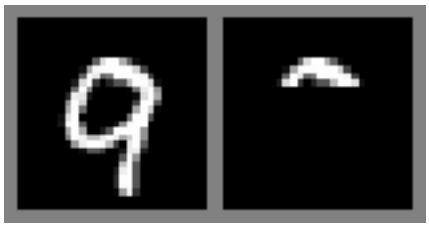
```
Original image and input image to sampling:
```

```
  0%|          | 0/28 [00:00<?, ?it/s]
```

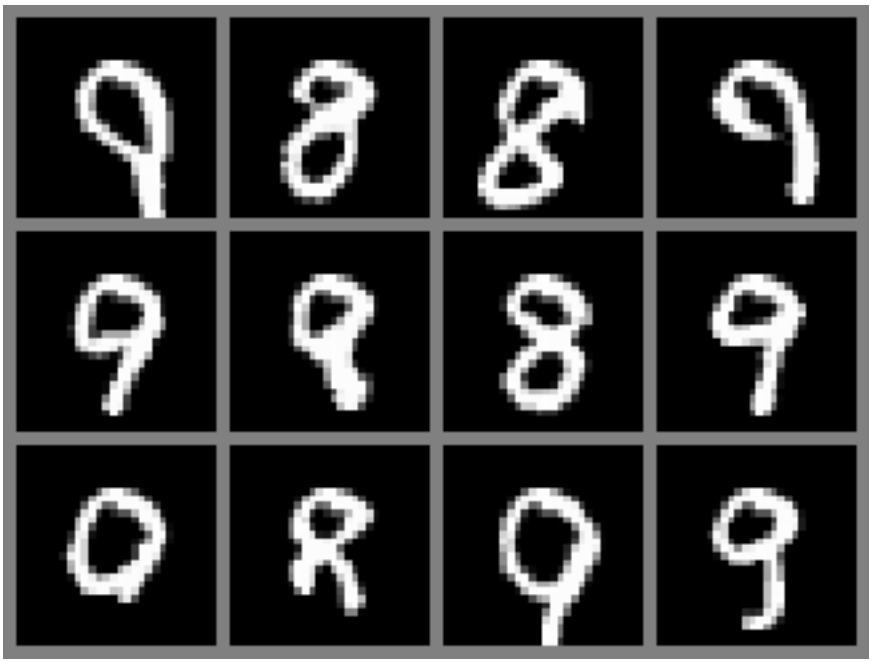
```
Autocompletion samples:
```



```
Original image and input image to sampling:
```



```
  0%|          | 0/28 [00:00<?, ?it/s]
Autocompletion samples:
```



For the first two digits (7 and 6), we see that the 12 samples all result in a shape which resemble the original digit. Nevertheless, there are some style difference in writing the 7, and some deformed sixes in the samples. When auto-completing the 9 below, we see that the model can fit multiple digits to it. We obtain diverse samples from 0, 8 and 9. This shows that despite having no latent space, we can still obtain diverse samples from an autoregressive model.

Visualization of the predictive distribution (softmax)

Autoregressive models use a softmax over 256 values to predict the next pixel. This gives the model a large flexibility as the probabilities for each pixel value can be learned independently if necessary. However, the values are actually not independent because the values 32 and 33 are much closer than 32 and 255. In the following, we visualize the softmax distribution that the model predicts to gain insights how it has learned the relationships of close-by pixels.

To do this, we first run the model on a batch of images and store the output softmax distributions:

[24]:
```
det_loader = data.DataLoader(train_set, batch_size=128, shuffle=False, drop_last=False,␣
↪collate_fn=numpy_collate)
imgs,_ = next(iter(det_loader))

out = trainer.model_bd.pred_logits(imgs)
out = nn.softmax(out, axis=-1)
mean_out = jax.device_get(out.mean(axis=[0,1,2,3]))
out = jax.device_get(out)
```

Before diving into the model, let's visualize the distribution of the pixel values in the whole dataset:

[25]:
```
sns.set()
plot_args = {"color": to_rgb("C0")+(0.5,), "edgecolor": "C0", "linewidth": 0.5, "width":␣
↪1.0}
plt.hist(imgs.reshape(-1), bins=256, density=True, **plot_args)
plt.yscale("log")
```

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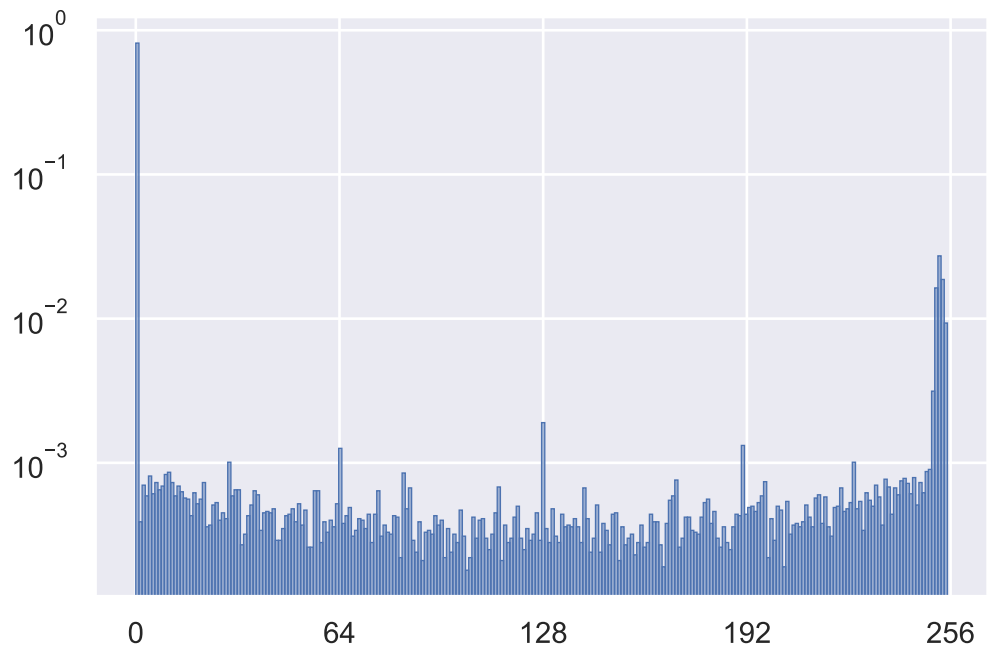
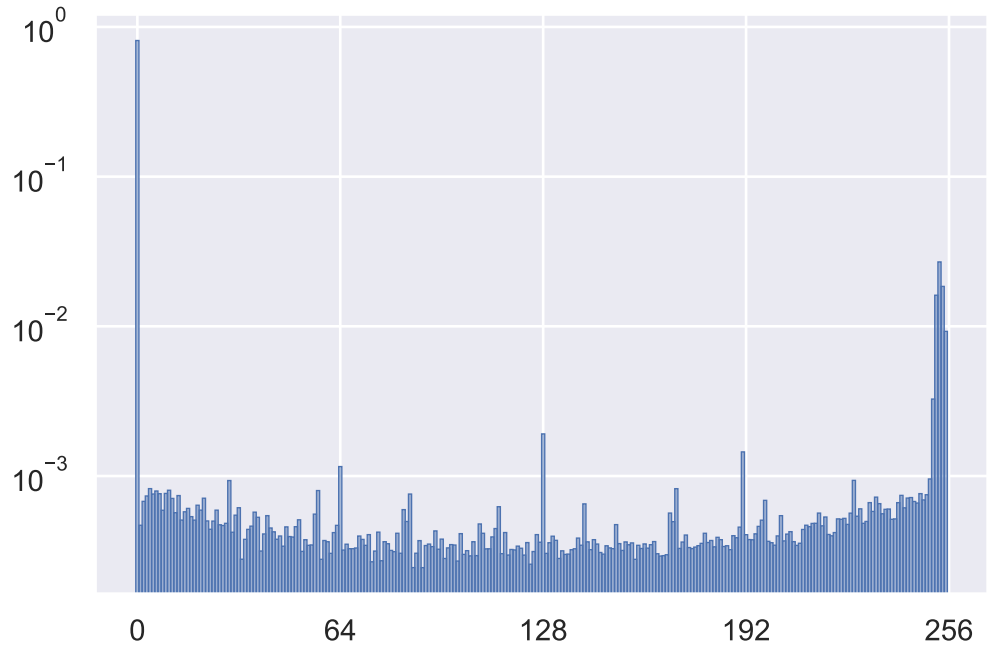
```
plt.xticks([0,64,128,192,256])
plt.show()
plt.close()
```



As we would expect from the seen images, the pixel value 0 (black) is the dominant value, followed by a batch of values between 250 and 255. Note that we use a log scale on the y-axis due to the big imbalance in the dataset. Interestingly, the pixel values 64, 128 and 191 also stand out which is likely due to the quantization used during the creation of the dataset. For RGB images, we would also see two peaks around 0 and 255, but the values in between would be much more frequent than in MNIST (see Figure 1 in the PixelCNN++ for a visualization on CIFAR10).

Next, we can visualize the distribution our model predicts (in average):

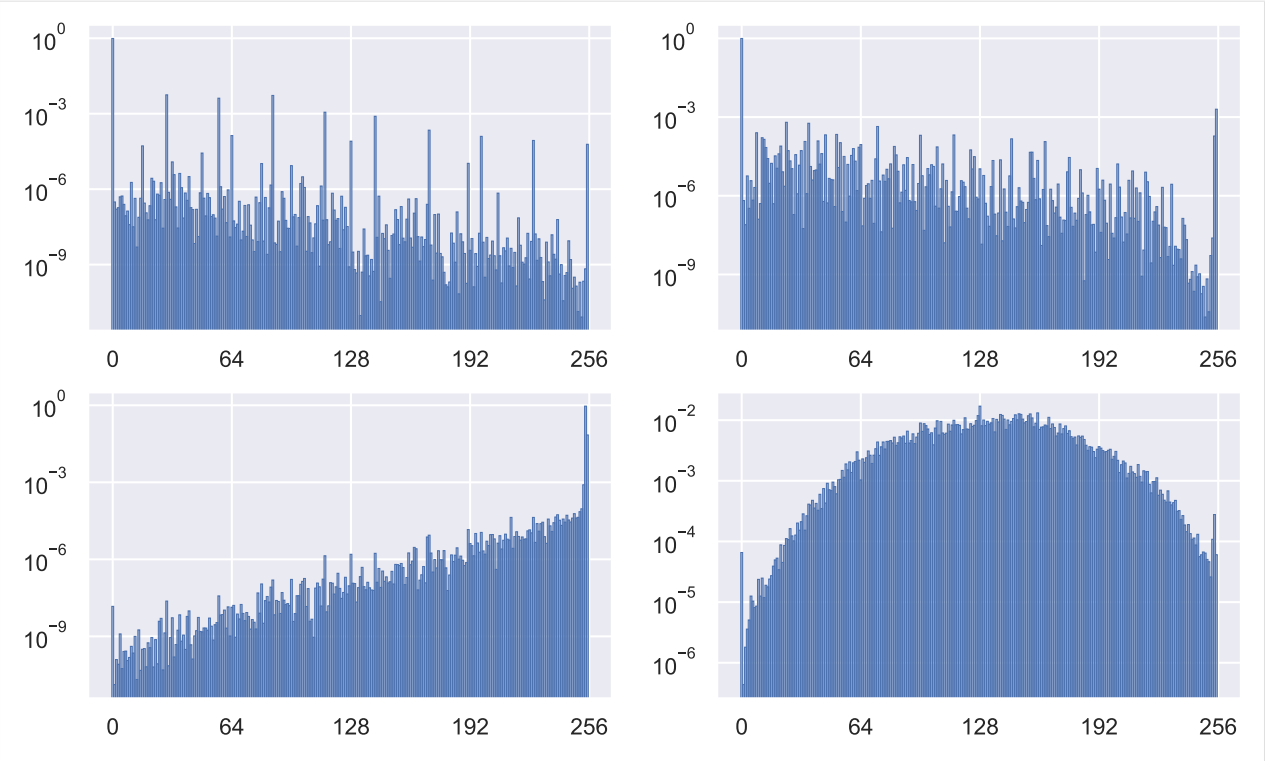
[26]:
```
plt.bar(np.arange(mean_out.shape[0]), mean_out, **plot_args)
plt.yscale("log")
plt.xticks([0,64,128,192,256])
plt.show()
plt.close()
```



This distribution is very close to the actual dataset distribution. This is in general a good sign, but we can see a slightly smoother histogram than above.

Finally, to take a closer look at learned value relations, we can visualize the distribution for individual pixel predictions to get a better intuition. For this, we pick 4 random images and pixels, and visualize their distribution below:

[27]:
```
fig, ax = plt.subplots(2,2, figsize=(10,6))
for i in range(4):
    ax_sub = ax[i//2][i%2]
    ax_sub.bar(np.arange(out.shape[-1], dtype=np.int32), out[i+4,14,14,0], **plot_args)
    ax_sub.set_yscale("log")
    ax_sub.set_xticks([0,64,128,192,256])
plt.show()
plt.close()
```



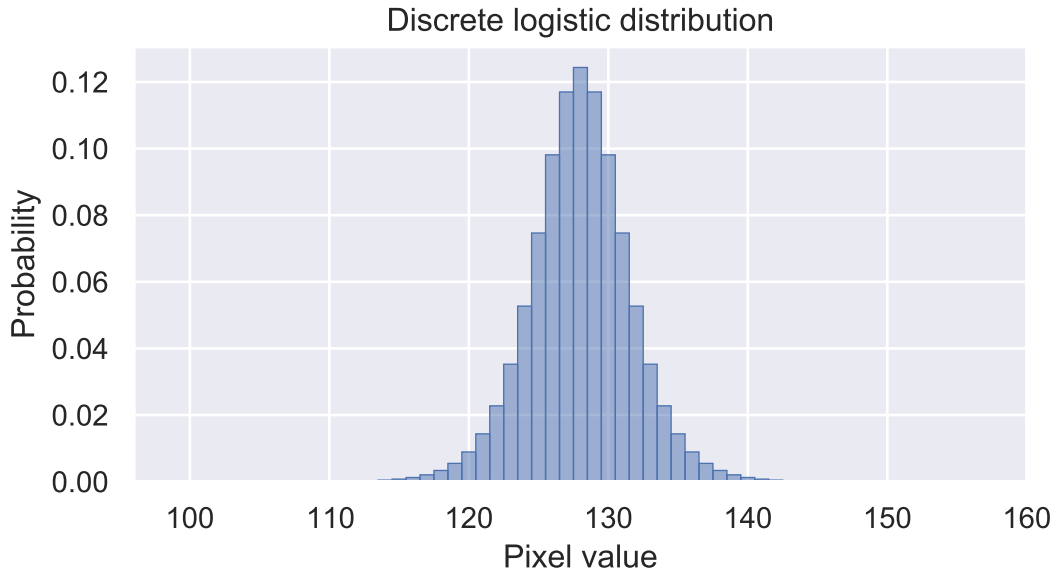
Overall we see a very diverse set of distributions, with a usual peak for 0 and close to 1. However, the distributions in the first row show a potentially undesirable behavior. For instance, the value 242 has a 1000x lower likelihood than 243 although they are extremely close and can often not be distinguished. This shows that the model might have not generlized well over pixel values. The better solution to this problem is to use discrete logitics mixtures instead of a softmax distribution. A discrete logistic distribution can be imagined as discretized, binned Gaussians. Using a mixture of discrete logistics instead of a softmax introduces an inductive bias to the model to assign close-by values similar likelihoods. We can visualize a discrete logistic below:

[28]:
```
mu = np.array([128])
sigma = np.array([2.0])

def discrete_logistic(x, mu, sigma):
    return nn.sigmoid((x+0.5-mu)/sigma) - nn.sigmoid((x-0.5-mu)/sigma)

x = np.arange(256)
p = discrete_logistic(x, mu, sigma)

# Visualization
plt.figure(figsize=(6,3))
plt.bar(x, p, **plot_args)
plt.xlim(96,160)
plt.title("Discrete logistic distribution")
plt.xlabel("Pixel value")
plt.ylabel("Probability")
plt.show()
plt.close()
```



Instead of the softmax, the model would output mean and standard deviations for the K logistics we use in the mixture. This is one of the improvements in autoregressive models that PixelCNN++ [3] has introduced compared to the original PixelCNN.

4.38.4 Conclusion

In this tutorial, we have looked at autoregressive image modeling, and implemented the PixelCNN architecture. With the usage of masked convolutions, we are able to apply a convolutional network in which a pixel is only influenced by all its predecessors. Separating the masked convolution into a horizontal and vertical stack allowed us to remove the known blind spot on the right upper row of a pixel. In experiments, autoregressive models outperformed normalizing flows in terms of bits per dimension, but are much slower to sample from. Improvements, that we have not implemented ourselves here, are discrete logistic mixtures, a downsampling architecture, and changing the pixel order in a diagonal fashion (see PixelSNAIL). Overall, autoregressive models are another, strong family of generative models, which however are mostly used in sequence tasks because of their linear scaling in sampling time than quadratic as on images.

4.38.5 References

[1] van den Oord, A., et al. "Pixel Recurrent Neural Networks." arXiv preprint arXiv:1601.06759 (2016). Link

[2] van den Oord, A., et al. "Conditional Image Generation with PixelCNN Decoders." In Advances in Neural Information Processing Systems 29, pp. 4790–4798 (2016). Link

[3] Salimans, Tim, et al. "PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications." arXiv preprint arXiv:1701.05517 (2017). Link

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If you found this tutorial helpful, consider -ing our repository.

For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.39 Tutorial 15 (JAX): Vision Transformers

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We note the training times for all models in the PyTorch and the JAX implementation below (PyTorch v1.11, JAX v0.3.13). The models were trained on the same hardware (NVIDIA RTX3090, 24 core CPU) and we slightly adjusted the tutorials to use the exact same training settings (200 epochs, data loading parameters, evaluation schedule, etc.). Overall, the JAX implementation is just slightly faster (1.1x) than PyTorch.

Models	PyTorch	JAX
Vision Transformer	28min 40sec	27min 10sec

In this tutorial, we will take a closer look at a recent new trend: Transformers for Computer Vision. Since Alexey Dosovitskiy et al. successfully applied a Transformer on a variety of image recognition benchmarks, there have been an incredible amount of follow-up works showing that CNNs might not be optimal architecture for Computer Vision anymore. But how do Vision Transformers work exactly, and what benefits and drawbacks do they offer in contrast to CNNs? We will answer these questions by implementing a Vision Transformer ourselves and train it on the popular, small dataset CIFAR10. We will compare these results to the convolutional architectures of Tutorial 5.

If you are not familiar with Transformers yet, take a look at Tutorial 6 where we discuss the fundamentals of Multi-Head Attention and Transformers. Let's start with importing our standard set of libraries.

[1]:
```
## Standard libraries
import os
import numpy as np
import math
import json
from functools import partial
from PIL import Image
from collections import defaultdict

## Imports for plotting
```

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```
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
from matplotlib.colors import to_rgb
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.reset_orig()

## tqdm for progress bars
from tqdm.auto import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch
import torch
import torch.utils.data as data
from torch.utils.tensorboard import SummaryWriter
import torchvision
from torchvision import transforms
from torchvision.datasets import CIFAR10

# Import tensorboard
%load_ext tensorboard
```

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```
# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial15_jax"

print("Device:", jax.devices()[0])
```

```
/tmp/ipykernel_2627394/2327484937.py:16: DeprecationWarning: `set_matplotlib_formats` is␣
↪deprecated since IPython 7.23, directly use `matplotlib_inline.backend_inline.set_
↪matplotlib_formats()`
  set_matplotlib_formats('svg', 'pdf') # For export
```

```
Device: gpu:0
```

We provide a pre-trained Vision Transformer which we download in the next cell. However, Vision Transformers can be relatively quickly trained on CIFAR10 with an overall training time of less than an hour on an NVIDIA TitanRTX. Feel free to experiment with training your own Transformer once you went through the whole notebook.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/"
# Files to download
pretrained_files = ["tutorial15/ViT.ckpt", "tutorial15/tensorboards/ViT/events.out.
↪tfevents.ViT",
                    "tutorial5/tensorboards/ResNet/events.out.tfevents.resnet"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name.split("/",1)[1])
    if "/" in file_name.split("/",1)[1]:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

We load the CIFAR10 dataset below. We use the same setup of the datasets and data augmentations as for the CNNs in Tutorial 5 to keep a fair comparison. The constants in the image normalization correspond to the values that scale and shift the data to a zero mean and standard deviation of one.

[3]:
```
# Transformations applied on each image => bring them into a numpy array
DATA_MEANS = np.array([0.49139968, 0.48215841, 0.44653091])
DATA_STD = np.array([0.24703223, 0.24348513, 0.26158784])
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
```

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```
    img = (img / 255. - DATA_MEANS) / DATA_STD
    return img

# We need to stack the batch elements
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
        return np.array(batch)

test_transform = image_to_numpy
# For training, we add some augmentation. Networks are too powerful and would overfit.
train_transform = transforms.Compose([transforms.RandomHorizontalFlip(),
                                      transforms.RandomResizedCrop((32,32),scale=(0.8,1.
↪0),ratio=(0.9,1.1)),
                                      image_to_numpy
                                     ])
# Loading the training dataset. We need to split it into a training and validation part
# We need to do a little trick because the validation set should not use the␣
↪augmentation.
train_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=train_transform,␣
↪download=True)
val_dataset = CIFAR10(root=DATASET_PATH, train=True, transform=test_transform,␣
↪download=True)
train_set, _ = torch.utils.data.random_split(train_dataset, [45000, 5000],␣
↪generator=torch.Generator().manual_seed(42))
_, val_set = torch.utils.data.random_split(val_dataset, [45000, 5000], generator=torch.
↪Generator().manual_seed(42))

# Loading the test set
test_set = CIFAR10(root=DATASET_PATH, train=False, transform=test_transform,␣
↪download=True)

# We define a set of data loaders that we can use for training and validation
train_loader = data.DataLoader(train_set,
                               batch_size=128,
                               shuffle=True,
                               drop_last=True,
                               collate_fn=numpy_collate,
                               num_workers=8,
                               persistent_workers=True)
val_loader   = data.DataLoader(val_set,
                               batch_size=128,
                               shuffle=False,
                               drop_last=False,
                               collate_fn=numpy_collate,
                               num_workers=4,
                               persistent_workers=True)
test_loader  = data.DataLoader(test_set,
```

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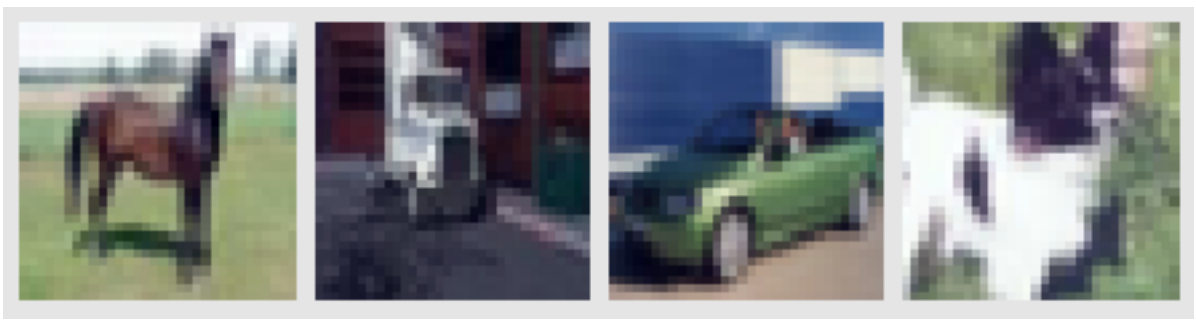
```
                                batch_size=128,
                                shuffle=False,
                                drop_last=False,
                                collate_fn=numpy_collate,
                                num_workers=4,
                                persistent_workers=True)
```

```
Files already downloaded and verified
Files already downloaded and verified
Files already downloaded and verified
```

[4]:
```
# Visualize some examples
def numpy_to_torch(array):
    array = jax.device_get(array)
    tensor = torch.from_numpy(array)
    tensor = tensor.permute(0, 3, 1, 2)
    return tensor

NUM_IMAGES = 4
CIFAR_images = np.stack([val_set[idx][0] for idx in range(NUM_IMAGES)], axis=0)
img_grid = torchvision.utils.make_grid(numpy_to_torch(CIFAR_images),
                                       nrow=4, normalize=True, pad_value=0.9)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Image examples of the CIFAR10 dataset")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```



4.39.1 Transformers for image classification

Transformers have been originally proposed to process sets since it is a permutation-equivariant architecture, i.e., producing the same output permuted if the input is permuted. To apply Transformers to sequences, we have simply added a positional encoding to the input feature vectors, and the model learned by itself what to do with it. So, why not do the same thing on images? This is exactly what Alexey Dosovitskiy et al. proposed in their paper "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale". Specifically, the Vision Transformer is a model for image classification that views images as sequences of smaller patches. As a preprocessing step, we split an image of, for example, 48×48 pixels into 9 16×16 patches. Each of those patches is considered to be a "word"/"token" and projected to a feature space. With adding positional encodings and a token for classification on top, we can apply a Transformer as usual to this sequence and start training it for our task. A nice GIF visualization of the architecture is shown below (figure credit - Phil Wang):

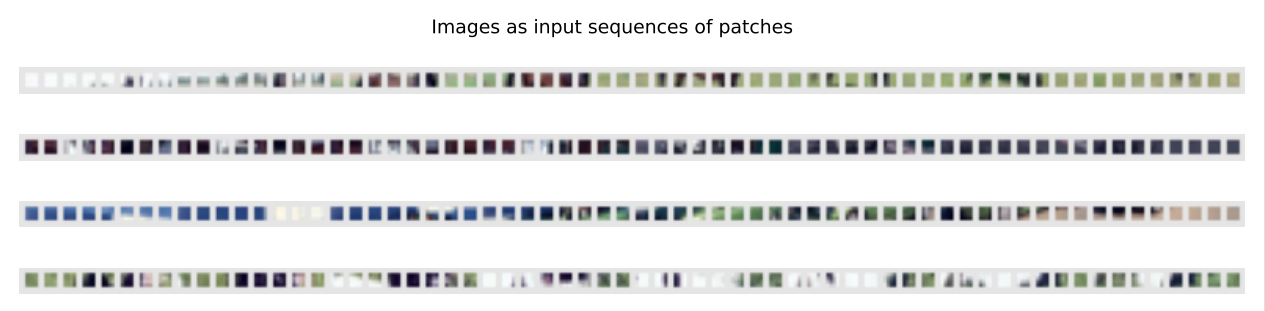
We will walk step by step through the Vision Transformer, and implement all parts by ourselves. First, let's implement the image preprocessing: an image of size $N \times N$ has to be split into $(N/M)^2$ patches of size $M \times M$. These represent the input words to the Transformer.

[5]:
```
def img_to_patch(x, patch_size, flatten_channels=True):
    """
    Inputs:
        x - torch.Tensor representing the image of shape [B, H, W, C]
        patch_size - Number of pixels per dimension of the patches (integer)
        flatten_channels - If True, the patches will be returned in a flattened format
                           as a feature vector instead of a image grid.
    """
    B, H, W, C = x.shape
    x = x.reshape(B, H//patch_size, patch_size, W//patch_size, patch_size, C)
    x = x.transpose(0, 1, 3, 2, 4, 5)    # [B, H', W', p_H, p_W, C]
    x = x.reshape(B, -1, *x.shape[3:])   # [B, H'*W', p_H, p_W, C]
    if flatten_channels:
        x = x.reshape(B, x.shape[1], -1) # [B, H'*W', p_H*p_W*C]
    return x
```

Let's take a look at how that works for our CIFAR examples above. For our images of size 32×32, we choose a patch size of 4. Hence, we obtain sequences of 64 patches of size 4×4. We visualize them below:

[6]:
```
img_patches = img_to_patch(CIFAR_images, patch_size=4, flatten_channels=False)

fig, ax = plt.subplots(CIFAR_images.shape[0], 1, figsize=(14,3))
fig.suptitle("Images as input sequences of patches")
for i in range(CIFAR_images.shape[0]):
    img_grid = torchvision.utils.make_grid(numpy_to_torch(img_patches[i]),
                                           nrow=64, normalize=True, pad_value=0.9)
    img_grid = img_grid.permute(1, 2, 0)
    ax[i].imshow(img_grid)
    ax[i].axis('off')
plt.show()
plt.close()
```



Compared to the original images, it is much harder to recognize the objects from those patch lists now. Still, this is the input we provide to the Transformer for classifying the images. The model has to learn itself how it has to combine the patches to recognize the objects. The inductive bias in CNNs that an image is a grid of pixels, is lost in this input format.

After we have looked at the preprocessing, we can now start building the Transformer model. Since we have discussed the fundamentals of Multi-Head Attention in Tutorial 6, we will use the Flax module `nn.MultiHeadDotProductAttention` (docs) here. Further, we use the Pre-Layer Normalization version of the Transformer blocks proposed by Ruibin Xiong et al. in 2020. The idea is to apply Layer Normalization not in between residual blocks, but instead as a first layer in the residual blocks. This reorganization of the layers supports better gradient flow and removes the necessity of a warm-up stage. A visualization of the difference between the standard Post-LN and the Pre-LN version is shown below.

The implementation of the Pre-LN attention block looks as follows:

[7]:
```
class AttentionBlock(nn.Module):
    embed_dim : int   # Dimensionality of input and attention feature vectors
    hidden_dim : int  # Dimensionality of hidden layer in feed-forward network
    num_heads : int   # Number of heads to use in the Multi-Head Attention block
    dropout_prob : float = 0.0  # Amount of dropout to apply in the feed-forward network

    def setup(self):
        self.attn = nn.MultiHeadDotProductAttention(num_heads=self.num_heads)
        self.linear = [
            nn.Dense(self.hidden_dim),
            nn.gelu,
            nn.Dropout(self.dropout_prob),
            nn.Dense(self.embed_dim)
        ]
        self.layer_norm_1 = nn.LayerNorm()
        self.layer_norm_2 = nn.LayerNorm()
        self.dropout = nn.Dropout(self.dropout_prob)

    def __call__(self, x, train=True):
        inp_x = self.layer_norm_1(x)
        attn_out = self.attn(inputs_q=inp_x, inputs_kv=inp_x)
        x = x + self.dropout(attn_out, deterministic=not train)

        linear_out = self.layer_norm_2(x)
        for l in self.linear:
            linear_out = l(linear_out) if not isinstance(l, nn.Dropout) else l(linear_
↪out, deterministic=not train)
```

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```
        x = x + self.dropout(linear_out, deterministic=not train)
        return x
```

[8]:
```
## Test AttentionBlock implementation
# Example features as input
main_rng, x_rng = random.split(main_rng)
x = random.normal(x_rng, (3, 16, 128))
# Create attention block
attnblock = AttentionBlock(embed_dim=128, hidden_dim=512, num_heads=4, dropout_prob=0.1)
# Initialize parameters of attention block with random key and inputs
main_rng, init_rng, dropout_init_rng = random.split(main_rng, 3)
params = attnblock.init({'params': init_rng, 'dropout': dropout_init_rng}, x, True)[
↪'params']
# Apply encoder block with parameters on the inputs
# Since dropout is stochastic, we need to pass a rng to the forward
main_rng, dropout_apply_rng = random.split(main_rng)
out = attnblock.apply({'params': params}, x, train=True, rngs={'dropout': dropout_apply_
↪rng})
print('Out', out.shape)

del attnblock, params
```

```
Out (3, 16, 128)
```

Now we have all modules ready to build our own Vision Transformer. Besides the Transformer encoder, we need the following modules:

- A **linear projection** layer that maps the input patches to a feature vector of larger size. It is implemented by a simple linear layer that takes each $M \times M$ patch independently as input.
- A **classification token** that is added to the input sequence. We will use the output feature vector of the classification token (CLS token in short) for determining the classification prediction.
- Learnable **positional encodings** that are added to the tokens before being processed by the Transformer. Those are needed to learn position-dependent information, and convert the set to a sequence. Since we usually work with a fixed resolution, we can learn the positional encodings instead of having the pattern of sine and cosine functions.
- An **MLP head** that takes the output feature vector of the CLS token, and maps it to a classification prediction. This is usually implemented by a small feed-forward network or even a single linear layer.

With those components in mind, let's implement the full Vision Transformer below:

[9]:
```
class VisionTransformer(nn.Module):
    embed_dim : int     # Dimensionality of input and attention feature vectors
    hidden_dim : int    # Dimensionality of hidden layer in feed-forward network
    num_heads : int     # Number of heads to use in the Multi-Head Attention block
    num_channels : int  # Number of channels of the input (3 for RGB)
    num_layers : int    # Number of layers to use in the Transformer
    num_classes : int   # Number of classes to predict
    patch_size : int    # Number of pixels that the patches have per dimension
    num_patches : int   # Maximum number of patches an image can have
    dropout_prob : float = 0.0  # Amount of dropout to apply in the feed-forward network

    def setup(self):
```

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```
        # Layers/Networks
        self.input_layer = nn.Dense(self.embed_dim)
        self.transformer = [AttentionBlock(self.embed_dim,
                                           self.hidden_dim,
                                           self.num_heads,
                                           self.dropout_prob) for _ in range(self.num_
↪layers)]
        self.mlp_head = nn.Sequential([
            nn.LayerNorm(),
            nn.Dense(self.num_classes)
        ])
        self.dropout = nn.Dropout(self.dropout_prob)

        # Parameters/Embeddings
        self.cls_token = self.param('cls_token',
                                    nn.initializers.normal(stddev=1.0),
                                    (1, 1, self.embed_dim))
        self.pos_embedding = self.param('pos_embedding',
                                        nn.initializers.normal(stddev=1.0),
                                        (1, 1+self.num_patches, self.embed_dim))


    def __call__(self, x, train=True):
        # Preprocess input
        x = img_to_patch(x, self.patch_size)
        B, T, _ = x.shape
        x = self.input_layer(x)

        # Add CLS token and positional encoding
        cls_token = self.cls_token.repeat(B, axis=0)
        x = jnp.concatenate([cls_token, x], axis=1)
        x = x + self.pos_embedding[:,:T+1]

        # Apply Transforrmer
        x = self.dropout(x, deterministic=not train)
        for attn_block in self.transformer:
            x = attn_block(x, train=train)

        # Perform classification prediction
        cls = x[:,0]
        out = self.mlp_head(cls)
        return out
```

[10]:
```
## Test VisionTransformer implementation
# Example features as input
main_rng, x_rng = random.split(main_rng)
x = random.normal(x_rng, (5, 32, 32, 3))
# Create vision transformer
visntrans = VisionTransformer(embed_dim=128,
                              hidden_dim=512,
                              num_heads=4,
                              num_channels=3,
```

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```
                                num_layers=6,
                                num_classes=10,
                                patch_size=4,
                                num_patches=64,
                                dropout_prob=0.1)
# Initialize parameters of the Vision Transformer with random key and inputs
main_rng, init_rng, dropout_init_rng = random.split(main_rng, 3)
params = visntrans.init({'params': init_rng, 'dropout': dropout_init_rng}, x, True)[
↪'params']
# Apply encoder block with parameters on the inputs
# Since dropout is stochastic, we need to pass a rng to the forward
main_rng, dropout_apply_rng = random.split(main_rng)
out = visntrans.apply({'params': params}, x, train=True, rngs={'dropout': dropout_apply_
↪rng})
print('Out', out.shape)

del visntrans, params
```

```
Out (5, 10)
```

Finally, we can put everything into a trainer module as usual. We use `optax.adamw` as the optimizer, which is Adam with a corrected weight decay implementation. Since we use the Pre-LN Transformer version, we do not need to use a learning rate warmup stage anymore. Instead, we use the same learning rate scheduler as the CNNs in our previous tutorial on image classification.

[11]:
```
class TrainerModule:

    def __init__(self, exmp_imgs, lr=1e-3, weight_decay=0.01, seed=42, **model_hparams):
        """
        Module for summarizing all training functionalities for classification on␣
↪CIFAR10.

        Inputs:
            exmp_imgs - Example imgs, used as input to initialize the model
            lr - Learning rate of the optimizer to use
            weight_decay - Weight decay to use in the optimizer
            seed - Seed to use in the model initialization
        """
        super().__init__()
        self.lr = lr
        self.weight_decay = weight_decay
        self.seed = seed
        self.rng = jax.random.PRNGKey(self.seed)
        # Create empty model. Note: no parameters yet
        self.model = VisionTransformer(**model_hparams)
        # Prepare logging
        self.log_dir = os.path.join(CHECKPOINT_PATH, 'ViT/')
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model(exmp_imgs)
```

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```
    def create_functions(self):
        # Function to calculate the classification loss and accuracy for a model
        def calculate_loss(params, rng, batch, train):
            imgs, labels = batch
            rng, dropout_apply_rng = random.split(rng)
            logits = self.model.apply({'params': params},
                                      imgs,
                                      train=train,
                                      rngs={'dropout': dropout_apply_rng})
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).mean()
            return loss, (acc, rng)
        # Training function
        def train_step(state, rng, batch):
            loss_fn = lambda params: calculate_loss(params, rng, batch, train=True)
            # Get loss, gradients for loss, and other outputs of loss function
            (loss, (acc, rng)), grads = jax.value_and_grad(loss_fn, has_aux=True)(state.
↪params)
            # Update parameters and batch statistics
            state = state.apply_gradients(grads=grads)
            return state, rng, loss, acc
        # Eval function
        def eval_step(state, rng, batch):
            # Return the accuracy for a single batch
            _, (acc, rng) = calculate_loss(state.params, rng, batch, train=False)
            return rng, acc
        # jit for efficiency
        self.train_step = jax.jit(train_step)
        self.eval_step = jax.jit(eval_step)

    def init_model(self, exmp_imgs):
        # Initialize model
        self.rng, init_rng, dropout_init_rng = random.split(self.rng, 3)
        self.init_params = self.model.init({'params': init_rng, 'dropout': dropout_init_
↪rng},
                                           exmp_imgs,
                                           train=True)['params']
        self.state = None

    def init_optimizer(self, num_epochs, num_steps_per_epoch):
        # We decrease the learning rate by a factor of 0.1 after 60% and 85% of the␣
↪training
        lr_schedule = optax.piecewise_constant_schedule(
            init_value=self.lr,
            boundaries_and_scales=
                {int(num_steps_per_epoch*num_epochs*0.6): 0.1,
                 int(num_steps_per_epoch*num_epochs*0.85): 0.1}
        )
        optimizer = optax.chain(
            optax.clip_by_global_norm(1.0),  # Clip gradients at norm 1
            optax.adamw(lr_schedule, weight_decay=self.weight_decay)
        )
```

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```
        # Initialize training state
        self.state = train_state.TrainState.create(
                                        apply_fn=self.model.apply,
                                        params=self.init_params if self.state is None␣
↪else self.state.params,
                                        tx=optimizer)

    def train_model(self, train_loader, val_loader, num_epochs=200):
        # Train model for defined number of epochs
        # We first need to create optimizer and the scheduler for the given number of␣
↪epochs
        self.init_optimizer(num_epochs, len(train_loader))
        # Track best eval accuracy
        best_eval = 0.0
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(epoch=epoch_idx)
            if epoch_idx % 2 == 0:
                eval_acc = self.eval_model(val_loader)
                self.logger.add_scalar('val/acc', eval_acc, global_step=epoch_idx)
                if eval_acc >= best_eval:
                    best_eval = eval_acc
                    self.save_model(step=epoch_idx)
                self.logger.flush()

    def train_epoch(self, epoch):
        # Train model for one epoch, and log avg loss and accuracy
        metrics = defaultdict(list)
        for batch in tqdm(train_loader, desc='Training', leave=False):
            self.state, self.rng, loss, acc = self.train_step(self.state, self.rng,␣
↪batch)
            metrics['loss'].append(loss)
            metrics['acc'].append(acc)
        for key in metrics:
            avg_val = np.stack(jax.device_get(metrics[key])).mean()
            self.logger.add_scalar('train/'+key, avg_val, global_step=epoch)

    def eval_model(self, data_loader):
        # Test model on all images of a data loader and return avg loss
        correct_class, count = 0, 0
        for batch in data_loader:
            self.rng, acc = self.eval_step(self.state, self.rng, batch)
            correct_class += acc * batch[0].shape[0]
            count += batch[0].shape[0]
        eval_acc = (correct_class / count).item()
        return eval_acc

    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir,
                                    target=self.state.params,
                                    step=step,
                                    overwrite=True)
```

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```
    def load_model(self, pretrained=False):
        # Load model. We use different checkpoint for pretrained models
        if not pretrained:
            params = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir, target=None)
        else:
            params = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'ViT.ckpt'), target=None)
        self.state = train_state.TrainState.create(
                                    apply_fn=self.model.apply,
                                    params=params,
                                    tx=self.state.tx if self.state else optax.
↪adamw(self.lr)  # Default optimizer
                                   )

    def checkpoint_exists(self):
        # Check whether a pretrained model exist for this autoencoder
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'ViT.ckpt'))
```

4.39.2 Experiments

Commonly, Vision Transformers are applied to large-scale image classification benchmarks such as ImageNet to leverage their full potential. However, here we take a step back and ask: can Vision Transformer also succeed on classical, small benchmarks such as CIFAR10? To find this out, we train a Vision Transformer from scratch on the CIFAR10 dataset. Let's first create a training function for our PyTorch Lightning module which also loads the pre-trained model if you have downloaded it above.

[12]:
```
def train_model(*args, num_epochs=200, **kwargs):
    # Create a trainer module with specified hyperparameters
    trainer = TrainerModule(*args, **kwargs)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(train_loader, val_loader, num_epochs=num_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    # Test trained model
    val_acc = trainer.eval_model(val_loader)
    test_acc = trainer.eval_model(test_loader)
    return trainer, {'val': val_acc, 'test': test_acc}
```

Now, we can already start training our model. As seen in our implementation, we have a couple of hyperparameters that we have to set. When creating this notebook, we have performed a small grid search over hyperparameters and listed the best hyperparameters in the cell below. Nevertheless, it is worth discussing the influence that each hyperparameter has, and what intuition we have for choosing its value.

First, let's consider the patch size. The smaller we make the patches, the longer the input sequences to the Transformer become. While in general, this allows the Transformer to model more complex functions, it requires a longer computation time due to its quadratic memory usage in the attention layer. Furthermore, small patches can make the task more difficult since the Transformer has to learn which patches are close-by, and which are far away. We experimented with patch sizes of 2, 4, and 8 which gives us the input sequence lengths of 256, 64, and 16 respectively. We found 4 to result in the best performance and hence pick it below.

Next, the embedding and hidden dimensionality have a similar impact on a Transformer as to an MLP. The larger the

sizes, the more complex the model becomes, and the longer it takes to train. In Transformers, however, we have one more aspect to consider: the query-key sizes in the Multi-Head Attention layers. Each key has the feature dimensionality of `embed_dim/num_heads`. Considering that we have an input sequence length of 64, a minimum reasonable size for the key vectors is 16 or 32. Lower dimensionalities can restrain the possible attention maps too much. We observed that more than 8 heads are not necessary for the Transformer, and therefore pick an embedding dimensionality of `256`. The hidden dimensionality in the feed-forward networks is usually 2-4x larger than the embedding dimensionality, and thus we pick `512`.

Finally, the learning rate for Transformers is usually relatively small, and in papers, a common value to use is 3e-5. However, since we work with a smaller dataset and have a potentially easier task, we found that we are able to increase the learning rate to 3e-4 without any problems. To reduce overfitting, we use a dropout value of 0.2. Remember that we also use small image augmentations as regularization during training.

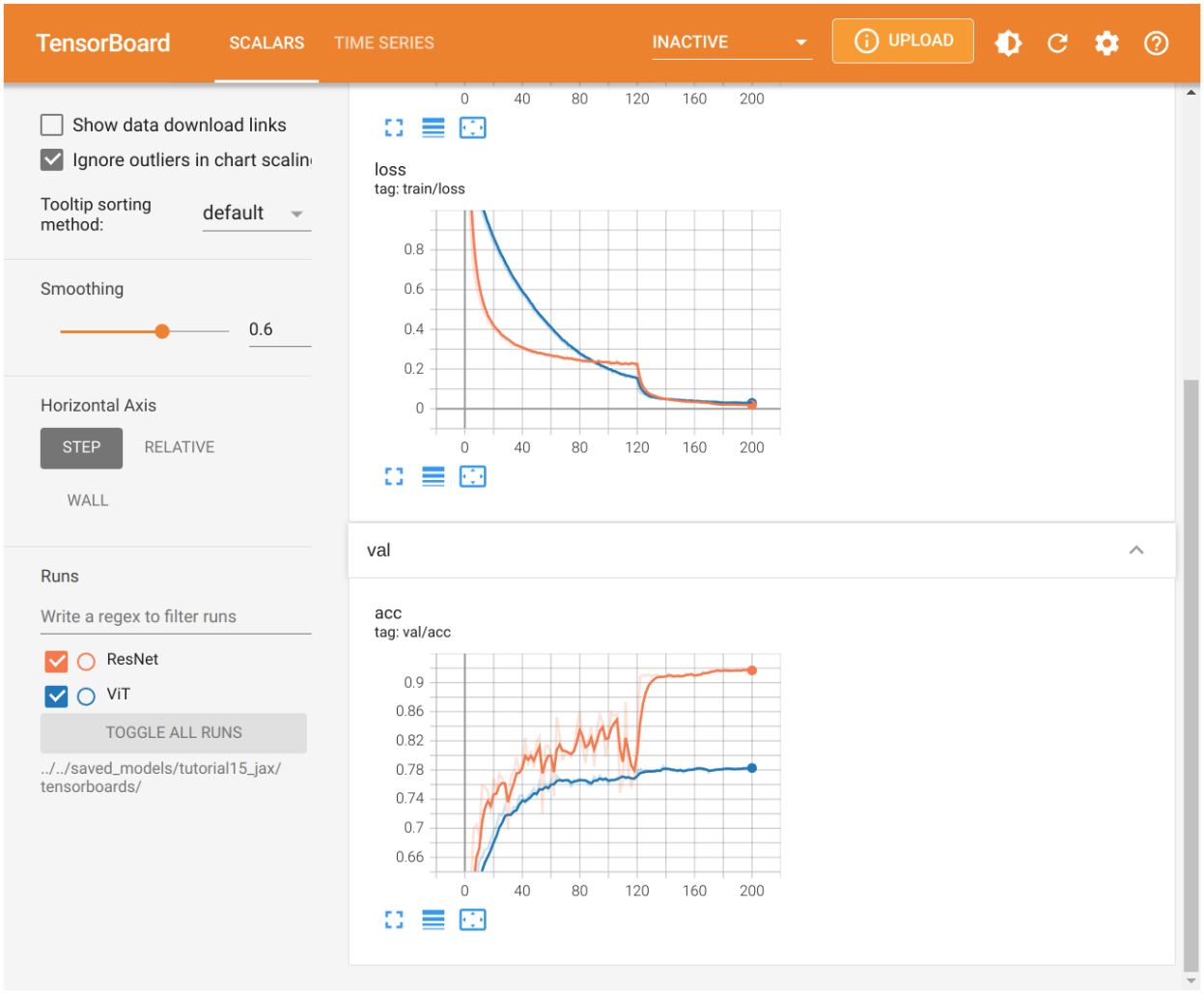
Feel free to explore the hyperparameters yourself by changing the values below. In general, the Vision Transformer did not show to be too sensitive to the hyperparameter choices on the CIFAR10 dataset.

[13]:
```
model, results = train_model(exmp_imgs=next(iter(train_loader))[0],
                             embed_dim=256,
                             hidden_dim=512,
                             num_heads=8,
                             num_layers=6,
                             patch_size=4,
                             num_channels=3,
                             num_patches=64,
                             num_classes=10,
                             dropout_prob=0.2,
                             lr=3e-4)
print("ViT results", results)
```

```
ViT results {'val': 0.7856000661849976, 'test': 0.784000039100647}
```

The Vision Transformer achieves a validation and test performance of about 78%. In comparison, almost all CNN architectures that we have tested in Tutorial 5 obtained a classification performance of around 90%. This is a considerable gap and shows that although Vision Transformers perform strongly on ImageNet with potential pretraining, they cannot come close to simple CNNs on CIFAR10 when being trained from scratch. The differences between a CNN and Transformer can be well observed in the training curves. Let's look at them in a tensorboard below:

[14]:
```
# Opens tensorboard in notebook. Adjust the path to your CHECKPOINT_PATH!
%tensorboard --logdir ../../saved_models/tutorial15_jax/tensorboards/
```



The tensorboard compares the Vision Transformer to a ResNet trained on CIFAR10. When looking at the training losses, we see that the ResNet learns much more quickly in the first iterations. While the learning rate might have an influence on the initial learning speed, we see the same trend in the validation accuracy. The ResNet achieves the best performance of the Vision Transformer after just 5 epochs (2000 iterations). Further, while the ResNet training loss and validation accuracy have a similar trend, the validation performance of the Vision Transformers only marginally changes after 10k iterations while the training loss has almost just started going down. Yet, the Vision Transformer is also able to achieve close to 100% accuracy on the training set.

All those observed phenomenons can be explained with a concept that we have visited before: inductive biases. Convolutional Neural Networks have been designed with the assumption that images are translation invariant. Hence, we apply convolutions with shared filters across the image. Furthermore, a CNN architecture integrates the concept of distance in an image: two pixels that are close to each other are more related than two distant pixels. Local patterns are combined into larger patterns until we perform our classification prediction. All those aspects are inductive biases of a CNN. In contrast, a Vision Transformer does not know which two pixels are close to each other, and which are far apart. It has to learn this information solely from the sparse learning signal of the classification task. This is a huge disadvantage when we have a small dataset since such information is crucial for generalizing to an unseen test dataset. With large enough datasets and/or good pre-training, a Transformer can learn this information without the need for inductive biases, and instead is more flexible than a CNN. Especially long-distance relations between local patterns can be difficult to process in CNNs, while in Transformers, all patches have the distance of one. This is why Vision Transformers are so strong on large-scale datasets such as ImageNet but underperform a lot when being applied to a small dataset such as CIFAR10.

4.39.3 Conclusion

In this tutorial, we have implemented our own Vision Transformer from scratch and applied it to the task of image classification. Vision Transformers work by splitting an image into a sequence of smaller patches, use those as input to a standard Transformer encoder. While Vision Transformers achieved outstanding results on large-scale image recognition benchmarks such as ImageNet, they considerably underperform when being trained from scratch on small-scale datasets like CIFAR10. The reason is that in contrast to CNNs, Transformers do not have the inductive biases of translation invariance and the feature hierarchy (i.e. larger patterns consist of many smaller patterns). However, these aspects can be learned when enough data is provided, or the model has been pre-trained on other large-scale tasks. Considering that Vision Transformers have just been proposed end of 2020, there is likely a lot more to come on Transformers for Computer Vision.

References

Dosovitskiy, Alexey, et al. "An image is worth 16x16 words: Transformers for image recognition at scale." International Conference on Learning Representations (2021). link

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Tolstikhin, Ilya, et al. "MLP-mixer: An all-MLP Architecture for Vision." arXiv preprint arXiv:2105.01601 (2021). link

Xiong, Ruibin, et al. "On layer normalization in the transformer architecture." International Conference on Machine Learning. PMLR, 2020. link

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.40 Tutorial 17 (JAX): Self-Supervised Contrastive Learning with SimCLR

Filled notebook:
Pre-trained models:
PyTorch version:
Author: Phillip Lippe

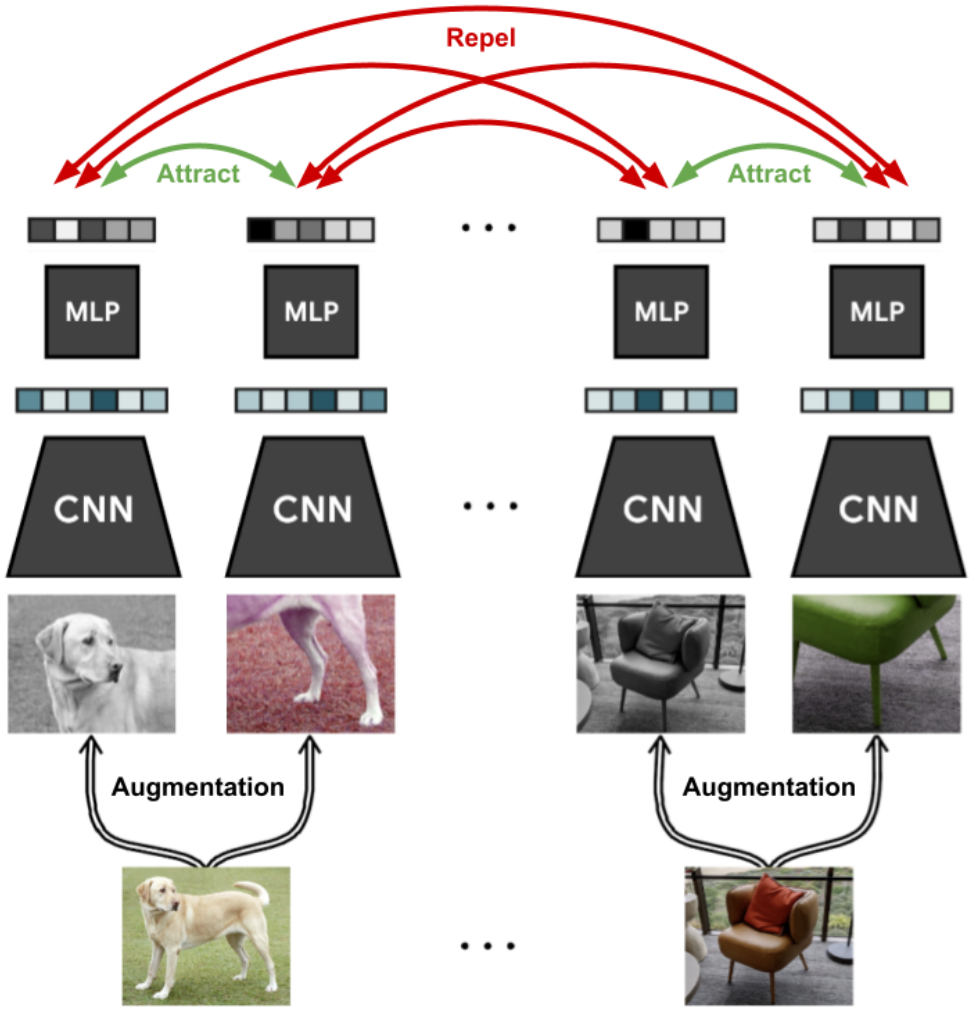
Note: This notebook is written in JAX+Flax. It is a 1-to-1 translation of the original notebook written in PyTorch+PyTorch Lightning with almost identical results. For an introduction to JAX, check out our Tutorial 2 (JAX): Introduction to JAX+Flax. Further, throughout the notebook, we comment on major differences to the PyTorch version and provide explanations for the major parts of the JAX code.

Speed comparison: We will report the speed comparisons of the PyTorch and JAX implementation soon.

Models	PyTorch	JAX
SimCLR	-min -sec	-min -sec
Logistic Regression	-min -sec	-min -sec
Supervised ResNet-18	-min -sec	-min -sec

In this tutorial, we will take a closer look at self-supervised contrastive learning. Self-supervised learning, or also sometimes called unsupervised learning, describes the scenario where we have given input data, but no accompanying labels to train in a classical supervised way. However, this data still contains a lot of information from which we can learn: how are the images different from each other? What patterns are descriptive for certain images? Can we cluster the images? And so on. Methods for self-supervised learning try to learn as much as possible from the data alone, so it can quickly be finetuned for a specific classification task. The benefit of self-supervised learning is that a large dataset can often easily be obtained. For instance, if we want to train a vision model on semantic segmentation for autonomous driving, we can collect large amounts of data by simply installing a camera in a car, and driving through a city for an hour. In contrast, if we would want to do supervised learning, we would have to manually label all those images before training a model. This is extremely expensive, and would likely take a couple of months to manually label the same amount of data. Further, self-supervised learning can provide an alternative to transfer learning from models pretrained on ImageNet since we could pretrain a model on a specific dataset/situation, e.g. traffic scenarios for autonomous driving.

Within the last two years, a lot of new approaches have been proposed for self-supervised learning, in particular for images, that have resulted in great improvements over supervised models when few labels are available. The subfield that we will focus on in this tutorial is contrastive learning. Contrastive learning is motivated by the question mentioned above: how are images different from each other? Specifically, contrastive learning methods train a model to cluster an image and its slightly augmented version in latent space, while the distance to other images should be maximized. A very recent and simple method for this is SimCLR, which is visualized below (figure credit - Ting Chen et al.).



The general setup is that we are given a dataset of images without any labels, and want to train a model on this data such that it can quickly adapt to any image recognition task afterward. During each training iteration, we sample a batch of images as usual. For each image, we create two versions by applying data augmentation techniques like cropping, Gaussian noise, blurring, etc. An example of such is shown on the left with the image of the dog. We will go into the details and effects of the chosen augmentation techniques later. On those images, we apply a CNN like ResNet and obtain as output a 1D feature vector on which we apply a small MLP. The output features of the two augmented images are then trained to be close to each other, while all other images in that batch should be as different as possible. This way, the model has to learn to recognize the content of the image that remains unchanged under the data augmentations, such as objects which we usually care about in supervised tasks.

We will now implement this framework ourselves and discuss further details along the way. Let's first start with importing our standard libraries below:

[1]:
```
## Standard libraries
import os
import numpy as np
from typing import Sequence, Any
from collections import defaultdict

## Imports for plotting
import matplotlib.pyplot as plt
```

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```
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.set()

## tqdm for loading bars
from tqdm.auto import tqdm

## To run JAX on TPU in Google Colab, uncomment the two lines below
# import jax.tools.colab_tpu
# jax.tools.colab_tpu.setup_tpu()

## JAX
import jax
import jax.numpy as jnp
from jax import random
# Seeding for random operations
main_rng = random.PRNGKey(42)

## Flax (NN in JAX)
try:
    import flax
except ModuleNotFoundError: # Install flax if missing
    !pip install --quiet flax
    import flax
from flax import linen as nn
from flax.training import train_state, checkpoints

## Optax (Optimizers in JAX)
try:
    import optax
except ModuleNotFoundError: # Install optax if missing
    !pip install --quiet optax
    import optax

## PyTorch
import torch
import torch.utils.data as data
from torch.utils.tensorboard import SummaryWriter
import torchvision
from torchvision import transforms
from torchvision.datasets import STL10

# Import tensorboard
%load_ext tensorboard

# Path to the folder where the datasets are/should be downloaded (e.g. CIFAR10)
DATASET_PATH = "../../data"
```

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```
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/tutorial17_jax"

print('Device:', jax.devices()[0])
```

```
Device: gpu:0
```

As in many tutorials before, we provide pre-trained models. Note that those models are slightly larger as normal (~100MB overall) since we use the default ResNet-18 architecture. If you are running this notebook locally, make sure to have sufficient disk space available.

[2]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/JAX/tutorial17/"
# Files to download
pretrained_files = ["SimCLR.ckpt", "ResNet.ckpt",
                    "tensorboards/SimCLR/events.out.tfevents.SimCLR",
                    "tensorboards/classification/ResNet/events.out.tfevents.ResNet"]
pretrained_files += [f"LogisticRegression_{size}.ckpt" for size in [10, 20, 50, 100, 200,
↪ 500]]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/",1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

4.40.1 SimCLR

We will start our exploration of contrastive learning by discussing the effect of different data augmentation techniques, and how we can implement an efficient data loader for such, specialized for JAX. Next, we implement SimCLR with Flax, and finally train it on a large, unlabeled dataset.

Data Augmentation for Contrastive Learning

To allow efficient training, we need to prepare the data loading such that we sample two different, random augmentations for each image in the batch. The easiest way to do this is by creating a transformation that, when being called, applies a set of data augmentations to an image twice. This is implemented in the class `ContrastiveTransformations` below:

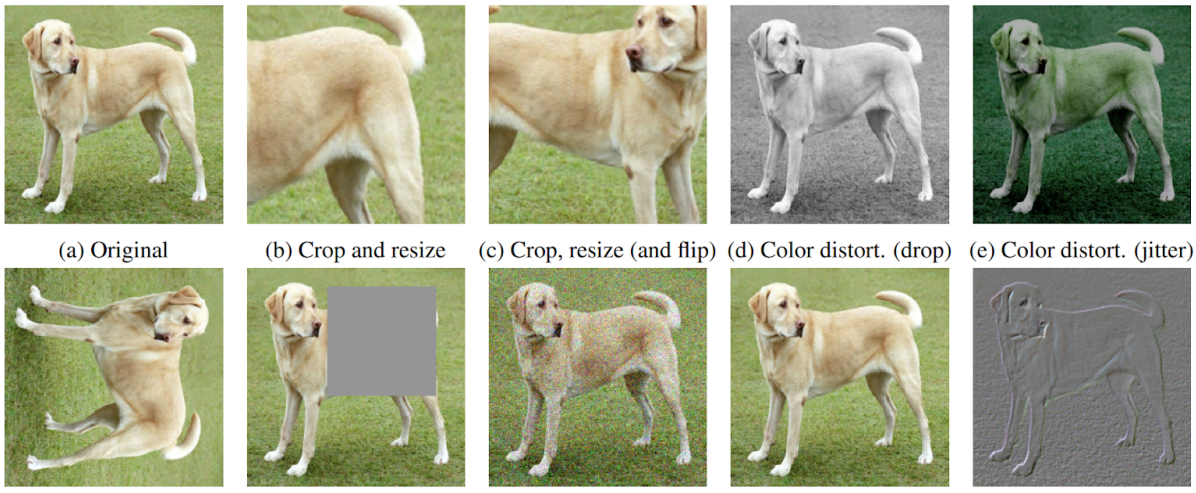
[3]:
```
class ContrastiveTransformations(object):

    def __init__(self, base_transforms, n_views=2):
        self.base_transforms = base_transforms
        self.n_views = n_views

    def __call__(self, x):
        return [self.base_transforms(x) for i in range(self.n_views)]
```

The contrastive learning framework can easily be extended to have more *positive* examples by sampling more than two augmentations of the same image. However, the most efficient training is usually obtained by using only two.

Next, we can look at the specific augmentations we want to apply. The choice of the data augmentation to use is the most crucial hyperparameter in SimCLR since it directly affects how the latent space is structured, and what patterns might be learned from the data. Let's first take a look at some of the most popular data augmentations (figure credit - Ting Chen and Geoffrey Hinton):



(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

(f) Rotate $\{90°, 180°, 270°\}$ (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

All of them can be used, but it turns out that two augmentations stand out in their importance: crop-and-resize, and color distortion. Interestingly, however, they only lead to strong performance if they have been used together as discussed by Ting Chen et al. in their SimCLR paper. When performing randomly cropping and resizing, we can distinguish between two situations: (a) cropped image A provides a local view of cropped image B, or (b) cropped images C and D show neighboring views of the same image (figure credit - Ting Chen and Geoffrey Hinton).

While situation (a) requires the model to learn some sort of scale invariance to make crops A and B similar in latent space, situation (b) is more challenging since the model needs to recognize an object beyond its limited view. However, without color distortion, there is a loophole that the model can exploit, namely that different crops of the same image usually look very similar in color space. Consider the picture of the dog above. Simply from the color of the fur and the green color tone of the background, you can reason that two patches belong to the same image without actually recognizing the dog in the picture. In this case, the model might end up focusing only on the color histograms of the images, and ignore other more generalizable features. If, however, we distort the colors in the two patches randomly

and independently of each other, the model cannot rely on this simple feature anymore. Hence, by combining random cropping and color distortions, the model can only match two patches by learning generalizable representations.

Overall, for our experiments, we apply a set of 5 transformations following the original SimCLR setup: random horizontal flip, crop-and-resize, color distortion, random grayscale, and gaussian blur. In comparison to the original implementation, we reduce the effect of the color jitter slightly (0.5 instead of 0.8 for brightness, contrast, and saturation, and 0.1 instead of 0.2 for hue). In our experiments, this setting obtained better performance and was faster and more stable to train. If, for instance, the brightness scale highly varies in a dataset, the original settings can be more beneficial since the model can't rely on this information anymore to distinguish between images.

Image Augmentations with JAX

In the PyTorch version of this tutorial, we implement all these augmentations with transformation from the torchvision library. This requires a considerable amount of compute from the CPU to prepare the data in time for using it on the GPU. As alternative, we show here an implementation with JAX-native transformations in Pix that are executed on GPU on batch-level, using `jax.vmap` and `jax.jit`. Still, one transformation that can be difficult in JAX is resize-and-crop, since the resize creates arrays of dynamic shapes. Hence, we use the `RandomResizedCrop` transformation from torchvision:

[4]:
```
def image_to_numpy(img):
    img = np.array(img, dtype=np.float32)
    img = img / 255.
    return img


contrast_transforms = transforms.Compose([transforms.RandomResizedCrop(size=96),
                                          image_to_numpy])
```

Pix is an image-processing library in JAX, developed by Deep mind, that implements most common data augmentations. Let's first import it below:

[5]:
```
try:
    import dm_pix
except ModuleNotFoundError: # Install pix if missing
    !pip install --quiet dm_pix
    import dm_pix
```

As a first step, we implement a function that augments a single image and applies a random horizontal flip, color jitter (brightness, contrast, saturation, and hue), random grayscaling, and gaussian blur. Since these are operations with stochaticity/randomness, we also pass a random seed with it that we can split for each operation.

[6]:
```
def augment_image(rng, img):
    rngs = random.split(rng, 8)
    # Random left-right flip
    img = dm_pix.random_flip_left_right(rngs[0], img)
    # Color jitter
    img_jt = img
    img_jt = img_jt * random.uniform(rngs[1], shape=(1,), minval=0.5, maxval=1.5)  #␣
↪Brightness
    img_jt = jax.lax.clamp(0.0, img_jt, 1.0)
    img_jt = dm_pix.random_contrast(rngs[2], img_jt, lower=0.5, upper=1.5)
    img_jt = jax.lax.clamp(0.0, img_jt, 1.0)
    img_jt = dm_pix.random_saturation(rngs[3], img_jt, lower=0.5, upper=1.5)
    img_jt = jax.lax.clamp(0.0, img_jt, 1.0)
```

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```
    img_jt = dm_pix.random_hue(rngs[4], img_jt, max_delta=0.1)
    img_jt = jax.lax.clamp(0.0, img_jt, 1.0)
    should_jt = random.bernoulli(rngs[5], p=0.8)
    img = jnp.where(should_jt, img_jt, img)
    # Random grayscale
    should_gs = random.bernoulli(rngs[6], p=0.2)
    img = jax.lax.cond(should_gs,  # Only apply grayscale if true
                       lambda x: dm_pix.rgb_to_grayscale(x, keep_dims=True),
                       lambda x: x,
                       img)
    # Gaussian blur
    sigma = random.uniform(rngs[7], shape=(1,), minval=0.1, maxval=2.0)
    img = dm_pix.gaussian_blur(img, sigma=sigma[0], kernel_size=9)
    # Normalization
    img = img * 2.0 - 1.0
    return img
```

You might have noticed that we do not use the function `dm_pix.random_brightness` for the brightness augmentation. The reason is that the implementation follows TensorFlow's brightness augmentation by adding a constant value to each pixel, while the implementation in torchvision and PIL scales the pixel values by the factor. To stay closer to the PyTorch implementation, we implement it ourselves by scaling the pixel values.

Now that we have a function to augment a single image, let's transform this function to allow for a batch of images. This can be done using `jax.vmap`, with which we can vectorize the function both over images and seeds, such that each image is differently augmented. To not have to pass N seeds for a batch of N images, we can simply split one seed N times before calling the augmentation function. Finally, let's optimize the whole augmentation pipeline by just-in-time compilation:

[7]:
```
parallel_augment = jax.jit(lambda rng, imgs: jax.vmap(augment_image)(random.split(rng,␣
↪imgs.shape[0]), imgs))
```

In contrast to the PyTorch implementation, this augmentation will be performed on GPU, integrated in the training step for contrastive learning. The benefit of this is that we require much less CPU compute power and don't have to worry much about having enough workers etc. in the data loader. However, the apparent disadvantage is that we strictly block the GPU for the augmentations. But will this even be noticable in practice? We can easily check that by timing the execution for our augmentations on an arbitrary batch of images:

[8]:
```
img_rng, augm_rng = random.split(random.PRNGKey(42))
rand_imgs = random.uniform(img_rng, (512, 96, 96, 3))
_ = parallel_augment(augm_rng, rand_imgs)
```

[9]:
```
%%timeit
_ = parallel_augment(augm_rng, rand_imgs)
```

```
8.3 ms ± 4.55 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

Even for this very large batch of images, the augmentation takes only a few milliseconds on a common GPU, while a training step of a ResNet-18, as we will see later, takes several magnitudes more (e.g. about 200ms on an NVIDIA GTX1080Ti). Hence, we will not really notice this extra computation during training, while being much more efficient in CPU usage.

STL10 dataset

After discussing the data augmentation techniques, we can now focus on the dataset. In this tutorial, we will use the STL10 dataset, which, similarly to CIFAR10, contains images of 10 classes: airplane, bird, car, cat, deer, dog, horse, monkey, ship, truck. However, the images have a higher resolution, namely 96×96 pixels, and we are only provided with 500 labeled images per class. Additionally, we have a much larger set of $100,000$ unlabeled images which are similar to the training images but are sampled from a wider range of animals and vehicles. This makes the dataset ideal to showcase the benefits that self-supervised learning offers.

Luckily, the STL10 dataset is provided through torchvision. Keep in mind, however, that since this dataset is relatively large and has a considerably higher resolution than CIFAR10, it requires more disk space (~3GB) and takes a bit of time to download. For our initial discussion of self-supervised learning and SimCLR, we will create two data loaders with our contrastive transformations above: the `unlabeled_data` will be used to train our model via contrastive learning, and `train_data_contrast` will be used as a validation set in contrastive learning.

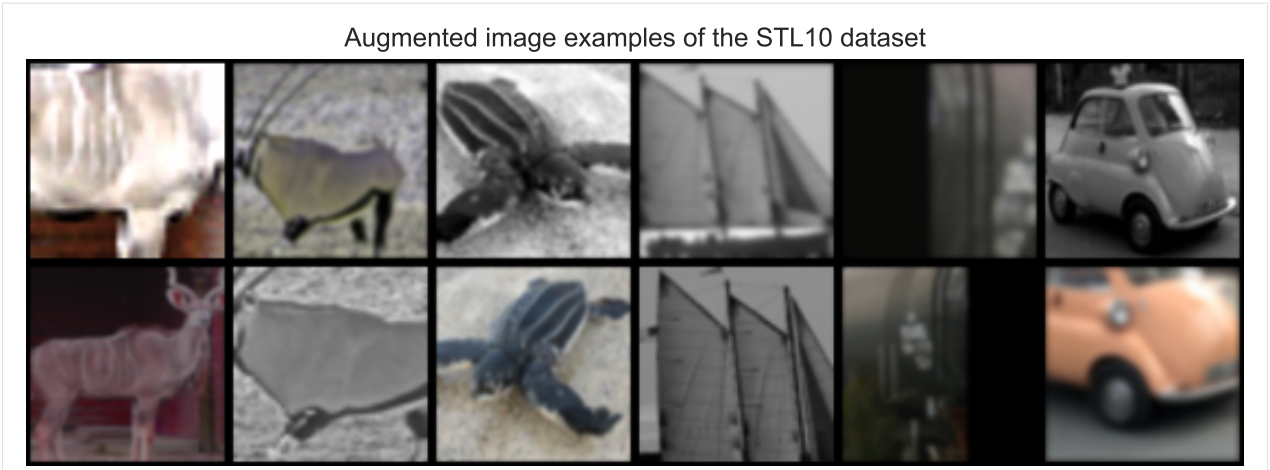
[10]:
```
unlabeled_data = STL10(root=DATASET_PATH, split='unlabeled', download=True,
                       transform=ContrastiveTransformations(contrast_transforms, n_
↪views=2))
train_data_contrast = STL10(root=DATASET_PATH, split='train', download=True,
                            transform=ContrastiveTransformations(contrast_transforms, n_
↪views=2))
```

```
Files already downloaded and verified
Files already downloaded and verified
```

Finally, before starting with our implementation of SimCLR, let's look at some example image pairs sampled with our augmentations:

[11]:
```
# Visualize some examples
NUM_IMAGES = 6
imgs = np.stack([parallel_augment(random.PRNGKey(idx), np.stack(unlabeled_data[idx][0],␣
↪axis=0)) for idx in range(NUM_IMAGES)], axis=2)
imgs = (imgs + 1.0) / 2.0
img_grid = np.pad(imgs, ((0,0), (2,2), (0,0), (2,2), (0,0)))
img_grid = img_grid.reshape(img_grid.shape[0]*img_grid.shape[1],-1,img_grid.shape[-1])

plt.figure(figsize=(10,5))
plt.title('Augmented image examples of the STL10 dataset')
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```



We see the wide variety of our data augmentation, including randomly cropping, grayscaling, gaussian blur, and color distortion. Thus, it remains a challenging task for the model to match two, independently augmented patches of the same image.

SimCLR implementation

Using the data loader pipeline above, we can now implement SimCLR. At each iteration, we get for every image x two differently augmented versions, which we refer to as $\tilde{x}_i$ and $\tilde{x}_j$. Both of these images are encoded into a one-dimensional feature vector, between which we want to maximize similarity which minimizes it to all other images in the batch. The encoder network is split into two parts: a base encoder network $f(\cdot)$, and a projection head $g(\cdot)$. The base network is usually a deep CNN as we have seen in e.g. Tutorial 5 before, and is responsible for extracting a representation vector from the augmented data examples. In our experiments, we will use the common ResNet-18 architecture as $f(\cdot)$, and refer to the output as $f(\tilde{x}_i) = h_i$. The projection head $g(\cdot)$ maps the representation h into a space where we apply the contrastive loss, i.e., compare similarities between vectors. It is often chosen to be a small MLP with non-linearities, and for simplicity, we follow the original SimCLR paper setup by defining it as a two-layer MLP with ReLU activation in the hidden layer. Note that in the follow-up paper, SimCLRv2, the authors mention that larger/wider MLPs can boost the performance considerably. This is why we apply an MLP with four times larger hidden dimensions, but deeper MLPs showed to overfit on the given dataset. The general setup is visualized below (figure credit - Ting Chen et al.):

After finishing the training with contrastive learning, we will remove the projection head $g(\cdot)$, and use $f(\cdot)$ as a pre-trained feature extractor. The representations z that come out of the projection head $g(\cdot)$ have been shown to perform worse than those of the base network $f(\cdot)$ when finetuning the network for a new task. This is likely because the representations z are trained to become invariant to many features like the color that can be important for downstream tasks. Thus, $g(\cdot)$ is only needed for the contrastive learning stage.

Now that the architecture is described, let's take a closer look at how we train the model. As mentioned before, we want to maximize the similarity between the representations of the two augmented versions of the same image, i.e., z_i and z_j in the figure above, while minimizing it to all other examples in the batch. SimCLR thereby applies the InfoNCE loss, originally proposed by Aaron van den Oord et al. for contrastive learning. In short, the InfoNCE loss compares the similarity of z_i and z_j to the similarity of z_i to any other representation in the batch by performing a softmax over the similarity values. The loss can be formally written as:

$$\ell_{i,j} = -\log \frac{\exp(\text{sim}(z_i, z_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\text{sim}(z_i, z_k)/\tau)} = -\text{sim}(z_i, z_j)/\tau + \log \left[\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\text{sim}(z_i, z_k)/\tau) \right]$$

The function sim is a similarity metric, and the hyperparameter τ is called temperature determining how peaked the distribution is. Since many similarity metrics are bounded, the temperature parameter allows us to balance the influence of many dissimilar image patches versus one similar patch. The similarity metric that is used in SimCLR is cosine similarity, as defined below:

$$\text{sim}(z_i, z_j) = \frac{z_i^\top \cdot z_j}{||z_i|| \cdot ||z_j||}$$

The maximum cosine similarity possible is 1, while the minimum is -1. In general, we will see that the features of two different images will converge to a cosine similarity around zero since the minimum, -1, would require z_i and z_j to be in the exact opposite direction in all feature dimensions, which does not allow for great flexibility.

Finally, now that we have discussed all details, let's implement SimCLR below as a Flax module. To not implement ResNet-18 ourselves, we use flaxmodels as we have already done in Tutorial 6.

[12]:
```
# Import and install flaxmodels if needed
try:
    import flaxmodels
except ModuleNotFoundError:
    !pip install --upgrade git+https://github.com/matthias-wright/flaxmodels.git
    import flaxmodels
```

[13]:
```
class SimCLR(nn.Module):
    hidden_dim : int
    temperature : float

    def setup(self):
        # Base model f(.) - ResNet 18 with last layer being size of 4*hidden_dim
        self.convnet = flaxmodels.ResNet18(output='activations',
                                           pretrained=False,
                                           normalize=False,
                                           num_classes=4*self.hidden_dim)
        # Network g(.) as MLP with last fc layer of convnet
        self.head = nn.Sequential([
            nn.relu,
            nn.Dense(self.hidden_dim)
        ])

    def __call__(self, imgs, train=True):
        # Encode all images
        model_feats = self.convnet(imgs, train=train)
        feats = self.head(model_feats['fc'])

        # Calculate cosine similarity between all images
        cos_sim = optax.cosine_similarity(feats[:,None,:], feats[None,:,:])
        cos_sim /= self.temperature
        # Masking cosine similarities to itself
        diag_range = jnp.arange(feats.shape[0], dtype=jnp.int32)
        cos_sim = cos_sim.at[diag_range, diag_range].set(-9e15)
        # Find positive example -> batch_size//2 away from the original example
        shifted_diag = jnp.roll(diag_range, imgs.shape[0]//2)
        pos_logits = cos_sim[diag_range, shifted_diag]
        # InfoNCE loss
        nll = - pos_logits + nn.logsumexp(cos_sim, axis=-1)
```

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```
        nll = nll.mean()

        # Logging
        metrics = {'loss': nll}
        # Determine ranking position of positive example
        comb_sim = jnp.concatenate([pos_logits[:,None],
                                    cos_sim.at[shifted_diag, diag_range].set(-9e15)],
                                   axis=-1)
        sim_argsort = (-comb_sim).argsort(axis=-1).argmin(axis=-1)
        # Logging of ranking position
        metrics['acc_top1'] = (sim_argsort == 0).mean()
        metrics['acc_top5'] = (sim_argsort < 5).mean()
        metrics['acc_mean_pos'] = (sim_argsort + 1).mean()

        return nll, metrics

    def encode(self, imgs, train=False):
        # Return features before g(.)
        model_feats = self.convnet(imgs, train=train)
        return model_feats['block4_1'].mean(axis=(1,2))
```

Alternatively to performing the validation on the contrastive learning loss as well, we could also take a simple, small downstream task, and track the performance of the base network $f(\cdot)$ on that. However, in this tutorial, we will restrict ourselves to the STL10 dataset where we use the task of image classification on STL10 as our test task.

Training

Now that we have implemented SimCLR and the data loading pipeline, we are ready to train the model. We will use the same training function setup as usual. We extend the TrainState with a `batch_stats` attribute for the batch statistics, and an PRNG key `rng` for the augmentations during training.

[14]:
```
class TrainState(train_state.TrainState):
    # Batch statistics from BatchNorm
    batch_stats : Any
    # PRNGKey for augmentations
    rng : Any
```

The class `TrainerModule` will build the foundation for our training code and will be specialized for the different parts/models in this tutorial.

[15]:
```
class TrainerModule:

    def __init__(self,
                 model_name : str,
                 model_class : Any,
                 eval_key : str,
                 exmp_imgs : Any,
                 lr : float = 1e-3,
                 weight_decay : float = 0.01,
                 seed : int = 42,
                 check_val_every_n_epoch : int = 1,
                 **model_hparams):
```

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```
        """
        Module for summarizing all common training functionalities.

        Inputs:
            model_name - Folder name in which to save the checkpoints
            model_class - Module class of the model to train
            eval_key - Name of the metric to check for saving the best model
            exmp_imgs - Example imgs, used as input to initialize the model
            lr - Learning rate of the optimizer to use
            weight_decay - Weight decay to use in the optimizer
            seed - Seed to use in the model initialization
            check_val_every_n_epoch - With which frequency to validate the model
        """
        super().__init__()
        self.lr = lr
        self.weight_decay = weight_decay
        self.seed = seed
        self.check_val_every_n_epoch = check_val_every_n_epoch
        # Create empty model. Note: no parameters yet
        self.eval_key = eval_key
        self.model_name = model_name
        self.model = model_class(**model_hparams)
        # Prepare logging
        self.log_dir = os.path.join(CHECKPOINT_PATH, f'{self.model_name}/')
        self.logger = SummaryWriter(log_dir=self.log_dir)
        # Create jitted training and eval functions
        self.create_functions()
        # Initialize model
        self.init_model(exmp_imgs)

    def create_functions(self):
        # To be implemented in sub-classes
        raise NotImplementedError

    def init_model(self, exmp_imgs):
        # Initialize model
        rng = random.PRNGKey(self.seed)
        rng, init_rng = random.split(rng)
        variables = self.model.init(init_rng, exmp_imgs)
        self.state = TrainState(step=0,
                                apply_fn=self.model.apply,
                                params=variables['params'],
                                batch_stats=variables.get('batch_stats'),
                                rng=rng,
                                tx=None, opt_state=None)

    def init_optimizer(self, num_epochs, num_steps_per_epoch):
        # By default, we decrease the learning rate with cosine annealing
        lr_schedule = optax.warmup_cosine_decay_schedule(
            init_value=0.0,
            peak_value=self.lr,
            warmup_steps=0.0,
```

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```
            decay_steps=int(num_epochs * num_steps_per_epoch),
            end_value=2e-2*self.lr
        )
        optimizer = optax.adamw(lr_schedule, weight_decay=self.weight_decay)
        self.create_train_state(optimizer)

    def create_train_state(self, optimizer):
        # Initialize training state
        self.state = TrainState.create(apply_fn=self.state.apply_fn,
                                       params=self.state.params,
                                       batch_stats=self.state.batch_stats,
                                       rng=self.state.rng,
                                       tx=optimizer)

    def train_model(self, train_loader, val_loader, num_epochs=200):
        # Train model for defined number of epochs
        # We first need to create optimizer and the scheduler for the given number of␣
↪epochs
        self.init_optimizer(num_epochs, len(train_loader))
        # Track best eval metric
        best_eval = 0.0
        for epoch_idx in tqdm(range(1, num_epochs+1)):
            self.train_epoch(train_loader, epoch=epoch_idx)
            if epoch_idx % self.check_val_every_n_epoch == 0:
                eval_metrics = self.eval_model(val_loader)
                for key in eval_metrics:
                    self.logger.add_scalar(f'val/{key}', eval_metrics[key], global_
↪step=epoch_idx)
                if eval_metrics[self.eval_key] >= best_eval:
                    best_eval = eval_metrics[self.eval_key]
                    self.save_model(step=epoch_idx)
                self.logger.flush()

    def train_epoch(self, data_loader, epoch):
        # Train model for one epoch, and log avg metrics
        metrics = defaultdict(float)
        for batch in tqdm(data_loader, desc='Training', leave=False):
            self.state, batch_metrics = self.train_step(self.state, batch)
            for key in batch_metrics:
                metrics[key] += batch_metrics[key]
        num_train_steps = len(data_loader)
        for key in metrics:
            avg_val = metrics[key].item() / num_train_steps
            self.logger.add_scalar('train/'+key, avg_val, global_step=epoch)

    def eval_model(self, data_loader):
        # Test model on all images of a data loader and return avg metrics
        metrics = defaultdict(float)
        count = 0
        for batch_idx, batch in enumerate(data_loader):
            batch_metrics = self.eval_step(self.state, random.PRNGKey(batch_idx), batch)
            batch_size = (batch[0] if isinstance(batch, (tuple, list)) else batch).
↪shape[0]
```

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```
            count += batch_size
            for key in batch_metrics:
                metrics[key] += batch_metrics[key] * batch_size
        metrics = {key: metrics[key].item() / count for key in metrics}
        return metrics

    def save_model(self, step=0):
        # Save current model at certain training iteration
        checkpoints.save_checkpoint(ckpt_dir=self.log_dir,
                                    target={'params': self.state.params,
                                            'batch_stats': self.state.batch_stats},
                                    step=step,
                                    overwrite=True)

    def load_model(self, pretrained=False):
        # Load model. We use different checkpoint for pretrained models
        if not pretrained:
            state_dict = checkpoints.restore_checkpoint(ckpt_dir=self.log_dir,␣
↪target=None)
        else:
            state_dict = checkpoints.restore_checkpoint(ckpt_dir=os.path.join(CHECKPOINT_
↪PATH, f'{self.model_name}.ckpt'), target=None)
        num_params = sum([np.prod(p.shape) for p in jax.tree_leaves(state_dict)])
        self.state = TrainState.create(apply_fn=self.state.apply_fn,
                                       params=state_dict['params'],
                                       batch_stats=state_dict['batch_stats'],
                                       rng=self.state.rng,
                                       tx=self.state.tx if self.state.tx else optax.
↪sgd(self.lr)  # Default optimizer
                                      )

    def checkpoint_exists(self):
        # Check whether a pretrained model exist
        return os.path.isfile(os.path.join(CHECKPOINT_PATH, f'{self.model_name}.ckpt'))
```

We specialize this training module for SimCLR below. For saving the best model checkpoint, we track the metric `acc_top5`, which describes how often the correct image patch is within the top-5 most similar examples in the batch. This is usually less noisy than the top-1 metric, making it a better metric to choose the best model from.

[16]:
```
class SimCLRTrainer(TrainerModule):

    def __init__(self, **kwargs):
        super().__init__(model_name='SimCLR',
                         model_class=SimCLR,
                         eval_key='acc_top5',
                         **kwargs)

    def create_functions(self):
        # Function to calculate the InfoNCE loss for a batch of images
        def calculate_loss(params, batch_stats, rng, batch, train):
            batch = parallel_augment(rng, batch)
            outs = self.model.apply({'params': params, 'batch_stats': batch_stats},
```

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```
                                    batch,
                                    train=train,
                                    mutable=['batch_stats'] if train else False)
            (loss, metrics), new_model_state = outs if train else (outs, None)
            return loss, (metrics, new_model_state)
        # Training function
        def train_step(state, batch):
            rng, forward_rng = random.split(state.rng)
            loss_fn = lambda params: calculate_loss(params,
                                                    state.batch_stats,
                                                    forward_rng,
                                                    batch,
                                                    train=True)
            (_, (metrics, new_model_state)), grads = jax.value_and_grad(loss_fn,
                                                                        has_
↪aux=True)(state.params)
            # Update parameters, batch statistics and PRNG key
            state = state.apply_gradients(grads=grads,
                                          batch_stats=new_model_state['batch_stats'],
                                          rng=rng)
            return state, metrics
        # Eval function
        def eval_step(state, rng, batch):
            _, (metrics, _) = calculate_loss(state.params,
                                             state.batch_stats,
                                             rng,
                                             batch,
                                             train=False)
            return metrics
        # jit for efficiency
        self.train_step = jax.jit(train_step)
        self.eval_step = jax.jit(eval_step)
```

Finally, let's prepare the data loaders and write a full training function:

[17]:
```
def numpy_collate_contrastive(batch):
    imgs1, imgs2 = [[b[0][i] for b in batch] for i in range(2)]
    return np.stack(imgs1 + imgs2, axis=0)


batch_size = 256
simclr_train_loader = data.DataLoader(unlabeled_data,
                                      batch_size=batch_size,
                                      shuffle=True,
                                      drop_last=True,
                                      collate_fn=numpy_collate_contrastive,
                                      num_workers=3,
                                      persistent_workers=True,
                                      generator=torch.Generator().manual_seed(42))
simclr_val_loader = data.DataLoader(train_data_contrast,
                                    batch_size=batch_size,
                                    shuffle=False,
```

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```
                                    drop_last=False,
                                    collate_fn=numpy_collate_contrastive,
                                    num_workers=3,
                                    persistent_workers=True)
```

A common observation in contrastive learning is that the larger the batch size, the better the models perform. A larger batch size allows us to compare each image to more negative examples, leading to overall smoother loss gradients. However, in our case, we experienced that a batch size of 256 was sufficient to get good results.

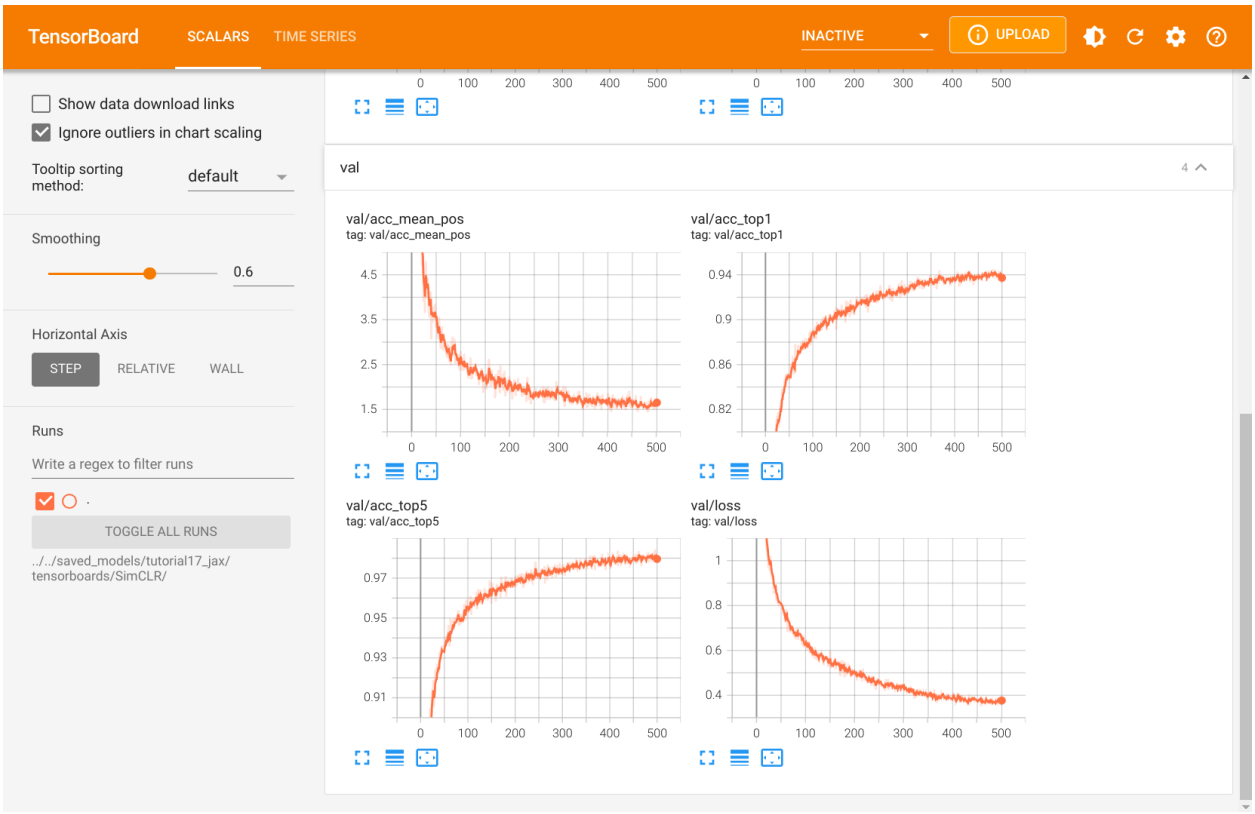
[18]:
```
def train_simclr(num_epochs=500, **kwargs):
    # Create a trainer module with specified hyperparameters
    trainer = SimCLRTrainer(exmp_imgs=parallel_augment(random.PRNGKey(0),
                                                       next(iter(simclr_train_loader))),
                            **kwargs)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(simclr_train_loader, simclr_val_loader, num_epochs=num_
↪epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)
    return trainer
```

With everything ready, let's train the model:

[19]:
```
simclr_trainer = train_simclr(hidden_dim=128,
                              lr=5e-4,
                              temperature=0.07,
                              weight_decay=1e-4,
                              num_epochs=500)
```

To get an intuition of how training with contrastive learning behaves, we can take a look at the TensorBoard below:

[20]:
```
%tensorboard --logdir ../../saved_models/tutorial17_jax/tensorboards/SimCLR/
```



One thing to note is that contrastive learning benefits a lot from long training. The shown plot above is from a training that took approx. 16 hrs on a NVIDIA GTX 1080Ti. Training the model for even longer might reduce its loss further, but we did not experience any gains from it for the downstream task on image classification. In general, contrastive learning can also benefit from using larger models, if sufficient unlabeled data is available.

4.40.2 Logistic Regression

After we have trained our model via contrastive learning, we can deploy it on downstream tasks and see how well it performs with little data. A common setup, which also verifies whether the model has learned generalized representations, is to perform Logistic Regression on the features. In other words, we learn a single, linear layer that maps the representations to a class prediction. Since the base network $f(\cdot)$ is not changed during the training process, the model can only perform well if the representations of h describe all features that might be necessary for the task. Further, we do not have to worry too much about overfitting since we have very few parameters that are trained. Hence, we might expect that the model can perform well even with very little data.

First, let's implement a simple Logistic Regression setup for which we assume that the images already have been encoded in their feature vectors. If very little data is available, it might be beneficial to dynamically encode the images during training so that we can also apply data augmentations. However, the way we implement it here is much more efficient and can be trained within a few seconds. Further, using data augmentations did not show any significant gain in this simple setup.

[21]:
```
class LogisticRegression(nn.Module):
    num_classes : int

    @nn.compact
    def __call__(self, x):
        return nn.Dense(self.num_classes)(x)
```

[22]:
```
class LGTrainer(TrainerModule):

    def __init__(self, model_suffix, **kwargs):
        super().__init__(model_name=f'LogisticRegression_{model_suffix}',
                         model_class=LogisticRegression,
                         eval_key='acc',
                         check_val_every_n_epoch=10,
                         **kwargs)

    def init_optimizer(self, num_epochs, num_steps_per_epoch):
        # We decrease the learning rate with a stepwise function
        lr_schedule = optax.piecewise_constant_schedule(
            init_value=self.lr,
            boundaries_and_scales=
                {int(num_steps_per_epoch*num_epochs*0.6): 0.1,
                 int(num_steps_per_epoch*num_epochs*0.8): 0.1}
        )
        optimizer = optax.adamw(lr_schedule, weight_decay=self.weight_decay)
        self.create_train_state(optimizer)

    def create_functions(self):
        # Function to calculate the classification loss and accuracy
        def calculate_loss(params, batch):
            imgs, labels = batch
            logits = self.model.apply({'params': params}, imgs)
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).mean()
            metrics = {'loss': loss, 'acc': acc}
            return loss, metrics
        # Training function
        def train_step(state, batch):
            (_, metrics), grads = jax.value_and_grad(calculate_loss,
                                                     has_aux=True)(state.params, batch)
            state = state.apply_gradients(grads=grads)
            return state, metrics
        # Eval function
        def eval_step(state, rng, batch):
            _, metrics = calculate_loss(state.params, batch)
            return metrics
        # jit for efficiency
        self.train_step = jax.jit(train_step)
        self.eval_step = jax.jit(eval_step)
```

The data we use is the training and test set of STL10. The training contains 500 images per class, while the test set has 800 images per class.

[23]:
```
def numpy_collate(batch):
    if isinstance(batch[0], np.ndarray):
        return np.stack(batch)
    elif isinstance(batch[0], (tuple,list)):
        transposed = zip(*batch)
        return [numpy_collate(samples) for samples in transposed]
    else:
```

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```
        return np.array(batch)


img_transforms = transforms.Compose([image_to_numpy,
                                     lambda img: (img * 2.0 - 1.0)])

train_img_data = STL10(root=DATASET_PATH, split='train', download=True,
                       transform=img_transforms)
test_img_data = STL10(root=DATASET_PATH, split='test', download=True,
                      transform=img_transforms)

print("Number of training examples:", len(train_img_data))
print("Number of test examples:", len(test_img_data))
```

```
Files already downloaded and verified
Files already downloaded and verified
Number of training examples: 5000
Number of test examples: 8000
```

Next, we implement a small function to encode all images in our datasets. The output representations are then used as inputs to the Logistic Regression model.

[24]:
```
class NumpyDataset(data.Dataset):
    # data.TensorDataset for numpy arrays

    def __init__(self, *arrays):
        self.arrays = arrays

    def __len__(self):
        return self.arrays[0].shape[0]

    def __getitem__(self, idx):
        return [arr[idx] for arr in self.arrays]
```

[25]:
```
def prepare_data_features(encode_fn, dataset):
    # Encode all images
    data_loader = data.DataLoader(dataset, batch_size=64,
                                  shuffle=False,
                                  drop_last=False,
                                  collate_fn=numpy_collate)
    feats, labels = [], []
    for batch_imgs, batch_labels in tqdm(data_loader):
        batch_feats = encode_fn(batch_imgs)
        feats.append(jax.device_get(batch_feats))
        labels.append(batch_labels)

    feats = np.concatenate(feats, axis=0)
    labels = np.concatenate(labels, axis=0)

    # Sort images by labels for easier postprocessing later
    idxs = labels.argsort()
    labels, feats = labels[idxs], feats[idxs]
```

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```
    return NumpyDataset(feats, labels)
```

Let's apply the function to both training and test set below.

[26]:
```
encode_fn = jax.jit(lambda img: simclr_trainer.model.bind(
                                        {'params': simclr_trainer.state.params,
                                         'batch_stats': simclr_trainer.state.batch_
↪stats}).encode(img))
train_feats_simclr = prepare_data_features(encode_fn, train_img_data)
test_feats_simclr = prepare_data_features(encode_fn, test_img_data)
```

```
  0%|          | 0/79 [00:00<?, ?it/s]
```

```
  0%|          | 0/125 [00:00<?, ?it/s]
```

Finally, we can write a training function as usual. We evaluate the model on the test set every 10 epochs to allow early stopping, but the low frequency of the validation ensures that we do not overfit too much on the test set.

[27]:
```
def train_logreg(batch_size, train_feats_data, test_feats_data, model_suffix, num_
↪epochs=100, **kwargs):
    # Data loaders
    train_loader = data.DataLoader(train_feats_data,
                                   batch_size=batch_size,
                                   shuffle=True,
                                   drop_last=False,
                                   generator=torch.Generator().manual_seed(42),
                                   collate_fn=numpy_collate)
    test_loader = data.DataLoader(test_feats_data,
                                  batch_size=batch_size,
                                  shuffle=False,
                                  drop_last=False,
                                  collate_fn=numpy_collate)

    # Create a trainer module with specified hyperparameters
    trainer = LGTrainer(exmp_imgs=next(iter(train_loader))[0],
                        model_suffix=model_suffix,
                        **kwargs)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(train_loader, test_loader, num_epochs=num_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)

    # Test best model on train and validation set
    train_result = trainer.eval_model(train_loader)
    test_result = trainer.eval_model(test_loader)
    result = {"train": train_result["acc"], "test": test_result["acc"]}

    return trainer, result
```

Despite the training dataset of STL10 already only having 500 labeled images per class, we will perform experiments with even smaller datasets. Specifically, we train a Logistic Regression model for datasets with only 10, 20, 50, 100, 200, and all 500 examples per class. This gives us an intuition on how well the representations learned by contrastive

learning can be transfered to a image recognition task like this classification. First, let's define a function to create the intended sub-datasets from the full training set:

[28]:
```
def get_smaller_dataset(original_dataset, num_imgs_per_label):
    new_arrays = [t.reshape(10, -1, *t.shape[1:])[:,:num_imgs_per_label].reshape(-1, *t.
↪shape[1:])
                  for t in original_dataset.arrays]
    new_dataset = NumpyDataset(*new_arrays)
    return new_dataset
```

Next, let's run all models. Despite us training 6 models, this cell could be run within a minute or two without the pretrained models.

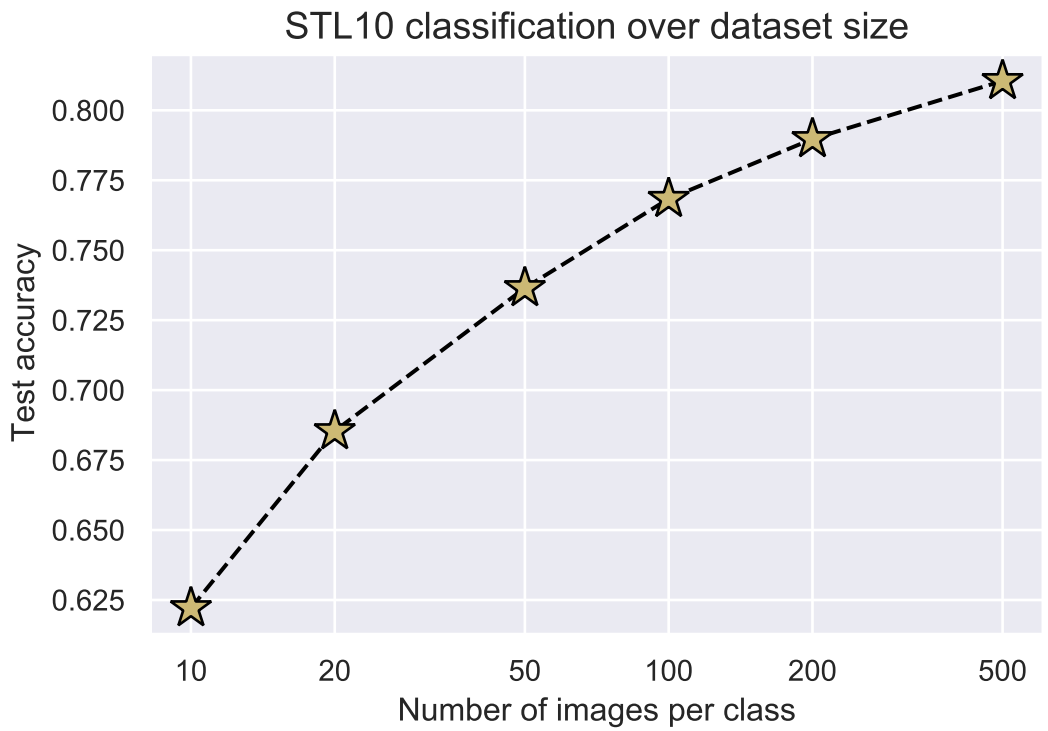
[29]:
```
results = {}
for num_imgs_per_label in [10, 20, 50, 100, 200, 500]:
    sub_train_set = get_smaller_dataset(train_feats_simclr, num_imgs_per_label)
    _, small_set_results = train_logreg(batch_size=64,
                                        train_feats_data=sub_train_set,
                                        test_feats_data=test_feats_simclr,
                                        model_suffix=num_imgs_per_label,
                                        num_classes=10,
                                        lr=1e-3,
                                        weight_decay=1e-3)
    results[num_imgs_per_label] = small_set_results
```

Finally, let's plot the results.

[30]:
```
dataset_sizes = sorted([k for k in results])
test_scores = [results[k]["test"] for k in dataset_sizes]

fig = plt.figure(figsize=(6,4))
plt.plot(dataset_sizes, test_scores, '--', color="#000", marker="*", markeredgecolor="
↪#000", markerfacecolor="y", markersize=16)
plt.xscale("log")
plt.xticks(dataset_sizes, labels=dataset_sizes)
plt.title("STL10 classification over dataset size", fontsize=14)
plt.xlabel("Number of images per class")
plt.ylabel("Test accuracy")
plt.minorticks_off()
plt.show()

for k, score in zip(dataset_sizes, test_scores):
    print(f'Test accuracy for {k:3d} images per label: {100*score:4.2f}%')
```




```
Test accuracy for  10 images per label: 62.21%
Test accuracy for  20 images per label: 68.54%
Test accuracy for  50 images per label: 73.65%
Test accuracy for 100 images per label: 76.84%
Test accuracy for 200 images per label: 78.97%
Test accuracy for 500 images per label: 81.05%
```

As one would expect, the classification performance improves the more data we have. However, with only 10 images per class, we can already classify more than 60% of the images correctly. This is quite impressive, considering that the images are also higher dimensional than e.g. CIFAR10. With the full dataset, we achieve an accuracy of 81%. The increase between 50 to 500 images per class might suggest a linear increase in performance with an exponentially larger dataset. However, with even more data, we could also finetune $f(\cdot)$ in the training process, allowing for the representations to adapt more to the specific classification task given.

To set the results above into perspective, we will train the base network, a ResNet-18, on the classification task from scratch.

4.40.3 Baseline

As a baseline to our results above, we will train a standard ResNet-18 with random initialization on the labeled training set of STL10. The results will give us an indication of the advantages that contrastive learning on unlabeled data has compared to using only supervised training. The implementation of the model is straightforward since the ResNet architecture is provided in the flaxmodels library.

[31]:
```
class ResNet(nn.Module):
    num_classes : int

    @nn.compact
```

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```
    def __call__(self, x, train=True):
        return flaxmodels.ResNet18(output='logits',
                                   pretrained=False,
                                   normalize=False,
                                   num_classes=self.num_classes)(x, train=train)
```

It is clear that the ResNet easily overfits on the training data since its parameter count is more than 1000 times larger than the dataset size. To make the comparison to the contrastive learning models fair, we apply data augmentations similar to the ones we used before: horizontal flip, crop-and-resize, grayscale, and gaussian blur. Color distortions as before are not used because the color distribution of an image showed to be an important feature for the classification. Hence, we observed no noticeable performance gains when adding color distortions to the set of augmentations. Similarly, we restrict the resizing operation before cropping to the max. 125% of its original resolution, instead of 1250% as done in SimCLR. This is because, for classification, the model needs to recognize the full object, while in contrastive learning, we only want to check whether two patches belong to the same image/object. Hence, the chosen augmentations below are overall weaker than in the contrastive learning case.

Following the same setup as for SimCLR, we apply the resizing augmentation in the data loading, and the remaining augmentations efficiently on GPU.

[32]:
```
train_transforms = transforms.Compose([transforms.RandomResizedCrop(size=96, scale=(0.8,␣
↪1.0)),
                                       image_to_numpy])

train_img_aug_data = STL10(root=DATASET_PATH, split='train', download=True,
                           transform=train_transforms)
```

```
Files already downloaded and verified
```

[33]:
```
def augment_image_for_classification(rng, img):
    rngs = random.split(rng, 3)
    # Random left-right flip
    img = dm_pix.random_flip_left_right(rngs[0], img)
    # Random grayscale
    should_gs = random.bernoulli(rngs[1], p=0.2)
    img = jax.lax.cond(should_gs,  # Only apply grayscale if true
                       lambda x: dm_pix.rgb_to_grayscale(x, keep_dims=True),
                       lambda x: x,
                       img)
    # Gaussian blur
    sigma = random.uniform(rngs[2], shape=(1,), minval=0.1, maxval=0.5)
    img = dm_pix.gaussian_blur(img, sigma=sigma[0], kernel_size=9)
    # Normalization
    img = img * 2.0 - 1.0
    return img

resnet_augm = jax.jit(lambda rng, imgs: jax.vmap(augment_image_for_
↪classification)(random.split(rng, imgs.shape[0]), imgs))
```

Using this augmentation function, we can define our trainer module, which is an extension of the Logistic Regression trainer to tracking BatchNorm statistics and augmentations.

[34]:
```
class RNTrainer(TrainerModule):
```

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```
    def __init__(self, **kwargs):
        super().__init__(model_name=f'ResNet',
                         model_class=ResNet,
                         eval_key='acc',
                         check_val_every_n_epoch=2,
                         **kwargs)

    def init_optimizer(self, num_epochs, num_steps_per_epoch):
        # We decrease the learning rate with a stepwise function
        lr_schedule = optax.piecewise_constant_schedule(
            init_value=self.lr,
            boundaries_and_scales=
                {int(num_steps_per_epoch*num_epochs*0.7): 0.1,
                 int(num_steps_per_epoch*num_epochs*0.9): 0.1}
        )
        optimizer = optax.adamw(lr_schedule, weight_decay=self.weight_decay)
        self.create_train_state(optimizer)

    def create_functions(self):
        # Function to calculate the classification loss and accuracy
        def calculate_loss(params, batch_stats, rng, batch, train):
            imgs, labels = batch
            if train:
                imgs = resnet_augm(rng, imgs)
            outs = self.model.apply({'params': params, 'batch_stats': batch_stats},
                                    imgs,
                                    train=train,
                                    mutable=['batch_stats'] if train else False)
            logits, new_model_state = outs if train else (outs, None)
            loss = optax.softmax_cross_entropy_with_integer_labels(logits, labels).mean()
            acc = (logits.argmax(axis=-1) == labels).mean()
            metrics = {'loss': loss, 'acc': acc}
            return loss, (metrics, new_model_state)
        # Training function
        def train_step(state, batch):
            rng, forward_rng = random.split(state.rng)
            loss_fn = lambda params: calculate_loss(params,
                                                    state.batch_stats,
                                                    forward_rng,
                                                    batch,
                                                    train=True)
            # Get loss, gradients for loss, and other outputs of loss function
            (_, (metrics, new_model_state)), grads = jax.value_and_grad(loss_fn,
                                                                        has_
↪aux=True)(state.params)
            # Update parameters, batch statistics and PRNG key
            state = state.apply_gradients(grads=grads,
                                          batch_stats=new_model_state['batch_stats'],
                                          rng=rng)
            return state, metrics
        # Eval function
        def eval_step(state, rng, batch):
```

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```
            _, (metrics, _) = calculate_loss(state.params,
                                             state.batch_stats,
                                             rng,
                                             batch,
                                             train=False)
            return metrics
        # jit for efficiency
        self.train_step = jax.jit(train_step)
        self.eval_step = jax.jit(eval_step)
```

The training function for the ResNet is almost identical to the Logistic Regression setup. Note that we allow the ResNet to perform validation every 2 epochs to also check whether the model overfits strongly in the first iterations or not.

[35]:
```
def train_resnet(batch_size, num_epochs=100, **kwargs):
    # Data loaders
    train_loader = data.DataLoader(train_img_aug_data,
                                   batch_size=batch_size,
                                   shuffle=True,
                                   drop_last=False,
                                   generator=torch.Generator().manual_seed(42),
                                   num_workers=3,
                                   persistent_workers=True,
                                   collate_fn=numpy_collate)
    test_loader = data.DataLoader(test_img_data,
                                  batch_size=batch_size,
                                  shuffle=False,
                                  drop_last=False,
                                  num_workers=3,
                                  persistent_workers=True,
                                  collate_fn=numpy_collate)

    # Create a trainer module with specified hyperparameters
    trainer = RNTrainer(exmp_imgs=next(iter(train_loader))[0],
                        **kwargs)
    if not trainer.checkpoint_exists():  # Skip training if pretrained model exists
        trainer.train_model(train_loader, test_loader, num_epochs=num_epochs)
        trainer.load_model()
    else:
        trainer.load_model(pretrained=True)

    # Test best model on validation/test set
    test_result = trainer.eval_model(test_loader)
    result = {"test": test_result["acc"]}

    return trainer, result
```

Finally, let's train the model and check its results:

[36]:
```
resnet_model, resnet_result = train_resnet(batch_size=64,
                                           num_classes=10,
                                           lr=1e-3,
                                           weight_decay=2e-4,
```

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```
                                                num_epochs=100)
print(f"Accuracy on test set: {resnet_result['test']:4.2%}")
```

```
Accuracy on test set: 71.64%
```

The ResNet trained from scratch achieves 71.64% on the test set. This is almost 8% less than the contrastive learning model, and even slightly less than SimCLR achieves with 1/10 of the data. This shows that self-supervised, contrastive learning provides considerable performance gains by leveraging large amounts of unlabeled data when little labeled data is available.

4.40.4 Conclusion

In this tutorial, we have discussed self-supervised contrastive learning and implemented SimCLR as an example method. We have applied it to the STL10 dataset and showed that it can learn generalizable representations that we can use to train simple classification models. With 500 images per label, it achieved an 8% higher accuracy than a similar model solely trained from supervision and performs on par with it when only using a tenth of the labeled data. Our experimental results are limited to a single dataset, but recent works such as Ting Chen et al. showed similar trends for larger datasets like ImageNet. Besides the discussed hyperparameters, the size of the model seems to be important in contrastive learning as well. If a lot of unlabeled data is available, larger models can achieve much stronger results and come close to their supervised baselines. Further, there are also approaches for combining contrastive and supervised learning, leading to performance gains beyond supervision (see Khosla et al.). Moreover, contrastive learning is not the only approach to self-supervised learning that has come up in the last two years and showed great results. Other methods include distillation-based methods like BYOL and redundancy reduction techniques like Barlow Twins. There is a lot more to explore in the self-supervised domain, and more, impressive steps ahead are to be expected.

References

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If you found this tutorial helpful, consider -ing our repository.
For any questions, typos, or bugs that you found, please raise an issue on GitHub.

4.41 GDL - Regular Group Convolutions

Filled notebook:

Pre-trained models:
Authors: David Knigge

4.41.1 0. Introduction

In this notebook, we will be implementing regular group convolutional networks from scratch, only making use of PyTorch primitives. The goal is to get familiar with the practical considerations to take into account when actually implementing these convolutional networks.

You will be asked to fill in some gaps yourself. The pieces of code you are expected to fill in are surrounded by demarcations, like so:

```
a = 1
b = 2

# We calculate c = a + b

### YOUR CODE STARTS HERE ###
c = ...
### AND ENDS HERE ###
```

And you'd be expected to fill in something along the lines of `c = a + b` for `c = ...`. We've included some assertions to test for correctness of resulting tensor shapes.

We've also scattered some questions throughout the notebook to test your understanding of the implementation and concepts used. Please include your answers to these questions (and any other observations you deem relevant!) in your report.

If you'd like a refresher of the lecture, here we give a brief overview of the operations we are going to work with / implement. These will be treated more extensively below. For simplicity of notation, here we assume each CNN layer consists of only a single channel. Questions and feedback may be forwarded to David Knigge; d.m.knigge@uva.nl.

0.1 Brief recap on CNNs

Conventional CNNs make use of the convolution operator, here defined over $\mathbb{R}^2$ for a signal $f : \mathbb{R}^2 \to \mathbb{R}$ and a kernel $k : \mathbb{R}^2 \to \mathbb{R}$ at $\mathbf{x} \in \mathbb{R}^2$:

$$(f * k)(\mathbf{x}) = \int_{\mathbb{R}^2} f(\tilde{\mathbf{x}}) k(\tilde{\mathbf{x}} - \mathbf{x}) \mathrm{d}\tilde{\mathbf{x}},$$

As we can see, the convolution operation comes down to an inner product of the function f and a shifted kernel k.

Sidenote: In reality CNNs implement a discretised version of this operation;

$$\begin{aligned}(f * k)(\mathbf{x}) &= \sum_{\tilde{\mathbf{x}} \in \mathbb{Z}^2} f(\tilde{\mathbf{x}}) k(\mathbf{x} - \tilde{\mathbf{x}}) \Delta\tilde{\mathbf{x}} \\ &= \sum_{\tilde{\mathbf{x}} \in \mathbb{Z}^2} f(\tilde{\mathbf{x}}) k(\mathbf{x} - \tilde{\mathbf{x}})\end{aligned}$$

> Where above, since pixels in an image are generally evenly spaced, we set $\Delta\tilde{\mathbf{x}} = 1$. For this recap we stay in the continuous domain for simplicity.

In convolution layers, like PyTorch's `Conv2D` implementation, the above operation is carried out for every $\mathbf{x} \in \mathbb{Z}^2$ (limited of course to the domain over which the image is defined). Because the same set of weights is used throughout the input, the output of this operation is equivariant to transformations from the translation group $\mathbb{R}^2$. Furthermore f, k usually consist of a number of channels, which are all summed over.

In this tutorial, we will use PyTorch's `torch.nn.functional.conv2d()` function to perform this integration operation at every position in input feature map. This saves us having to implement the convolution operation ourselves.

0.2 Brief recap on GCNNs

In regular group convolutions, the goal is to have a CNN of which are not only equivariant to translations $\mathbb{R}^2$, but which are also equivariant to another (usually broader) group of interest G. We focus specifically on groups which are combinations of translations $\mathbb{R}^2$ and some group of interest H. In this tutorial we keep to the group of 90 degree rotations in 2D; the Cyclic group of order 4 $H = C_4$.

We will operate on 2D images, generally defined on $\mathbb{R}^2$, as such, the first step in constructing a network which can track under which *pose* (read: transformation from a group $G = \mathbb{R}^2 \rtimes H$) a feature in the input occurs, we need to transfer our signal to a domain in which the same feature under a different pose is disentangled. This happens through *the lifting convolution*, which maps features in our input signal $f_{in} : \mathbb{R}^2 \to \mathbb{R}$ to a feature map on the group $f_{out} : G \to \mathbb{R}$. For a signal and kernel f, k both defined on $\mathbb{R}^2$, and a group element $g = (\boldsymbol{x}, h) \in G = \mathbb{R}^2 \rtimes H$:

$$(f *_{\text{lifting}} k)(g) = \int_{\mathbb{R}^2} f(\tilde{\mathbf{x}}) k_h(\tilde{\mathbf{x}} - \mathbf{x}) \, \mathrm{d}\tilde{\mathbf{x}}.$$

Where k_h is the kernel $k : \mathbb{R}^2 \to \mathbb{R}$ transformed under the regular representation $\mathcal{L}_h$ of a group element $h \in H$; $k_h = \frac{1}{|h|} \mathcal{L}_h[k]$.

> Sidenote: The factor $\frac{1}{|h|}$, with $|h|$ the determinant of the matrix representation of h in $\mathbb{R}^2$, accounts for a possible change in volume on $\mathbb{R}^2$ that h might have. Working with the cyclic group, we don't encounter this problem (the determinant of a rotation matrix is 1, volumes are invariant to rotations on $\mathbb{R}^2$), but if you'd like to implement equivariance to for example the dilation group, this becomes important.

Next, now that we have a feature map defined on the group; $f_{out} : G \to \mathbb{R}$, we apply group convolutions, extending the convolution operation to an integral over the entire group G;

$$\begin{aligned}
(f *_{\text{group}} k)(g) &= \int_G f(\tilde{g}) k(g^{-1} \cdot \tilde{g}) \mathrm{d}\tilde{g} \\
&= \int_{\mathbb{R}^2} \int_H f(\tilde{\mathbf{x}}, \tilde{h}) \mathcal{L}_x \mathcal{L}_h k(\tilde{\mathbf{x}}, \tilde{h}) \frac{1}{|h|} \, \mathrm{d}\tilde{\mathbf{x}} \, \mathrm{d}\tilde{h} \\
&= \int_{\mathbb{R}^2} \int_H f(\tilde{\mathbf{x}}, \tilde{h}) k(h^{-1}(\tilde{\mathbf{x}} - \mathbf{x}), h^{-1} \cdot \tilde{h}) \frac{1}{|h|} \, \mathrm{d}\tilde{\mathbf{x}} \, \mathrm{d}\tilde{h}.
\end{aligned}$$

The main difference with the lifting convolution is that the signal and kernel f, k are both functions on G;$G \to \mathbb{R}$, and the integral reflects this by extending over the entire group G. Other than that, there is little difference!

After a number of such group convolutional layers, we will want to ultimately obtain a representation that is invariant to the group action. We can do this by performing a projection which collapses our function defined over G to a single point, with an operation that is invariant to the group action (summing, averaging, max, min).

After this short refresher, let's get to coding!

0.3 Installing and importing some useful packages

Here we install and import some libraries that we will use throughout this tutorial. We use the PyTorch as our deep learning framework of choice. Note that for ease of model training and tracking, we additionally make use of PyTorch Lightning.

[1]:
```
## Standard libraries
import os
import numpy as np
import math
from PIL import Image
from functools import partial

## Imports for plotting
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline

## PyTorch
import torch
import torch.nn as nn
import torch.utils.data as data
import torch.optim as optim
## Torchvision
import torchvision
from torchvision.datasets import MNIST
from torchvision import transforms
## PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip3 install pytorch-lightning>=1.4 --quiet
    import pytorch_lightning as pl
import pytorch_lightning as pl
from pytorch_lightning.callbacks import LearningRateMonitor, ModelCheckpoint
```

[2]:
```
# Path to the folder where the datasets are be downloaded (e.g. MNIST)
DATASET_PATH = "../../data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "../../saved_models/DL2/GDL"

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.determinstic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
```

[3]:
```
import urllib.request
from urllib.error import HTTPError
# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/DL2/GDL/"
# Files to download
```

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```
files = ["paprika.tiff"]
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try to download the file from the GDrive␣
↪folder, or contact the author with the full output including the following error:\n",␣
↪e)
```

```
Downloading https://raw.githubusercontent.com/phlippe/saved_models/main/DL2/GDL/paprika.
↪tiff...
```

4.41.2 1. Group theory

1.1 What is a group?

To start off, we recap some of the group theoretical preliminaries. Recall that a group is defined by a tuple $(G, \cdot)$, where G is a set of group elements and $\cdot$ the binary group action which tells us how elements $g \in G$ combine. The group action $\cdot$ needs to satisfy:

1. Closure. G is closed under $\cdot$; for all $g_1, g_2 \in G$ we have $g_1 \cdot g_2 \in G$.
2. Identity. There exists an identity element e s.t. for each $g \in G$, we have $e \cdot g = g \cdot e = g$.
3. Inverse. For every element $g \in G$ we have an element $g^{-1} \in G$, s.t. $g \cdot g^{-1} = e$.
4. Associativity. For every set of elements $g_1, g_2, g_3 \in G$, we have $(g_1 \cdot g_2) \cdot g_3 = g_1 \cdot (g_2 \cdot g_3)$.

The group can have an action on functions defined on $\mathbb{R}^2$, which we can instantiate through the *regular representation* $\mathcal{L}_g^{\mathbb{G} \to \mathbb{R}^2}$. For simplicity, we write $\mathcal{L}_g$. It is given by:

$$\mathcal{L}_g f(\mathbf{x}) = f(g^{-1} \cdot \mathbf{x})$$

Where we write the action of g^{-1} on x as $g^{-1} \cdot \mathbf{x}$. This is where the regular group convolution gets its name; because of its use of the regular representation to transform the kernels k used throughout the network.

1.2 Implementing a group in python

Let's start out with a baseclass in which we outline which functions we are going to need when working with groups in our setting. As we're going to use `torch` in our implementation of group convolutional neural networks, let us implement the group as a `torch` module as well.

We first specify a base class `GroupBase` in which we specify all necessary properties and operations that we need in our treatment of group convolutional neural networks. The idea is that in our implementation of group convolutions, implementing these functions is necessary and sufficient for extending group convolutional neural networks to other groups. In other words; if you'd like to implement group convolutions equivariant to a new group you find interesting,

just inherit this baseclass, implement its methods, and you're good to go. (In practice this only faithfully works for discrete, compact groups).

[4]:
```
class GroupBase(torch.nn.Module):

    def __init__(self, dimension, identity):
        """ Implements a group.

        @param dimension: Dimensionality of the group (number of dimensions in the basis␣
↪of the algebra).
        @param identity: Identity element of the group.
        """
        super().__init__()
        self.dimension = dimension
        self.register_buffer('identity', torch.Tensor(identity))

    def elements(self):
        """ Obtain a tensor containing all group elements in this group.

        """
        raise NotImplementedError()

    def product(self, h, h_prime):
        """ Defines group product on two group elements.

        @param h: Group element 1
        @param h_prime: Group element 2
        """
        raise NotImplementedError()

    def inverse(self, h):
        """ Defines inverse for group element.

        @param h: A group element from subgroup H.
        """
        raise NotImplementedError()

    def left_action_on_R2(self, h, x):
        """ Group action of an element from the subgroup H on a vector in R2.

        @param h: A group element from subgroup H.
        @param x: Vectors in R2.
        """
        raise NotImplementedError()

    def matrix_representation(self, h):
        """ Obtain a matrix representation in R^2 for an element h.

        @param h: Group element
        """
        raise NotImplementedError()

    def determinant(self, h):
```

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```
        """ Calculate the determinant of the representation of a group element
        h.

        @param g:
        """
        raise NotImplementedError()

    def normalize_group_parameterization(self, h):
        """ Map the group elements to an interval [-1, 1]. We use this to create
        a standardized input for obtaining weights over the group.

        @param g:
        """
        raise NotImplementedError()
```

1.3 Implementing the cyclic group C_4

As an example, let's discuss a relatively simple group; the group of all 90 rotations of the plane, otherwise known as the cyclic group C_4. Note:

- The set of group elements of C_4 is given by $G := \{e, g, g^2, g^3\}$. We can parameterise these group elements using rotation angles θ, i.e. $e = 0, g = \frac{1}{2}\pi, g^2 = \pi, \ldots$
- The group product is then given by $g \cdot g' := \theta + \theta' \mod 2\pi$.
- The inverse is given by: $g^{-1} = -\theta \mod 2\pi$.
- The group C_4 has an action on the euclidean plane in 2 dimensions $\mathbb{R}^2$ given by a rotation matrix;

$$R_\theta : \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}.$$

  This gives us the regular representation $\mathcal{L}_\theta$ on functions f defined over $\mathbb{R}^2$:

$$\mathcal{L}_\theta f(\mathbf{x}) = f(R_{-\theta \mod 2\pi}\mathbf{x}).$$

Let's implement this group!

[ ]:
```
class CyclicGroup(GroupBase):

    def __init__(self, order):
        super().__init__(
            dimension=1,
            identity=[0.]
        )

        assert order > 1
        self.order = torch.tensor(order)

    def elements(self):
        """ Obtain a tensor containing all group elements in this group.

        @returns elements: Tensor containing group elements of shape [self.order]
```

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```
        """
        return torch.linspace(
            start=0,
            end=2 * np.pi * float(self.order - 1) / float(self.order),
            steps=self.order,
            device=self.identity.device
        )

    def product(self, h, h_prime):
        """ Defines group product on two group elements of the cyclic group C4.

        @param h: Group element 1
        @param h_prime: Group element 2

        @returns product: Tensor containing h \cdot h_prime with \cdot the group action.
        """
        # As we directly parameterize the group by its rotation angles, this
        # will be a simple addition. Don't forget the closure property though!

        ## YOUR CODE STARTS HERE ##
        product = ...
        ## AND ENDS HERE ##

        return product

    def inverse(self, h):
        """ Defines group inverse for an element of the cyclic group C4.

        @param h: Group element

        @returns inverse: Tensor containing h^{-1}.
        """
        # Implement the inverse operation. Keep the closure property in mind!

        ## YOUR CODE STARTS HERE ##
        inverse = ...
        ## AND ENDS HERE ##

        return inverse

    def left_action_on_R2(self, h, x):
        """ Group action of an element from the subgroup H on a vector in R2.

        @param h: A group element from subgroup H.
        @param x: Vectors in R2.

        @returns transformed_x: Tensor containing \rho(h)x.
        """
        # Transform the vector x with h, recall that we are working with a left-regular␣
↪representation,
        # meaning we transform vectors in R^2 through left-matrix multiplication.
        transformed_x = torch.tensordot(self.matrix_representation(h), x, dims=1)
```

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```
        return transformed_x

    def matrix_representation(self, h):
        """ Obtain a matrix representation in R^2 for an element h.

        @param h: A group element.

        @returns representation: Tensor containing matrix representation of h, shape [2,␣
↪2].
        """
        ## YOUR CODE STARTS HERE ##
        representation = ...
        ## AND ENDS HERE ##

        return representation

    def normalize_group_elements(self, h):
        """ Normalize values of group elements to range between -1 and 1.
        The group elements range from 0 to 2pi * (self.order - 1) / self.order,
        so we normalize accordingly.

        @param h: A group element.
        @return normalized_h: Tensor containing normalized value corresponding to␣
↪element h.
        """
        largest_elem = 2 * np.pi * (self.order - 1) / self.order
        normalized_h = (2*h / largest_elem) - 1.
        return normalized_h
```

[ ]:
```
# Some tests to verify our implementation.
c4 = CyclicGroup(order=4)
e, g1, g2, g3 = c4.elements()

assert c4.product(e, g1) == g1 and c4.product(g1, g2) == g3
assert c4.product(g1, c4.inverse(g1)) == e

assert torch.allclose(c4.matrix_representation(e), torch.eye(2))
assert torch.allclose(c4.matrix_representation(g2), torch.tensor([[-1, 0], [0, -1]]).
↪float(), atol=1e-6)

assert torch.allclose(c4.left_action_on_R2(g1, torch.tensor([0., 1.])), torch.tensor([-1.
↪, 0.]), atol=1e-7)
```

1.4 Visualizing the group action

Let's play around with the group implementation we have just created! We'll have a look at the group action on some vegetables.

[ ]:
```
# Load image from disk.
img = Image.open(os.path.join(CHECKPOINT_PATH, "paprika.tiff"))

# Convert to torch tensor.
img_tensor = transforms.ToTensor()(img)
img
```

To obtain pixel values for the transformed image grid, we'll use a pytorch function: `grid_sample` function (link to docs). Feel free to go through the docs to understand precisely what this function does, but it should be enough just to know that we use this function for bilinear and trilinear interpolation to obtain kernel weight values for rotated kernel grids.

[ ]:
```
def bilinear_interpolation(signal, grid):
    """ Obtain signal values for a set of gridpoints through bilinear interpolation.

    @param signal: Tensor containing pixel values [C, H, W] or [N, C, H, W]
    @param grid: Tensor containing coordinate values [2, H, W] or [2, N, H, W]
    """
    # If signal or grid is a 3D array, add a dimension to support grid_sample.
    if len(signal.shape) == 3:
        signal = signal.unsqueeze(0)
    if len(grid.shape) == 3:
        grid = grid.unsqueeze(1)

    # Grid_sample expects [N, H, W, 2] instead of [2, N, H, W]
    grid = grid.permute(1, 2, 3, 0)

    # Grid sample expects YX instead of XY.
    grid = torch.roll(grid, shifts=1, dims=-1)

    return torch.nn.functional.grid_sample(
        signal,
        grid,
        padding_mode='zeros',
        align_corners=True,
        mode="bilinear"
    )

def trilinear_interpolation(signal, grid):
    """

    @param signal: Tensor containing pixel values [C, D, H, W] or [N, C, D, H, W]
    @param grid: Tensor containing coordinate values [3, D, H, W] or [3, N, D, H, W]
    """
    # If signal or grid is a 4D array, add a dimension to support grid_sample.
    if len(signal.shape) == 4:
        signal = signal.unsqueeze(0)
    if len(grid.shape) == 4:
        grid = grid.unsqueeze(1)
```

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```
    # Grid_sample expects [N, D, H, W, 3] instead of [3, N, D, H, W]
    grid = grid.permute(1, 2, 3, 4, 0)

    # Grid sample expects YX instead of XY.
    grid = torch.roll(grid, shifts=1, dims=-1)

    return torch.nn.functional.grid_sample(
        signal,
        grid,
        padding_mode='zeros',
        align_corners=True,
        mode="bilinear" # actually trilinear in this case...
    )
```

[ ]:
```
# This creates a grid of the pixel locations in our image of [2, 512, 512] since
# our image is 2 dimensional and has a width and height of 512 pixels.
img_grid = torch.stack(torch.meshgrid(
    torch.linspace(-1, 1, img_tensor.shape[-2]),
    torch.linspace(-1, 1, img_tensor.shape[-1]),
    indexing='ij'
))

# Let's create the group of 90 degree clockwise rotations.
c4 = CyclicGroup(order=4)
e, g1, g2, _ = c4.elements()

# Create a counterclockwise rotation of 270 degrees using only e, g1 and g2.

## YOUR CODE STARTS HERE ##
g3 = ...
## AND ENDS HERE ##

assert g3 == c4.elements()[-1]
```

[ ]:
```
# Transform the image grid we just created with the matrix representation of
# this group element.
transformed_img_grid = c4.left_action_on_R2(c4.inverse(g3), img_grid)

# Sample the image on the transformed grid points.
transformed_img = bilinear_interpolation(img_tensor, transformed_img_grid)[0]
```

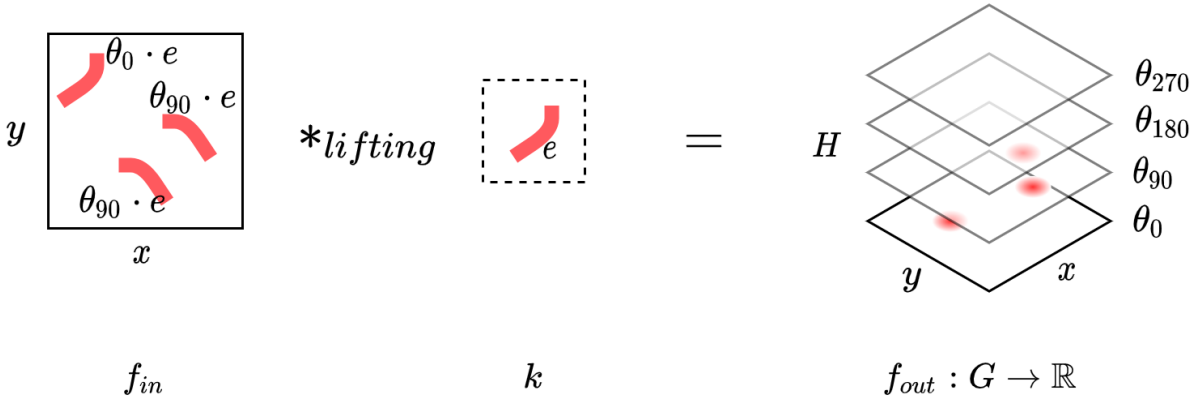
[ ]:
```
# If we turn this back into a PIL image we can see the result of our transformation!
transforms.ToPILImage()(transformed_img)
```

4.41.3 2. Group Equivariant Convolutional Networks

As discussed in the lecture, regular group convolutional neural networks consist of three main elements. The lifting convolution, group convolution and projection operation. We treat these in order.

2.1 Lifting convolution

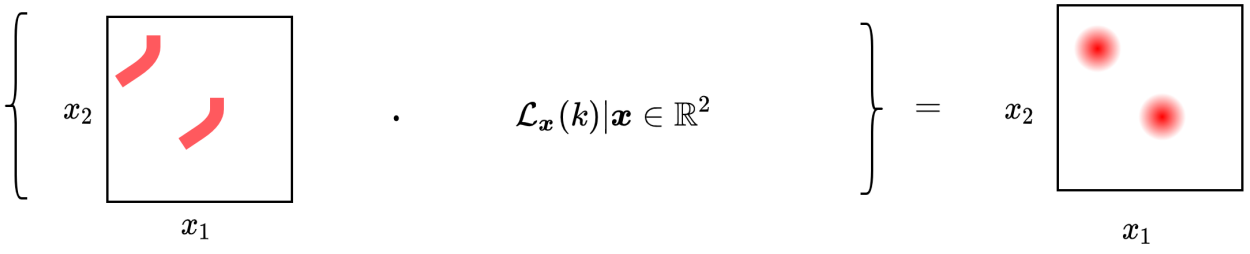
First is the lifting convolution, which disentangles features at any spatial location in the input f_{in} under transformations of H. You may think of this as registering at all locations, for a given feature e, the occurrences of transformed versions of this feature $\mathcal{L}_h(e)$, for $h \in H$. (Instead of $\mathcal{L}_h(e)$, we sometimes write $h \cdot e$ to denote the action of h on e.) The lifting convolution thus maps from $\mathbb{R}^2$ to $G = \mathbb{R}^2 \rtimes H$. As a result, our lifted feature map f_{out} has, besides the usual spatial dimensions, one or more additional group dimensions (dependent on the dimensionality of H).



For example, take the group of 90 deg rotations as H, and let's say e is a squiggle of sorts, of which we have three occurences in our input feature map f_{in}. Two are under a 90 deg rotation; $\theta_{90} \cdot e$, and one is under its canonical orientation; $\theta_0 \cdot e$. A lifting convolution with a kernel k which exactly matches the feature e would land responses at different offsets along the group dimension of the feature map; namely one at the spatial feature map corresponding to the group elements θ_0 and two at the spatial feature map corresponding to θ_{90}. See the above figure for an intuition.

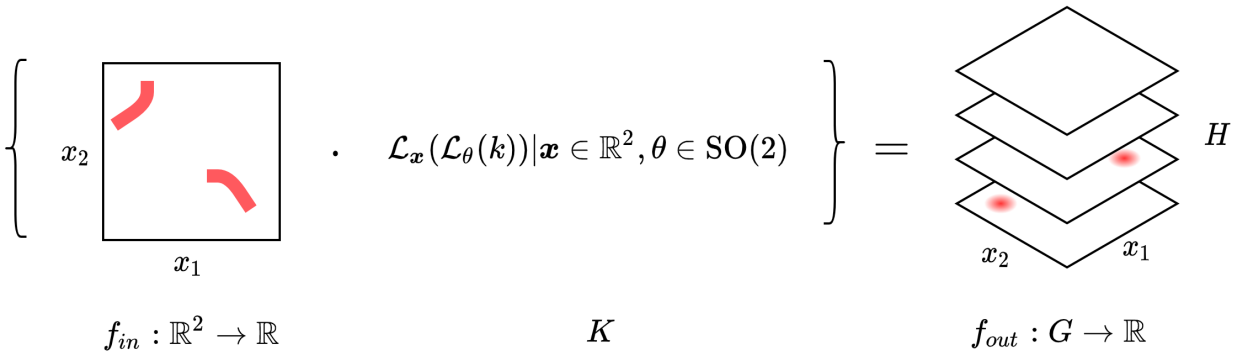
2.1.1 Overview

How do we get our convolution operation to pick up features under different transformations of H? Intuitively, it is not that different from the convolution operation as we are familiar with in CNNs. There, we enable the extraction of features at any location by sharing the same kernel over all spatial positions.



From our current group theoretic perspective, we interpret this as applying all possible translations $\boldsymbol{x} \in \mathbb{R}^2$ to our kernel k and recording the response we get when we take the inner product of the input f_{in} with this transformed

kernel $\mathcal{L}_{\mathbf{x}}(k)$. This operation starts with a feature map defined on $\mathbb{R}^2$ and also yields a feature map defined over $\mathbb{R}^2$. See above.



Now that we additionally want to register features under different group actions $\mathcal{L}_h$ for $h \in H$, we can do so by simply *also* transforming k with all of their group actions and recording the results. For example, in case of the rotation group C_4, we not only translate, but additionally rotate the kernel k by all possible 90 deg rotations, and record the responses for the resulting transformed kernels!

2.1.2 Implementing the lifting convolution kernel

Let's get to programming. First, we need to define a kernel k which we can transform under arbitrary group actions with $\mathcal{L}_h$. When working with images, a convolution kernel is generally defined as a set of independently sampled weights W defined over an equidistant discretisation of $\mathbb{R}^2$ (pixels are evenly spaced).

Recall that we can express the group action of a group H on functions (such as kernels k) defined over $\mathbb{R}^2$ through the regular representation $\mathcal{L}_h$. The regular representation transforms the function k through a transformation of the domain of the function k. In other words, the regular representation transforms the grid over which the kernel k is defined, to obtain the values for the transformed function $\mathcal{L}_h(k)$.

As such, to define a kernel k which we can transform with the regular representation of a group H, we need to construct a grid over which the kernel values are defined. We can then transform this grid by the action of each group element $h \in H$ to obtain a set of grids corresponding to transformed kernels for each of the group elements of H. Let's get to work!

Notes: * In implementing the actual lifting and group convolution operations, we will make use of PyTorch's `Conv2D` class. This simplifies our life a lot, since `Conv2D` takes cares of translating the kernels k over all input locations. Hence we do not need to implement the action of the translation group ourselves ($\mathcal{L}_{\mathbf{x}}$), but will still remain translation equivariant! Making our operations compatible with `Conv2D` requires a small amount of trickery, but we will get to that later.

[ ]:
```
class LiftingKernelBase(torch.nn.Module):

    def __init__(self, group, kernel_size, in_channels, out_channels):
        """ Implements a base class for the lifting kernel. Stores the R^2 grid
        over which the lifting kernel is defined and it's transformed copies
        under the action of a group H.

        """
        super().__init__()
        self.group = group

        self.kernel_size = kernel_size
```

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```
        self.in_channels = in_channels
        self.out_channels = out_channels

        # Create spatial kernel grid. These are the coordinates on which our
        # kernel weights are defined.
        self.register_buffer("grid_R2", torch.stack(torch.meshgrid(
            torch.linspace(-1., 1., self.kernel_size),
            torch.linspace(-1., 1., self.kernel_size),
            indexing='ij'
        )).to(self.group.identity.device))

        # Transform the grid by the elements in this group.
        self.register_buffer("transformed_grid_R2", self.create_transformed_grid_R2())

    def create_transformed_grid_R2(self):
        """Transform the created grid by the group action of each group element.
        This yields a grid (over H) of spatial grids (over R2). In other words,
        a list of grids, each index of which is the original spatial grid transformed by
        a corresponding group element in H.

        """
        # Obtain all group elements.

        ## YOUR CODE STARTS HERE ##
        group_elements = ...
        ## AND ENDS HERE ##

        # Transform the grid defined over R2 with the sampled group elements.
        # Recall how the left-regular representation acts on the domain of a
        # function on R2! (Hint: look closely at the equation given under 1.3)
        # We'd like to end up with a grid of shape [2, |H|, kernel_size, kernel_size].

        ## YOUR CODE STARTS HERE ##
        transformed_grid = ...
        ## AND ENDS HERE ##

        return transformed_grid


    def sample(self, sampled_group_elements):
        """ Sample convolution kernels for a given number of group elements

        arguments should include:
        :param sampled_group_elements: the group elements over which to sample
            the convolution kernels

        should return:
        :return kernels: filter bank extending over all input channels,
            containing kernels transformed for all output group elements.
        """
        raise NotImplementedError()
```

[ ]:
```
# Let's check whether our implementation works correctly. First we inspect the
# shape of our transformed grids to assess whether this is correct.
order = 4
lifting_kernel_base = LiftingKernelBase(
    group=CyclicGroup(order=order),
    kernel_size=7,
    in_channels=3,
    out_channels=1
)

# The grid has a shape of [2, |H|, kernel_size, kernel_size].
assert lifting_kernel_base.transformed_grid_R2.shape == torch.Size([2, 4, 7, 7])
```

[ ]:
```
plt.rcParams['figure.figsize'] = [12, 3]

# Create [group_elements] figures
fig, ax = plt.subplots(1, order)

# Get the grid
transformed_grid_R2 = lifting_kernel_base.transformed_grid_R2

# Visualize the transformed kernel grids. We mark the same cornerpoint by a
# blue 'x' in all grids as reference point.
for group_elem in range(order):
    ax[group_elem].scatter(
        transformed_grid_R2[1, group_elem, :, :],
        transformed_grid_R2[0, group_elem, :, :],
        c='r'
    )
    # Mark a corner point so we can see it transform.
    ax[group_elem].scatter(
        transformed_grid_R2[1, group_elem, 0, 0],
        transformed_grid_R2[0, group_elem, 0, 0],
        marker='x',
        c='b'
    )

fig.text(0.5, 0., 'Group elements', ha='center')
plt.show()
```

If your code is correctly implemented, you should see the counter-clockwise rotation action happening!

At this point we have a set of grids transformed under the operation of the group H. We now need to decide how we are going to sample kernel values at the grid points in each of these grids. This is where the first major hurdle in applying GCNNs occurs.

Whereas conventional CNNs get away with sharing the same set of weights over all spatial positions (which is due to the fact that we translate the kernel only with steps that match whole pixel-distances), for arbitrary groups H we may require kernel values for grid points that lie off the pixel grid of the kernel under its canonical transformation.

Of course, we could (and in fact will) use interpolation to obtain kernel values for grid locations between pixel locations, but this may be limiting in expressivity and will introduce interpolation artefacts!

Notes:

- When we are implementing equivariance for the group of 90 deg rotations, $H = C_4$, we of course could get

away without using interpolation, since all transformed grids lie share the same locations. We could implement the group action of this particular group through a permutation of the weights. But we'd like to be more general than that in this tutorial, so we'll go with interpolation instead! Luckily PyTorch has a function that allows us to sample an input on a grid; we will use PyTorch's `grid_sample` function for interpolation!

[ ]:
```
class InterpolativeLiftingKernel(LiftingKernelBase):

    def __init__(self, group, kernel_size, in_channels, out_channels):
        super().__init__(group, kernel_size, in_channels, out_channels)

        # Create and initialise a set of weights, we will interpolate these
        # to create our transformed spatial kernels.
        self.weight = torch.nn.Parameter(torch.zeros((
            self.out_channels,
            self.in_channels,
            self.kernel_size,
            self.kernel_size
        ), device=self.group.identity.device))

        # Initialize weights using kaiming uniform intialisation.
        torch.nn.init.kaiming_uniform_(self.weight.data, a=math.sqrt(5))

    def sample(self):
        """ Sample convolution kernels for a given number of group elements

        should return:
        :return kernels: filter bank extending over all input channels,
            containing kernels transformed for all output group elements.
        """
        # First, we fold the output channel dim into the input channel dim;
        # this allows us to transform the entire filter bank in one go using the
        # torch grid_sample function.

        ## YOUR CODE STARTS HERE ##
        weight = ...
        ## AND ENDS HERE ##

        # Sample the transformed kernels.
        transformed_weight = []
        for spatial_grid_idx in range(self.group.elements().numel()):
            transformed_weight.append(
                bilinear_interpolation(weight, self.transformed_grid_R2[:, spatial_grid_
↪idx, :, :])
            )
        transformed_weight = torch.stack(transformed_weight)

        # Separate input and output channels.
        transformed_weight = transformed_weight.view(
            self.group.elements().numel(),
            self.out_channels,
            self.in_channels,
            self.kernel_size,
            self.kernel_size
```

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```
        )

        # Put out channel dimension before group dimension. We do this
        # to be able to use pytorched Conv2D. Details below!
        transformed_weight = transformed_weight.transpose(0, 1)

        return transformed_weight
```

[ ]:
```
ik = InterpolativeLiftingKernel(
    group=CyclicGroup(order=4),
    kernel_size=7,
    in_channels=2,
    out_channels=1
)

weights = ik.sample()
weights.shape
```

Let's visualize the weights we sampled from our lifting convolution kernel!

[ ]:
```
# Pick an output channel to visualize
out_channel_idx = 0

# Create [in_channels, group_elements] figures
fig, ax = plt.subplots(ik.in_channels, ik.group.elements().numel())

for in_channel in range(ik.in_channels):
    for group_elem in range(ik.group.elements().numel()):
        ax[in_channel, group_elem].imshow(
            weights[out_channel_idx, group_elem, in_channel, :, :].detach().numpy()
        )

fig.text(0.5, 0.04, 'Group elements', ha='center')
fig.text(0.04, 0.5, 'Input channels', va='center', rotation='vertical')

plt.show()
```

As we can see, spatial kernel rotates under the action of the rotation group elements!

2.1.3 Implementing the lifting convolution

Finally, we can implement the lifting convolution operation! This class should take as input a feature map defined over $\mathbb{R}^2$, and spit out a feature map over $\mathbb{R}^2 \rtimes H$, where features under different transformations $h \in H$ are disentangled along the H axis!

Notes:

- To prevent having to implement our own implementation of the convolution operation, and to leverage the highly optimized pytorch `Conv2D` class, we use some neat tricks in our lifting (and group) convolution classes. Normally, a convolution layer applies a set of n spatial kernels throughout the input, where n is the number of output channels of the convolution operation. Because we now also have `num_group_elem` transformed versions of these kernels, which we want to apply everywhere in the input, we can trick PyTorch by having it treat every transformation of the same spatial kernel as a separate output channel. To do this, we simply reshape our

set of `[out_channels, num_group_elem, in_channels, kernel_size, kernel_size]` kernels into a set of `[out_channels x num_group_elem, in_channels, kernel_size, kernel_size]` kernels. See below!

- As mentioned, a great additional benefit of using the PyTorch `Conv2D` class is that we are not required to obtain translated kernels $\mathcal{L}_{\mathbf{x}}(k)$ ourselves, PyTorch takes care of that!

[ ]:
```
class LiftingConvolution(torch.nn.Module):

    def __init__(self, group, in_channels, out_channels, kernel_size, padding):
        super().__init__()

        self.kernel = InterpolativeLiftingKernel(
            group=group,
            kernel_size=kernel_size,
            in_channels=in_channels,
            out_channels=out_channels
        )

        self.padding = padding

    def forward(self, x):
        """ Perform lifting convolution

        @param x: Input sample [batch_dim, in_channels, spatial_dim_1,
            spatial_dim_2]
        @return: Function on a homogeneous space of the group
            [batch_dim, out_channels, num_group_elements, spatial_dim_1,
            spatial_dim_2]
        """

        # Obtain convolution kernels transformed under the group.

        ## YOUR CODE STARTS HERE ##
        conv_kernels = ...
        ## AND ENDS HERE ##

        # Apply lifting convolution. Note that using a reshape we can fold the
        # group dimension of the kernel into the output channel dimension. We
        # treat every transformed kernel as an additional output channel. This
        # way we can use pytorch's conv2d function!

        # Question: Do you see why we (can) do this?

        ## YOUR CODE STARTS HERE ##
        x = ...
        ## AND ENDS HERE ##

        # Reshape [batch_dim, in_channels * num_group_elements, spatial_dim_1,
        # spatial_dim_2] into [batch_dim, in_channels, num_group_elements,
        # spatial_dim_1, spatial_dim_2], separating channel and group
        # dimensions.
        x = x.view(
            -1,
```

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```
            self.kernel.out_channels,
            self.kernel.group.elements().numel(),
            x.shape[-1],
            x.shape[-2]
        )

        return x
```

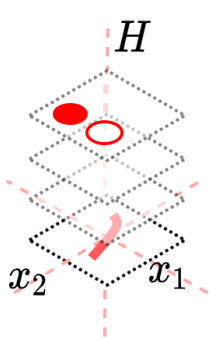
[ ]:
```
lifting_conv = LiftingConvolution(
    group=CyclicGroup(order=4),
    kernel_size=5,
    in_channels=3,
    out_channels=8,
    padding=False
)
```

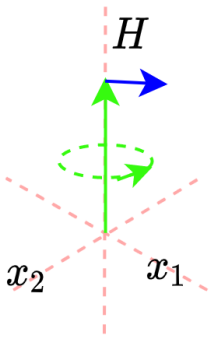
2.2 Group convolution

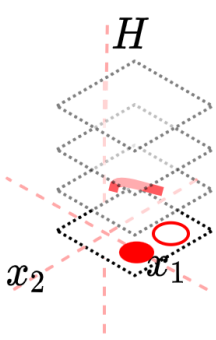
Now that we have a way to obtain feature maps defined over the group G from input functions defined over $\mathbb{R}^2$, let's move on to implementing a convolutional layer that fully operates on the group $G : \mathbb{R}^2 \rtimes H$. Note that the input feature map at this stage, f_{in}, has, besides the usual spatial dimensions defined over $\mathbb{R}^2$, one or more additional group dimensions defined over H. As such, the group convolution operation, $*_{group}$, maps from a function on the group f_{in} to another function on the group f_{out}.

2.2.1 Overview

Since the input to the group convolution layer now contains additional group dimensions; $f_{in} : \mathbb{R}^2 \rtimes H \to \mathbb{R}$, we need to convolve it with a kernel k_{group} that is also defined over the entire group; $k_{group} : \mathbb{R}^2 \rtimes H \to \mathbb{R}$. This is in contrast to the lifting convolution, where $k_{lifting}$ was only defined over the spatial domain $\mathbb{R}^2$. You could think of this kernel k_{group} as a stack of spatial kernels, a separate one for each group element $h \in H$. Importantly, since k is now *also* defined on a grid over H, the group H now also has an action *on* this H-axis of k. For example, in our case of $H = C_4$, elements $\theta \in C_4$ now not only have a rotating action on the spatial domain of the kernel, but also a translating action along the group axis. Hence, applying a group element $\theta \in C_4$ leads to a twist-shift of the k along the group axis. See below! (Remember $H = C_4$ is periodic)

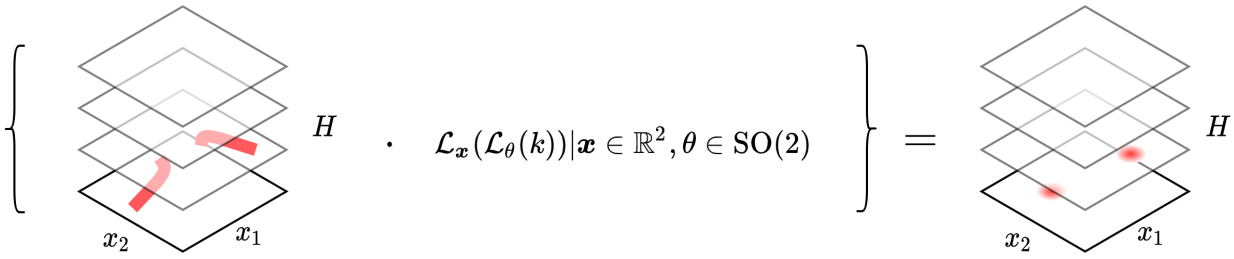






$k : G \to \mathbb{R}$ $\quad$ $\mathcal{L}_{\boldsymbol{x}_{(2,2)}} \mathcal{L}_{\theta_{90}}$ $\quad$ $\mathcal{L}_{\boldsymbol{x}_{(2,2)}} \mathcal{L}_{\theta_{90}}(k) : G \to \mathbb{R}$

Apart from this difference, the group convolution operator works in much the same way as the liting operator. We again transform the kernel k_{group} with the actions of the group H and $\mathbb{R}^2$ and obtain responses for the inner product of this kernel with the input (although again, we let PyTorch do all the work for the translation group). See below for an intuition.



$f_{in} : G \to \mathbb{R}$ $\quad$ K $\quad$ $f_{out} : G \to \mathbb{R}$

2.2.2 Implementing the group convolution kernel

Again, let's define a kernel k which we can transform with the group action. Now, our kernel grid is not only defined over $\mathbb{R}^2$, but additionally over H.

Notes:

- Since the grid over H is made up of elements $h' \in H$, transforming the grid over H with (another) group element $h \in H$ comes out to applying the group product of h with each grid element h'.
- Because we are working with semidirect product groups $\mathbb{R}^2 \rtimes H$, we can transform the $\mathbb{R}^2$ and H dimensions of our grids separately before combining them into a shared grid over $\mathbb{R}^2 \rtimes H$!

[ ]:
```
class GroupKernelBase(torch.nn.Module):

    def __init__(self, group, kernel_size, in_channels, out_channels):
        """ Implements base class for the group convolution kernel. Stores grid
        defined over the group R^2 \rtimes H and it's transformed copies under
        all elements of the group H.
```

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```
        """
        super().__init__()
        self.group = group

        self.kernel_size = kernel_size
        self.in_channels = in_channels
        self.out_channels = out_channels

        # Create a spatial kernel grid
        self.register_buffer("grid_R2", torch.stack(torch.meshgrid(
            torch.linspace(-1., 1., self.kernel_size),
            torch.linspace(-1., 1., self.kernel_size),
            indexing='ij'
        )).to(self.group.identity.device))

        # The kernel grid now also extends over the group H, as our input
        # feature maps contain an additional group dimension
        self.register_buffer("grid_H", self.group.elements())
        self.register_buffer("transformed_grid_R2xH", self.create_transformed_grid_
↪R2xH())

    def create_transformed_grid_R2xH(self):
        """Transform the created grid over R^2 \rtimes H by the group action of
        each group element in H.

        This yields a set of grids over the group. In other words, a list of
        grids, each index of which is the original grid over G transformed by
        a corresponding group element in H.
        """
        # Sample the group H.

        ## YOUR CODE STARTS HERE ##
        group_elements = ...
        ## AND ENDS HERE ##

        # Transform the grid defined over R2 with the sampled group elements.
        # We again would like to end up with a grid of shape [2, |H|, kernel_size,␣
↪kernel_size].

        ## YOUR CODE STARTS HERE ##
        transformed_grid_R2 = ...
        ## AND ENDS HERE ##

        # Transform the grid defined over H with the sampled group elements. We want a␣
↪grid of
        # shape [|H|, |H|]. Make sure to stack the transformed like above (over the 1st␣
↪dim).

        ## YOUR CODE STARTS HERE ##
        transformed_grid_H = ...
        ## AND ENDS HERE ##
```

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```
        # Rescale values to between -1 and 1, we do this to please the torch
        # grid_sample function.
        transformed_grid_H = self.group.normalize_group_elements(transformed_grid_H)

        # Create a combined grid as the product of the grids over R2 and H
        # repeat R2 along the group dimension, and repeat H along the spatial dimension
        # to create a [3, |H|, |H|, kernel_size, kernel_size] grid
        transformed_grid = torch.cat(
            (
                transformed_grid_R2.view(
                    2,
                    group_elements.numel(),
                    1,
                    self.kernel_size,
                    self.kernel_size,
                ).repeat(1, 1, group_elements.numel(), 1, 1),
                transformed_grid_H.view(
                    1,
                    group_elements.numel(),
                    group_elements.numel(),
                    1,
                    1,
                ).repeat(1, 1, 1, self.kernel_size, self.kernel_size)
            ),
            dim=0
        )
        return transformed_grid


    def sample(self, sampled_group_elements):
        """ Sample convolution kernels for a given number of group elements

        arguments should include:
        :param sampled_group_elements: the group elements over which to sample
            the convolution kernels

        should return:
        :return kernels: filter bank extending over all input channels,
            containing kernels transformed for all output group elements.
        """
        raise NotImplementedError()
```

Let's get some intuition for what is happening with our grid when we apply the group action of H to it. First we will inspect the action on $\mathbb{R}^2$.

In our current setting, H is one-dimensional, and as we can see, transforming the grid over H with all group elements of H leads to a translation over the group. Next, let's see what happens when we combine these grids.

[ ]:
```
gk_base = GroupKernelBase(
    group=CyclicGroup(order=4),
    kernel_size=7,
    in_channels=1,
    out_channels=1
```

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```
)

gk_base.transformed_grid_R2xH.shape
```

[ ]:
```
plt.rcParams['figure.figsize'] = [10, 3]

# Create [group_elements] figures.
fig, ax = plt.subplots(
    1,
    gk_base.group.elements().numel(),
    subplot_kw=dict(projection='3d')
)

# Flatten spatial and group grid dimensions.
transformed_grid_R2xH = gk_base.transformed_grid_R2xH.reshape(
    3,
    gk_base.group.elements().numel(),
    gk_base.group.elements().numel() * gk_base.kernel_size * gk_base.kernel_size
)

# Visualize the transformed kernel grids. We mark the same row by a blue 'x' in all grids␣
↪as reference point.
for group_elem in range(gk_base.group.elements().numel()):
    ax[group_elem].scatter(transformed_grid_R2xH[1, group_elem, 1:],
                           transformed_grid_R2xH[0, group_elem, 1:],
                           transformed_grid_R2xH[2, group_elem, 1:],
                           c='r')
    ax[group_elem].scatter(transformed_grid_R2xH[1, group_elem, 0],
                           transformed_grid_R2xH[0, group_elem, 0],
                           transformed_grid_R2xH[2, group_elem, 0],
                           marker='x',
                           c='b')

fig.text(0.5, 0.04, 'Group elements', ha='center')

plt.show()
```

As we can see, under the application of group elements $h' \in H$ the grid defined over $\mathbb{R}^2 \rtimes H$ rotates over the spatial dimensions, and shifts along the group dimension!

Let's now implement the group kernel using interpolation as well.

Notes: * For multidimensional groups H the following implementation won't work, as this would require kernels defined on grids with dimensionality > 3, which our implementation of trilinear interpolation with `grid_sample` does not support. To resolve this, one could implement the sampling of the weights along the H dimension using a translation of the weight matrix along the H dimensions, and only interpolate over the spatial dimensions. This is possible because we don't end up between grid points along the group dimension H (remember the closure constraint of the group product?). * The C_4 group exhibits periodicity along the group axis, so our kernels should too. Although we correctly implemented the group product to reflect this, `grid_sample` doesn't know about the periodicity of the weights in its interpolation. This shouldn't be a problem since, again because of the closure constraint, we should always end up exactly on grid points along the group axis, meaning no interpolation is necessary in that direction. In practice, because of the way `grid_sample` is implemented, we may encounter some small interpolation artefacts because of this.

[ ]:
```
class InterpolativeGroupKernel(GroupKernelBase):

    def __init__(self, group, kernel_size, in_channels, out_channels):
        super().__init__(group, kernel_size, in_channels, out_channels)

        # create and initialise a set of weights, we will interpolate these
        # to create our transformed spatial kernels. Note that our weight
        # now also extends over the group H.

        ## YOUR CODE STARTS HERE ##
        self.weight = ...
        ## AND ENDS HERE ##

        # initialize weights using kaiming uniform intialisation.
        torch.nn.init.kaiming_uniform_(self.weight.data, a=math.sqrt(5))

    def sample(self):
        """ Sample convolution kernels for a given number of group elements

        should return:
        :return kernels: filter bank extending over all input channels,
            containing kernels transformed for all output group elements.
        """
        # First, we fold the output channel dim into the input channel dim;
        # this allows us to transform the entire filter bank in one go using the
        # interpolation function.

        ## YOUR CODE STARTS HERE ##
        weight = self.weight.view(
            self.out_channels * self.in_channels,
            self.group.elements().numel(),
            self.kernel_size,
            self.kernel_size
        )
        ## AND ENDS HERE ##

        transformed_weight = []
        # We loop over all group elements and retrieve weight values for
        # the corresponding transformed grids over R2xH.
        for grid_idx in range(self.group.elements().numel()):
            transformed_weight.append(
                trilinear_interpolation(weight, self.transformed_grid_R2xH[:, grid_idx, :
↪, :, :])
            )
        transformed_weight = torch.stack(transformed_weight)

        # Separate input and output channels.
        transformed_weight = transformed_weight.view(
            self.group.elements().numel(),
            self.out_channels,
            self.in_channels,
            self.group.elements().numel(),
            self.kernel_size,
```

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```
            self.kernel_size
        )

        # Put out channel dimension before group dimension. We do this
        # to be able to use pytorched Conv2D. Details below!
        transformed_weight = transformed_weight.transpose(0, 1)

        return transformed_weight
```

[ ]:
```
igk = InterpolativeGroupKernel(
    group=CyclicGroup(order=4),
    kernel_size=5,
    in_channels=2,
    out_channels=8
)
```

[ ]:
```
weights = igk.sample()
weights.shape
```

Let's visualize the sampled group convolution kernels! We visualize our 3D kernels in 2D by folding the input group dimension into the first spatial dimension. In doing so, we create a 2D flattened version of the 3D group convolution kernel, where spatial kernels corresponding to the different group elements lie along the spatial dimension. Each channel goes from `[num_group_elem, kernel_size, kernel_size]` to `[num_group_elem x kernel_size, kernel_size]`.

To clearly see what happens to the group convolution kernel under transformation of the group H, we outline the spatial kernel corresponding to the first input group element in red. For subsequent transformations we can see this spatial kernel. See below!

[ ]:
```
plt.rcParams['figure.figsize'] = [10, 10]

# For ease of viewing, we fold the input group dimension into the spatial x dimension
weights_t = weights.view(
    igk.out_channels,
    igk.group.elements().numel(),
    igk.in_channels,
    igk.group.elements().numel() * igk.kernel_size,
    igk.kernel_size
)

# pick an output channel to visualize
out_channel_idx = 0

# create [in_channels, group_elements] figures
fig, ax = plt.subplots(igk.in_channels, igk.group.elements().numel())

for in_channel in range(igk.in_channels):
    for group_elem in range(igk.group.elements().numel()):
        ax[in_channel, group_elem].imshow(
            weights_t[out_channel_idx, group_elem, in_channel, :, :].detach()
        )
```

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```
        # Outline the spatial kernel corresponding to the first group element under␣
↪canonical transformation
        rect = matplotlib.patches.Rectangle(
            (-0.5, group_elem * weights_t.shape[-1] - 0.5), weights_t.shape[-1], weights_
↪t.shape[-1], linewidth=5, edgecolor='r', facecolor='none')
        ax[in_channel, group_elem].add_patch(rect)

fig.text(0.5, 0.04, 'Group elements', ha='center')
fig.text(0.04, 0.5, 'Input channels / input group elements', va='center', rotation=
↪'vertical')

plt.show()
```

We see the same twist shift motion as we saw with the kernel grids!

2.2.3 Implementing the group convolution

The next step is implementing the group convolution operation.

Notes: * We would still like to use PyTorch's `Conv2D` implementation, but we're now faced with an additional problem; the group dimension in the input feature map. Luckily we can resolve this problem in much the same way; normally a 2D convolution layer integrates over a local neighbourhood of all input channels. We would now additionally like to integrate over the entire group. Thus, we can simply treat the group dimensions in the input feature map as additional channel dimensions! We achieve this by folding our input group dimension into the input channel dimension; f_{in} is reshaped from `[batch, in_channels, num_group_elem, spatial_1, spatial_2]` into `[batch, in_channels x num_group_elem, spatial_1, spatial_2]`. * To match this, and to apply the same trick as we did in the lifting convolution to get results for each separate group element in the *output*, we also reshape our kernel from `[out_channels, num_group_elem, in_channels, num_group_elem, kernel_size, kernel_size]` to `[out_channels x num_group_elem, in_channels x num_group_elem, kernel_size, kernel_size]`. See below!

[ ]:
```
class GroupConvolution(torch.nn.Module):

    def __init__(self, group, in_channels, out_channels, kernel_size, padding):
        super().__init__()

        self.kernel = InterpolativeGroupKernel(
            group=group,
            kernel_size=kernel_size,
            in_channels=in_channels,
            out_channels=out_channels
        )

        self.padding = padding


    def forward(self, x):
        """ Perform lifting convolution

        @param x: Input sample [batch_dim, in_channels, group_dim, spatial_dim_1,
            spatial_dim_2]
        @return: Function on a homogeneous space of the group
```

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```
            [batch_dim, out_channels, num_group_elements, spatial_dim_1,
            spatial_dim_2]
        """

        # We now fold the group dimensions of our input into the input channel
        # dimension.

        ## YOUR CODE STARTS HERE ##
        x = ...
        ## AND ENDS HERE ##

        # We obtain convolution kernels transformed under the group.

        ## YOUR CODE STARTS HERE ##
        conv_kernels = ...
        ## AND ENDS HERE ##

        # Apply group convolution, note that the reshape folds the 'output' group
        # dimension of the kernel into the output channel dimension, and the
        # 'input' group dimension into the input channel dimension.

        # Question: Do you see why we (can) do this?

        ## YOUR CODE STARTS HERE ##
        x = ...
        ## AND ENDS HERE ##

        # Reshape [batch_dim, in_channels * num_group_elements, spatial_dim_1,
        # spatial_dim_2] into [batch_dim, in_channels, num_group_elements,
        # spatial_dim_1, spatial_dim_2], separating channel and group
        # dimensions.
        x = x.view(
            -1,
            self.kernel.out_channels,
            self.kernel.group.elements().numel(),
            x.shape[-1],
            x.shape[-2],
        )

        return x
```

2.3 Projection to obtain invariance and tying everything together

Up until now, our feature maps equivary with the group action of $\mathbb{R}^2 \rtimes H$; our feature maps are defined over $\mathbb{R}^2 \rtimes H$. Usually in a CNN, a series of convolutional layers build a representation, which is followed by a (number of) linear layer(s). To create a GCNN using our lifting and group convolution operations that is fully invariant to the action of the group, we must apply a projection operation invariant to the action of the group to our feature map, to reduce its dimensionality from `[batch, channels, num_group_elem, spatial_1, spatial_2]` to `[batch, channels]` or even . The representation that we obtain then is fully invariant to the group. This representation is pushed through a final linear layer to yield a classification.

Below, we build a small GCNN from our implemented PyTorch modules.

Notes: * We use a mean-pooling operation to pool over group and spatial dimensions, but we could also use max or min pooling, or any other operation invariant to the group.

[ ]:
```
from torch.nn import AdaptiveAvgPool3d


class GroupEquivariantCNN(torch.nn.Module):

    def __init__(self, group, in_channels, out_channels, kernel_size, num_hidden, hidden_
↪channels):
        super().__init__()

        # Create the lifing convolution.

        ## YOUR CODE STARTS HERE ##
        self.lifting_conv = ...
        ## AND ENDS HERE ##

        # Create a set of group convolutions.
        self.gconvs = torch.nn.ModuleList()

        ## YOUR CODE STARTS HERE ##
        for i in range(num_hidden):
            ...
        ## AND ENDS HERE ##

        # Create the projection layer. Hint: check the import at the top of
        # this cell.

        ## YOUR CODE STARTS HERE ##
        self.projection_layer = torch.nn.AdaptiveAvgPool3d(1)
        ## AND ENDS HERE ##

        # And a final linear layer for classification.
        self.final_linear = torch.nn.Linear(hidden_channels, out_channels)

    def forward(self, x):

        # Lift and disentangle features in the input.
        x = self.lifting_conv(x)
        x = torch.nn.functional.layer_norm(x, x.shape[-4:])
        x = torch.nn.functional.relu(x)
```

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```
        # Apply group convolutions.
        for gconv in self.gconvs:
            x = gconv(x)
            x = torch.nn.functional.layer_norm(x, x.shape[-4:])
            x = torch.nn.functional.relu(x)

        # to ensure equivariance, apply max pooling over group and spatial dims.
        x = self.projection_layer(x).squeeze()

        x = self.final_linear(x)
        return x
```

To compare, let's create a more or less identical CNN. The only difference here is that this network consists of regular convolution operations.

[ ]:
```
class CNN(torch.nn.Module):

    def __init__(self, in_channels, out_channels, kernel_size, num_hidden, hidden_
↪channels):
        super().__init__()

        self.first_conv = torch.nn.Conv2d(
            in_channels=in_channels,
            out_channels=hidden_channels,
            kernel_size=kernel_size,
            padding=0
        )

        self.convs = torch.nn.ModuleList()
        for i in range(num_hidden):
            self.convs.append(
                torch.nn.Conv2d(
                    in_channels=hidden_channels,
                    out_channels=hidden_channels,
                    kernel_size=kernel_size,
                    padding=0
                )
            )

        self.final_linear = torch.nn.Linear(hidden_channels, out_channels)

    def forward(self, x):

        x = self.first_conv(x)
        x = torch.nn.functional.layer_norm(x, x.shape[-3:])
        x = torch.nn.functional.relu(x)

        for conv in self.convs:
            x = conv(x)
            x = torch.nn.functional.layer_norm(x, x.shape[-3:])
            x = torch.nn.functional.relu(x)
```

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```
        # Apply average pooling over remaining spatial dimensions.
        x = torch.nn.functional.adaptive_avg_pool2d(x, 1).squeeze()

        x = self.final_linear(x)
        return x
```

4.41.4 3. Experimenting with our implementation

Note that for ease of model training and tracking, we additionally make use of `pytorch-lightning`. Although the specifics of this package aren't the focus of this tutorial, if you'd like a refresher please have a look at this excellent Deep Learning 1 tutorial by Phillip Lippe.

3.1 Generalization to the group action

To show the generalization capabilities of regular group convolutional networks, we will train this model on the MNIST training dataset, but evaluate it on an augmented version of the MNIST test set in which each image is randomly rotated by a continuous rotation between $[0, 2\pi]$.

[ ]:
```
# We normalize the training data.
train_transform = torchvision.transforms.Compose([torchvision.transforms.ToTensor(),
                                                  torchvision.transforms.Normalize((0.
↪1307,), (0.3081,))
                                                  ])

# To demonstrate the generalization capabilities our rotation equivariant layers bring,␣
↪we apply a random
# rotation between 0 and 360 deg to the test set.
test_transform = torchvision.transforms.Compose([torchvision.transforms.ToTensor(),
                                                 torchvision.transforms.RandomRotation(
                                                     [0, 360],
                                                     torchvision.transforms.
↪InterpolationMode.BILINEAR,
                                                     fill=0),
                                                 torchvision.transforms.Normalize((0.
↪1307,), (0.3081,))
                                                 ])

# We demonstrate our models on the MNIST dataset.
train_ds = torchvision.datasets.MNIST(root=DATASET_PATH, train=True, transform=train_
↪transform, download=True)
test_ds = torchvision.datasets.MNIST(root=DATASET_PATH, train=False, transform=test_
↪transform)
train_loader = torch.utils.data.DataLoader(train_ds, batch_size=64, shuffle=True)
test_loader = torch.utils.data.DataLoader(test_ds, batch_size=64, shuffle=False)

# Set the random seed for reproducibility.
pl.seed_everything(12)
```

Let's visualize some of the training and test images. As we can see the test images are randomly rotated.

[ ]:
```
NUM_IMAGES = 4
images = [train_ds[idx][0] for idx in range(NUM_IMAGES)]
orig_images = [Image.fromarray(train_ds.data[idx].numpy()) for idx in range(NUM_IMAGES)]
orig_images = [test_transform(img) for img in orig_images]

img_grid = torchvision.utils.make_grid(torch.stack(images + orig_images, dim=0), nrow=4,␣
↪normalize=True, pad_value=0.5)
img_grid = img_grid.permute(1, 2, 0)

plt.figure(figsize=(8,8))
plt.title("Images sampled from the MNIST train set, augmented with test transforms.")
plt.imshow(img_grid)
plt.axis('off')
plt.show()
plt.close()
```

[ ]:
```
class DataModule(pl.LightningModule):

    def __init__(self, model_name, model_hparams, optimizer_name, optimizer_hparams):
        """
        Inputs:
            model_name - Name of the model/CNN to run. Used for creating the model (see␣
↪function below)
            model_hparams - Hyperparameters for the model, as dictionary.
            optimizer_name - Name of the optimizer to use. Currently supported: Adam, SGD
            optimizer_hparams - Hyperparameters for the optimizer, as dictionary. This␣
↪includes learning rate, weight decay, etc.
        """
        super().__init__()
        # Exports the hyperparameters to a YAML file, and create "self.hparams" namespace
        self.save_hyperparameters()
        # Create model
        self.model = create_model(model_name, model_hparams)
        # Create loss module
        self.loss_module = nn.CrossEntropyLoss()

    def forward(self, imgs):
        return self.model(imgs)

    def configure_optimizers(self):
        # AdamW is Adam with a correct implementation of weight decay (see here for␣
↪details: https://arxiv.org/pdf/1711.05101.pdf)
        optimizer = optim.AdamW(
            self.parameters(), **self.hparams.optimizer_hparams)
        return [optimizer], []

    def training_step(self, batch, batch_idx):
        # "batch" is the output of the training data loader.
        imgs, labels = batch
        preds = self.model(imgs)
        loss = self.loss_module(preds, labels)
        acc = (preds.argmax(dim=-1) == labels).float().mean()
```

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```
        # Logs the accuracy per epoch to tensorboard (weighted average over batches)
        self.log('train_acc', acc, on_step=False, on_epoch=True)
        self.log('train_loss', loss)
        return loss  # Return tensor to call ".backward" on

    def validation_step(self, batch, batch_idx):
        imgs, labels = batch
        preds = self.model(imgs).argmax(dim=-1)
        acc = (labels == preds).float().mean()
        # By default logs it per epoch (weighted average over batches)
        self.log('val_acc', acc, prog_bar=True)

    def test_step(self, batch, batch_idx):
        imgs, labels = batch
        preds = self.model(imgs).argmax(dim=-1)
        acc = (labels == preds).float().mean()
        # By default logs it per epoch (weighted average over batches), and returns it␣
↪afterwards
        self.log('test_acc', acc, prog_bar=True)
```

We create a dictionary to keep track of our models

[ ]:
```
model_dict = {
    'CNN': CNN,
    'GCNN': GroupEquivariantCNN
}

def create_model(model_name, model_hparams):
    if model_name in model_dict:
        return model_dict[model_name](**model_hparams)
    else:
        assert False, f"Unknown model name \"{model_name}\". Available models are:
↪{str(model_dict.keys())}"
```

[ ]:
```
def train_model(model_name, save_name=None, **kwargs):
    """
    Inputs:
        model_name - Name of the model you want to run. Is used to look up the class in
↪"model_dict"
        save_name (optional) - If specified, this name will be used for creating the␣
↪checkpoint and logging directory.
    """
    if save_name is None:
        save_name = model_name

    # Create a PyTorch Lightning trainer with the generation callback
    trainer = pl.Trainer(default_root_dir=os.path.join(CHECKPOINT_PATH, save_name),     ␣
↪                    # Where to save models
                         accelerator='auto',
↪# We run on a single GPU (if possible)
                         max_epochs=10,                                                 ␣
↪                    # How many epochs to train for if no patience is set
```

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```
                         callbacks=[ModelCheckpoint(save_weights_only=True, mode="max",␣
↪monitor="val_acc"),  # Save the best checkpoint based on the maximum val_acc recorded.␣
↪Saves only weights and not optimizer
                                    LearningRateMonitor("epoch")])
    trainer.logger._default_hp_metric = None # Optional logging argument that we don't␣
↪need

    # Check whether pretrained model exists. If yes, load it and skip training
    pretrained_filename = os.path.join(CHECKPOINT_PATH, save_name + ".ckpt")

    if os.path.isfile(pretrained_filename):
        print(f"Found pretrained model at {pretrained_filename}, loading...")
        model = DataModule.load_from_checkpoint(pretrained_filename) # Automatically␣
↪loads the model with the saved hyperparameters
    else:
        pl.seed_everything(12) # To be reproducable
        model = DataModule(model_name=model_name, **kwargs)
        trainer.fit(model, train_loader, test_loader)
        model = DataModule.load_from_checkpoint(trainer.checkpoint_callback.best_model_
↪path) # Load best checkpoint after training

    # Test best model on test set
    val_result = trainer.test(model.to(device), test_loader, verbose=False)
    result = {"val": val_result[0]["test_acc"]}

    return model, result
```

Let's train the conventional CNN first!

[ ]:
```
cnn_model, cnn_results = train_model(model_name="CNN",
                                     model_hparams={"in_channels": 1,
                                                    "out_channels": 10,
                                                    "kernel_size": 5,
                                                    "num_hidden":4,
                                                    "hidden_channels":32},
                                     optimizer_name="Adam",
                                     optimizer_hparams={"lr": 1e-2,
                                                        "weight_decay": 1e-4},
                                     save_name='cnn-pretrained')
```

Next, we train the GCNN. Note that we reduce the number of channels by half to account for the increased kernel dimensionality. We do this to keep the number of trainable parameters more or less equal.

[ ]:
```
gcnn_model, gcnn_results = train_model(model_name="GCNN",
                                       model_hparams={"in_channels": 1,
                                                      "out_channels": 10,
                                                      "kernel_size": 5,
                                                      "num_hidden": 4,
                                                      "hidden_channels":16, # to account␣
↪for the increase in trainable parameters due to the extra dimension in our feature␣
↪maps, remove some hidden channels.
                                                      "group":CyclicGroup(order=4).
↪to(device)},
```

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```
                                        optimizer_name="Adam",
                                        optimizer_hparams={"lr": 1e-2,
                                                           "weight_decay": 1e-4},
                                        save_name='gcnn-pretrained')
```

Let us inspect the final results from both models. As we can see the GCNN performs considerably better than the CNN. This because the GCNN implementation is invariant to rotations of 90 deg, which makes it able to recognize the handwritten digits in the test set under such rotations. Of course, since the test images are rotated by continuous rotations between 0 and 360 deg, the GCNN model still doesn't obtain perfect accuracy. How could we further improve the GCNNs generalization?

[ ]:
```
print(f"CNN - Num Parameters {sum([np.prod(p.shape) for p in cnn_model.parameters()])} -␣
↪Val Accuracy {cnn_results['val']*100.:4.2f}%")
print(f"GCNN - Num Parameters {sum([np.prod(p.shape) for p in gcnn_model.parameters()])}␣
↪- Val Accuracy {gcnn_results['val']*100.:4.2f}%")
```

3.2 Inspecting the created feature maps

To better understand what happens inside our CNN and GCNN as we rotate an input image, let's visualize a single channel of a feature map in the second layer of the network for different rotations of an input image.

[ ]:
```
train_ds = torchvision.datasets.MNIST(root=DATASET_PATH, train=False, transform=None)

# Get an image from the test dataset.
digit, label = train_ds[123]

# Turn it into a tensor.
digit = transforms.ToTensor()(digit)

plt.figure(figsize=(6, 6))
plt.imshow(digit.squeeze())
plt.title(f'Label: {label}')
plt.show()
```

[ ]:
```
plt.rcParams['figure.figsize'] = [10, 3]

# Get a set of angles by which to rotate this image.
rots = torch.linspace(0, 360 - 360/8, 8)

# Rotate the input image and push it through the normalization transform.
rot_digit = torch.stack(tuple(torchvision.transforms.functional.rotate(digit, a.item(),␣
↪torchvision.transforms.functional.InterpolationMode.BILINEAR) for a in rots))
rot_digit = torchvision.transforms.Normalize((0.1307,), (0.3081,))(rot_digit)

# Create a subfigure for every rotated input.
fig, ax = plt.subplots(1, rots.numel())

for idx, rotation in enumerate(rots):
    ax[idx].imshow(
        rot_digit[idx, :, :].squeeze()
    )
```

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```
    ax[idx].set_title(f"{int(rotation)} deg")

fig.text(0.5, 0.04, 'Rotations of input image', ha='center')

plt.show()
```

[ ]:
```
# Forward it through the first few layers of the CNN.
cnn_out = cnn_model.model.first_conv(rot_digit)
cnn_out = torch.nn.functional.relu(torch.nn.functional.layer_norm(cnn_out, cnn_out.
↪shape[-3:]))
for i in range(2):
    cnn_out = cnn_model.model.convs[i](cnn_out)
    cnn_out = torch.nn.functional.relu(torch.nn.functional.layer_norm(cnn_out, cnn_out.
↪shape[-3:]))

# Let's also see what happens after we apply projection over remaining spatial dimensions.
projected_cnn_out = torch.nn.functional.adaptive_avg_pool2d(cnn_out, 1).squeeze()

# Forward it through the first few layers of the GCNN.
gcnn_out = gcnn_model.model.lifting_conv(rot_digit)
gcnn_out = torch.nn.functional.relu(torch.nn.functional.layer_norm(gcnn_out, gcnn_out.
↪shape[-4:]))
for i in range(2):
    gcnn_out = gcnn_model.model.gconvs[i](gcnn_out)
    gcnn_out = torch.nn.functional.relu(torch.nn.functional.layer_norm(gcnn_out, gcnn_
↪out.shape[-4:]))

# And let's see what happens if we apply the projection on this equivariant␣
↪representation.
projected_gcnn_out = torch.mean(gcnn_out, dim=(-3, -2, -1))
```

Let's first visualize the activations after the third convolution for a single channel of the regular CNN.

Question: What would you expect to see happening to the feature maps of the conventional CNN as the input is rotated?

[ ]:
```
plt.rcParams['figure.figsize'] = [10, 3]

# Pick a channel to visualize
channel_idx = 2

# Create a subfigure for every rotated input
fig, ax = plt.subplots(1, rots.numel())

for idx, rotation in enumerate(rots):
    ax[idx].imshow(
        cnn_out[idx, out_channel_idx, :, :].detach().numpy()
    )
    ax[idx].set_title(f"{int(rotation)} deg")

fig.text(0.5, 0.04, 'Rotations of input image', ha='center')

plt.show()
```

Question: Explain what you see in the above images; how should we interpret what is happening to the feature maps as the input is rotated?

Next, we'll visualize activations after the third convolution operation for the G-CNN.

Question: What do you expect to see happen to the feature maps in the G-CNN as the input is rotated?

[ ]:
```
plt.rcParams['figure.figsize'] = [10, 9]

# Pick a channel to visualize
channel_idx = 2

# Create a subfigure for every rotated input and every group element
fig, ax = plt.subplots(gcnn_out.shape[2], rots.numel())

for idx, rotation in enumerate(rots):
    for group_element_idx in range(gcnn_out.shape[2]):
        ax[group_element_idx ,idx].imshow(
            gcnn_out[idx, out_channel_idx, group_element_idx, :, :].detach().numpy()
        )
    ax[0, idx].set_title(f"{int(rotation)} deg")


fig.text(0.5, 0.04, 'Rotations of input image', ha='center')
fig.text(0.04, 0.5, '$H$ dimension in feature map', va='center', rotation='vertical')

plt.show()
```

Question: Explain what you see in the above images; how should we interpret what is happening to the feature maps as the input is rotated? What happens after a 45 degree rotation? And a 90 degree rotation?

Lastly, we inspect the representations we obtain after the projection step for the CNN and GCNN. We visualize all channels. These are the representations on which the final linear layer(s) perform classification.

[ ]:
```
plt.rcParams['figure.figsize'] = [8, 8]

# Create a subfigure for every rotated input
fig, ax = plt.subplots(rots.numel(), 1)

for idx, rotation in enumerate(rots):
    ax[idx].imshow(
        projected_cnn_out[idx, None, :].detach().numpy()
    )
    ax[idx].set_title(f"{int(rotation)} deg")
    ax[idx].set_yticks([])

fig.text(0.5, 0.04, 'Channels', ha='center')
fig.text(0.04, 0.5, 'Rotations of input image', va='center', rotation='vertical')

plt.show()
```

Question: What happens to the learned representations as the input is rotated? What consequences do you think this has on the performance of the model?

[ ]:
```
plt.rcParams['figure.figsize'] = [8, 8]

# Create a subfigure for every rotated input
fig, ax = plt.subplots(rots.numel(), 1)

for idx, rotation in enumerate(rots):
    ax[idx].imshow(
        projected_gcnn_out[idx, None, :].detach().numpy()
    )
    ax[idx].set_title(f"{int(rotation)} deg")
    ax[idx].set_yticks([])

fig.text(0.5, 0.04, 'Channels', ha='center')
fig.text(0.04, 0.5, 'Rotations of input image', va='center', rotation='vertical')

plt.show()
```

Question: Explain what you see above. What does this mean for the final of input samples that are rotated?

Question: Do you notice anything about the learned representations of 45 degree vs 90 degree rotated input samples? To what can we attribute this phenomenon do you think?

4.41.5 4. Concluding remarks

We've seen how to implement a basic regular group convolutional network equivariant to rotations of 90 degrees. A couple suggestions of things to ponder on. Include answers to these questions in your report:

- What other groups could be interesting in computer vision problems? (these often come with their own interesting challenges).
- We used interpolation to obtain our values for transformed kernels. As mentioned, this makes our networks prone to interpolation artefacts. Would our interpolation implementation work well for other groups? Could you maybe think of other ways of defining the kernel over a continuous domain?
- Here we worked with a one-dimensional group. What would it take to implement group convolutions for multi-dimensional groups H?

4.42 GDL - Steerable CNNs

Filled notebook:
Empty notebook:
Authors: Gabriele Cesa

During the lectures, you have learnt that the symmetries of a machine learning task can be modelled with **groups**. In the previous tutorial, you have also studied the framework of *Group-Convolutional Neural Networks* (**GCNNs**), which describes a neural architecture design equivariant to general groups.

The feature maps of a GCNN are functions over the elements of the group. A naive implementation of group-convolution requires computing and storing a response for each group element. For this reason, the GCNN framework is not particularly convenient to implement networks equivariant to groups with infinite elements.

Steerable CNNs are a more general framework which solves this issue. The key idea is that, instead of storing the value of a feature map on each group element, the model stores the *Fourier transform* of this feature map, up to a finite number of frequencies.

In this tutorial, we will first introduce some Representation theory and Fourier theory (*non-commutative harmonic analysis*) and, then, we will explore how this idea is used in practice to implement Steerable CNNs.

4.42.1 Prerequisite Knowledge

Throughout this tutorial, we will assume you are already familiar with some concepts of **group theory**, such as *groups*, *group actions* (in particular *on functions*), *semi-direct product* and *order of a group*, as well as basic **linear algebra**.

We start by importing the necessary packages. You can run the following command to install all the requirements:

```
> pip install torch torchvision numpy matplotlib git+https://github.com/AMLab-Amsterdam/
lie_learn escnn scipy
```

[1]:
```
import torch
import numpy as np
import scipy
import os

np.set_printoptions(precision=3, suppress=True, linewidth=10000, threshold=100000)

import matplotlib
%matplotlib inline
import matplotlib.pyplot as plt
# If the fonts in the plots are incorrectly rendered, comment out the next two lines
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
matplotlib.rcParams['lines.linewidth'] = 2.0

import urllib.request
from urllib.error import HTTPError

CHECKPOINT_PATH = "../../saved_models/DL2/GDL"
```

```
/opt/conda/lib/python3.8/site-packages/tqdm/auto.py:22: TqdmWarning: IProgress not found.
↪ Please update jupyter and ipywidgets. See https://ipywidgets.readthedocs.io/en/stable/
↪user_install.html
  from .autonotebook import tqdm as notebook_tqdm
/tmp/ipykernel_109/1932627903.py:13: DeprecationWarning: `set_matplotlib_formats` is␣
↪deprecated since IPython 7.23, directly use `matplotlib_inline.backend_inline.set_
↪matplotlib_formats()`
  set_matplotlib_formats('svg', 'pdf') # For export
```

[2]:
```
# Create checkpoint path if it doesn't exist yet
os.makedirs(CHECKPOINT_PATH, exist_ok=True)


# Files to download
pretrained_files = [
    "steerable_c4-pretrained.ckpt",
    "steerable_so2-pretrained.ckpt",
```

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```
    "steerable_c4-accuracies.npy",
    "steerable_so2-accuracies.npy",
]

# Github URL where saved models are stored for this tutorial
base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/DL2/GDL/"

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please contact the author with the full output␣
↪including the following error:\n", e)
```

4.42.2 1. Representation Theory and Harmonic Analysis of Compact Groups

We will make use of the `escnn` library throughout this tutorial. You can also find its documentation here.

[3]:
```
try:
    from escnn.group import *
except ModuleNotFoundError: # Google Colab does not have escnn installed by default.␣
↪Hence, we do it here if necessary
    !pip install --quiet git+https://github.com/AMLab-Amsterdam/lie_learn escnn
    from escnn.group import *
```

First, let's create a group. We will use the *Cyclic Group* $G = C_8$ as an example. This group contains the 8 planar rotations by multiples of $\frac{2\pi}{8}$. In `escnn`, a groups are instances of the abstract class `escnn.group.Group`, which provides some useful functionalities. We instantiate groups via a *factory method*. To build the cyclic group of order 8, we use this factory method:

[4]:
```
G = cyclic_group(N=8)

# We can verify that the order of this group is 8:
G.order()
```

[4]:
```
8
```

A group is a collection of group elements together with a binary operation to combine them. This is implemented in the class `escnn.group.GroupElement`. We can access the *identity* element $e \in G$ as

[5]:
```
G.identity
```

[5]:
```
0[2pi/8]
```

or sample a random element as

[6]:
```
G.sample()
```

[6]:
```
1[2pi/8]
```

Group elements can be combined via the binary operator `@`; we can also take the inverse of an element using `~`:

[7]:
```
a = G.sample()
b = G.sample()
print(a)
print(b)
print(a @ b)
print(~a)
```

```
6[2pi/8]
1[2pi/8]
7[2pi/8]
2[2pi/8]
```

Representation theory is a fundamental element in Steerable CNNs and to construct a Fourier theory over groups. In this first section, we will introduce the essential concepts.

1.1 Group Representation

A **linear group representation** ρ of a compact group G on a vector space (called *representation space*) $\mathbb{R}^d$ is a *group homomorphism* from G to the general linear group $GL(\mathbb{R}^d)$, i.e. it is a map $\rho : G \to \mathbb{R}^{d \times d}$ such that:

$$\rho(g_1 g_2) = \rho(g1)\rho(g2) \quad \forall g_1, g_2 \in G \,.$$

In other words, $\rho(g)$ is a $d \times d$ *invertible* matrix. We refer to d as the *size* of the representation.

Example: the Trivial Representation

The simplest example of *group representation* is the **trivial representation** which maps every element to $1 \in \mathbb{R}$, i.e. $\rho : g \mapsto 1$. One can verify that it satisfies the condition above. We can construct this representation as follows:

[8]:
```
rho = G.trivial_representation
```

`rho` is an instance of `escnn.group.Representation`. This class provides some functionalities to work with group representations. We can also use it as a callable function to compute the representation of a group element; this will return a squared matrix as a `numpy.array`. Let verify that the trivial representation does indeed verify the condition above:

[9]:
```
g1 = G.sample()
g2 = G.sample()
print(rho(g1) @ rho(g2))
print(rho(g1 @ g2))
```

```
[[1.]]
[[1.]]
```

Note that the trivial representation has size 1:

[10]:
```
rho.size
```

[10]:
```
1
```

Example: rotations

Another common example of group representations is given by 2D rotations. Let $SO(2)$ be the group of all planar rotations; note that we can identify each rotation by an angle $\theta \in [0, 2\pi)$. Then, the standard representation of planar rotations as 2×2 rotation matrices is a representation of $SO(2)$:

$$\rho : r_\theta \mapsto \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

where $r_\theta \in SO(2)$ is a counter-clockwise rotation by θ. Let's try to build this group and, then, verify that this is a representation:

[11]:
```
G = so2_group()
rho = G.standard_representation()

g1 = G.sample()
g2 = G.sample()
print(f'g1={g1}, g2={g2}, g1 * g2 = {g1 @ g2}')
print()
print('rho(g1) @ rho(g2)')
print(rho(g1) @ rho(g2))
print()
print('rho(g1 * g2)')
print(rho(g1 @ g2))
```

```
g1=4.83985258221817, g2=4.721165128388411, g1 * g2 = 3.277832403426995

rho(g1) @ rho(g2)
[[-0.991  0.136]
 [-0.136 -0.991]]

rho(g1 * g2)
[[-0.991  0.136]
 [-0.136 -0.991]]
```

QUESTION 1

Show that any representation $\rho : G \to \mathbb{R}^{d \times d}$ also satisfies the following two properties:

- let $e \in G$ be the identity element. Then, $\rho(e)$ is the identity matrix of size d.
- let $g \in G$ and g^{-1} be its inverse (i.e. $g \cdot g^{-1} = e$). Then, $\rho(g^{-1}) = \rho(g)^{-1}$.

ANSWER 1

First question. First, note that for any $g \in G$:

$$\rho(g) = \rho(g \cdot e) = \rho(g)\rho(e)$$

Because $\rho(g)$ is invertible, we can left multiply by $\rho(g)^{-1}$ to find that $\rho(e)$ is the identity.

Second question. Note that

$$\rho(e) = \rho(g \cdot g^{-1}) = \rho(g)\rho(g^{-1})$$

Using the fact $\rho(e)$ is the identity, by left-multiplying by $\rho(g)^{-1}$ we recover the original statement.

Direct Sum

We can combine representations to build a larger representation via the **direct sum**.

Given representations $\rho_1 : G \to \mathbb{R}^{d_1 \times d_1}$ and $\rho_2 : G \to \mathbb{R}^{d_2 \times d_2}$, their *direct sum* $\rho_1 \oplus \rho_2 : G \to \mathbb{R}^{(d_1+d_2)\times(d_1+d_2)}$ is defined as

$$(\rho_1 \oplus \rho_2)(g) = \begin{bmatrix} \rho_1(g) & 0 \\ 0 & \rho_2(g) \end{bmatrix}$$

Its action is therefore given by the independent actions of ρ_1 and ρ_2 on the orthogonal subspaces $\mathbb{R}^{d_1}$ and $\mathbb{R}^{d_2}$ of $\mathbb{R}^{d_1+d_2}$.

Let's see an example:

[12]:
```
rho_sum = rho + rho

g = G.sample()
print(rho(g))
print()
print(rho_sum(g))
```

```
[[-0.943 -0.332]
 [ 0.332 -0.943]]

[[-0.943 -0.332  0.     0.   ]
 [ 0.332 -0.943  0.     0.   ]
 [ 0.     0.    -0.943 -0.332]
 [ 0.     0.     0.332 -0.943]]
```

Note that the direct sum of two representations has size equal to the sum of their sizes:

[13]:
```
rho.size, rho_sum.size
```

[13]:
```
(2, 4)
```

We can combine arbitrary many representations in this way, e.g. $\rho \oplus \rho \oplus \rho \oplus \rho$:

[14]:
```
rho_sum = rho + rho + rho + rho

# or, more simply:
rho_sum = directsum([rho, rho, rho, rho])
rho_sum.size
```

[14]:
```
8
```

The Regular Representation

Another important representation is the **regular representation**. The regular representation describes the action of a group G on the vector space of functions over the group G. Assume for the moment that the group G is *finite*, i.e. $|G| < \infty$.

The set of functions over G is equivalent to the vector space $\mathbb{R}^{|G|}$. We can indeed interpret a vector $\mathbf{f} \in \mathbb{R}^{|G|}$ as a function over G, where the i-th entry of $\mathbf{f}$ is interpreted as the value of the function on the i-th element $g_i \in G$.

The **regular representation** of G is a $|G|$ dimensional representation. Recall the left action of G on a function $f : G \to \mathbb{R}$:

$$[g.f](h) := f(g^{-1}h)$$

The new function $g.f$ is still a function over G and belongs to the same vector space. If we represent the function f as a vector $\mathbf{f}$, the vector representing the function $g.f$ will have permuted entries with respect to $\mathbf{f}$. This permutation is the regular representation of $g \in G$.

QUESTION 2

Show that the space of functions over G is a vector space. To do so, show that functions satisfy the properties of a vector space; see here.

ANSWER 2

Let $f_1, f_2, f_3 : G \to \mathbb{R}$ be three functions and $\alpha, \beta \in \mathbb{R}$ scalars. The point-wise sum of two functions is the function $[f_1 + f_2] : G \to \mathbb{R}$ defined as

$$[f_1 + f_2](g) = f_1(g) + f_2(g)$$

The scalar multiplication is also defined pointwise as

$$[\alpha \cdot f_1](g) = \alpha f_1(G)$$

We now verify the required properties of a vector space.

- associativity: $[f_1 + (f_2 + f_3)](g) = f_1(g) + f_2(g) + f_3(g) = [(f_1 + f_2) + f_3](g)$
- commutativity: $[f_1 + f_2)](g) = f_1(g) + f_2(g) = f_2(g) + f_1(g) = [f_2 + f_1](g)$
- identity: define the function $\mathbf{O} : G \to 0$; $[f_1 + \mathbf{O}](g) = f_1(g) + \mathbf{O}(g) = f_1(g)$
- inverse: define $[-f_1](g) = -1 \cdot f_1(g)$; then $[f_1 + (-f_1)](g) = f_1(g) - f_1(g) = 0$
- compatibility: $[\alpha \cdot (\beta \cdot f_1)](g) = \alpha\beta f_1(g) = [(\alpha\beta) \cdot f_1](g)$
- identity (multiplication): $[1 \cdot f_1](g) = 1 f_1(g) = f_1(g)$
- distributivity (vector): $[\alpha \cdot (f_1 + f_2)](g) = \alpha(f_1 + f_2)(g) = \alpha f_1(g) + \alpha f_2(g)$
- distributivity (scalar): $[(\alpha + \beta) \cdot f_1](g) = (\alpha + \beta) f_1(g) = \alpha f_1(g) + \beta f_1(g)$

For finite groups, we can generate this representation. We assume that the i-th entry is associated with the element of $G = C_8$ corresponing to a rotation by $i\frac{2\pi}{8}$.

[15]:
```
G = cyclic_group(8)
rho = G.regular_representation
```

[16]:
```
# note that the size of the representation is equal to the group's order |G|
rho.size
```

[16]:
```
8
```

the identity element maps a function to itself, so the entries are not permuted

[17]:
```
rho(G.identity)
```

[17]:
```
array([[ 1.,  0., -0.,  0., -0., -0.,  0., -0.],
       [ 0.,  1.,  0., -0., -0., -0., -0., -0.],
       [-0.,  0.,  1., -0., -0.,  0., -0.,  0.],
       [ 0., -0., -0.,  1.,  0., -0., -0., -0.],
       [-0., -0., -0.,  0.,  1.,  0., -0., -0.],
       [-0., -0.,  0., -0.,  0.,  1., -0.,  0.],
       [ 0., -0., -0., -0., -0., -0.,  1., -0.],
       [-0., -0.,  0., -0., -0.,  0., -0.,  1.]])
```

The regular representation of the rotation by $1\frac{2\pi}{8}$ just cyclically shifts each entry to the next position since $r_{1\frac{2\pi}{8}}^{-1} r_{i\frac{2\pi}{8}} = r_{(i-1)\frac{2\pi}{8}}$:

[18]:
```
rho(G.element(1))
```

[18]:
```
array([[ 0., -0.,  0., -0., -0.,  0., -0.,  1.],
       [ 1.,  0., -0., -0., -0., -0.,  0., -0.],
       [-0.,  1.,  0., -0.,  0., -0., -0., -0.],
       [-0.,  0.,  1.,  0., -0.,  0., -0.,  0.],
       [-0., -0., -0.,  1.,  0., -0.,  0., -0.],
       [-0.,  0., -0.,  0.,  1.,  0.,  0., -0.],
       [-0., -0., -0., -0.,  0.,  1.,  0.,  0.],
       [-0.,  0., -0., -0.,  0., -0.,  1.,  0.]])
```

Let's see an example of the action on a function. We consider a function which is zero on all group elements apart from the identity ($i = 0$).

[19]:
```
f = np.zeros(8)
f[0] = 1
f
```

[19]:
```
array([1., 0., 0., 0., 0., 0., 0., 0.])
```

Observe that $\rho(e)\mathbf{f} = \mathbf{f}$, where $e = 0\frac{2\pi}{8}$ is the identity element.

[20]:
```
rho(G.identity) @ f
```

[20]:
```
array([ 1.,  0., -0.,  0., -0., -0.,  0., -0.])
```

$\mathbf{f}$ is non-zero only on the element e. If an element g acts on this function, it moves the non-zero value to the entry associated with g:

[21]:
```
rho(G.element(1)) @ f
```

[21]:
```
array([ 0.,  1., -0., -0., -0., -0., -0., -0.])
```

[22]:
```
rho(G.element(6)) @ f
```

[22]:
```
array([ 0., -0.,  0., -0., -0., -0.,  1., -0.])
```

QUESTION 3

Prove the result above.

ANSWER 3

Let's call $\delta_g : G \to \mathbb{R}$ the function defined as

$$\delta_g(h) = \begin{cases} 1 & \text{if } h = g \\ 0 & \text{otherwise} \end{cases}$$

which is zero everywhere apart from $g \in G$, where it is 1. The function δ_e is represented by the vector $\mathbf{f}$ above.

We now want to show that $[g.\delta_e](h) = \delta_g(h)$:

$$[g.\delta_e](h) = \delta_e(g^{-1}h) = \begin{cases} 1 & \text{if } g^{-1}h = e \\ 0 & \text{otherwise} \end{cases} = \begin{cases} 1 & \text{if } h = g \\ 0 & \text{otherwise} \end{cases} = \delta_g(h)$$

Equivalent Representations

Two representations ρ and ρ' of a group G on the same vector space $\mathbb{R}^d$ are called *equivalent* (or **isomorphic**) if and only if they are related by a change of basis $Q \in \mathbb{R}^{d \times d}$, i.e.

$$\forall g \in G \quad \rho(g) = Q\rho'(g)Q^{-1} \, .$$

Equivalent representations behave similarly since their composition is *basis-independent* as seen by

$$\rho'(g_1)\rho'(g_2) = Q\rho(g_1)Q^1Q\rho(g_2)Q^1 = Q\rho(g_1)\rho(g_2)Q^1 \, .$$

Direct sum and *change of basis matrices* provide a way to combine representations to construct larger and more complex representations. In the next example, we concatenate two trivial representations and two regular representations and apply a random change of basis Q. The final representation is formally defined as:

$$\rho(g) = Q \left(\rho_{\text{trivial}} \oplus \rho_{\text{regular}} \oplus \rho_{\text{regular}} \oplus \rho_{\text{trivial}} \right) Q^{-1}$$

[23]:
```
d = G.trivial_representation.size * 2 + G.regular_representation.size * 2
Q = np.random.randn(d, d)
rho = directsum(
    [G.trivial_representation, G.regular_representation, G.regular_representation, G.
↪trivial_representation],
    change_of_basis=Q
)
```

[24]:
```
rho.size
```

[24]:
```
18
```

Irreducible Representations (or *Irreps*)

Under minor conditions, any representation can be decomposed in this way, that is, any representation ρ of a compact group G can be written as a *direct sum* of a number of smaller representations, up to a *change of basis*. These "smaller representations" can not be decomposed further and play a very important role in the theory of group representations and steerable CNNs and are called **irreducible representations**, or simply **irreps**.

The set of *irreducible representations* of a group G is generally denoted as $\hat{G}$. We will often use the notation $\hat{G} = \{\rho_j\}_j$ to index this set.

We can access the irreps of a group via the `irrep()` method. The *trivial representation* is *always* an irreducible representation. For $G = C_8$, we access it with the index $j = 0$:

[25]:
```
rho_0 = G.irrep(0)

print(rho_0 == G.trivial_representation)

rho_0(G.sample())
```

```
True
```

[25]:
```
array([[1.]])
```

The next irrep $j = 1$ gives the representation of $i\frac{2\pi}{8}$ as the 2×2 rotation matrix by $\theta = i\frac{2\pi}{8}$:

[26]:
```
rho = G.irrep(1)
g = G.sample()

print(g)
print()
print(rho(g))
```

```
1[2pi/8]

[[ 0.707 -0.707]
 [ 0.707  0.707]]
```

Irreducible representations provide the building blocks to construct any representation ρ via direct sums and change of basis, i.e:

$$\rho = Q \left(\bigoplus_{j \in \mathcal{I}} \rho_j \right) Q^{-1}$$

where $\mathcal{I}$ is an index set (possibly with repetitions) over $\hat{G}$.

Internally, any `escnn.group.Representation` is indeed implemented as a list of irreps (representing the index set $\mathcal{I}$) and a change of basis Q. An irrep is identified by a *tuple* `id`.

Let's see an example. Let's take the regular representaiton of C_8 and check its decomposition into irreps:

[27]:
```
rho = G.regular_representation
rho.irreps
```

[27]:
```
[(0,), (1,), (2,), (3,), (4,)]
```

[28]:
```
rho.change_of_basis
```

[28]:
```
array([[ 0.354,  0.5  ,  0.   ,  0.5  ,  0.   ,  0.5  ,  0.   ,  0.354],
       [ 0.354,  0.354,  0.354,  0.   ,  0.5  , -0.354,  0.354, -0.354],
       [ 0.354,  0.   ,  0.5  , -0.5  ,  0.   , -0.   , -0.5  ,  0.354],
       [ 0.354, -0.354,  0.354, -0.   , -0.5  ,  0.354,  0.354, -0.354],
       [ 0.354, -0.5  ,  0.   ,  0.5  , -0.   , -0.5  ,  0.   ,  0.354],
       [ 0.354, -0.354, -0.354,  0.   ,  0.5  ,  0.354, -0.354, -0.354],
       [ 0.354, -0.   , -0.5  , -0.5  ,  0.   ,  0.   ,  0.5  ,  0.354],
       [ 0.354,  0.354, -0.354, -0.   , -0.5  , -0.354, -0.354, -0.354]])
```

[29]:
```
# let's access second irrep
rho_id = rho.irreps[1]
rho_1 = G.irrep(*rho_id)

# we verify it is the irrep j=1 we described before
rho_1(g)
```

[29]:
```
array([[ 0.707, -0.707],
       [ 0.707,  0.707]])
```

Finally, let's verify that this direct sum and this change of basis indeed yield the regular representation

[30]:
```
# evaluate all the irreps in rho.irreps:
irreps = [
          G.irrep(*irrep)(g) for irrep in rho.irreps
]

# build the direct sum
direct_sum = np.asarray(scipy.sparse.block_diag(irreps, format='csc').todense())

print('Regular representation of', g)
print(rho(g))
print()
print('Direct sum of the irreps:')
print(direct_sum)
print()
print('Apply the change of basis on the direct sum of the irreps:')
print(rho.change_of_basis @ direct_sum @ rho.change_of_basis_inv)
print()
print('Are the two representations equal?', np.allclose(rho(g), rho.change_of_basis @␣
↪direct_sum @ rho.change_of_basis_inv))
```

```
Regular representation of 1[2pi/8]
[[ 0. -0.  0. -0. -0.  0. -0.  1.]
 [ 1.  0. -0. -0. -0. -0.  0. -0.]
 [-0.  1.  0. -0.  0. -0. -0. -0.]
```

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```
 [-0.  0.  1.  0. -0.  0. -0.  0.]
 [-0. -0. -0.  1.  0. -0.  0. -0.]
 [-0.  0. -0.  0.  1.  0.  0. -0.]
 [-0. -0. -0. -0.  0.  1.  0.  0.]
 [-0.  0. -0. -0.  0. -0.  1.  0.]]

Direct sum of the irreps:
[[ 1.     0.     0.     0.     0.     0.     0.     0.   ]
 [ 0.     0.707 -0.707  0.     0.     0.     0.     0.   ]
 [ 0.     0.707  0.707  0.     0.     0.     0.     0.   ]
 [ 0.     0.     0.     0.    -1.     0.     0.     0.   ]
 [ 0.     0.     0.     1.     0.     0.     0.     0.   ]
 [ 0.     0.     0.     0.     0.    -0.707 -0.707  0.   ]
 [ 0.     0.     0.     0.     0.     0.707 -0.707  0.   ]
 [ 0.     0.     0.     0.     0.     0.     0.    -1.   ]]

Apply the change of basis on the direct sum of the irreps:
[[ 0. -0.  0. -0. -0.  0. -0.  1.]
 [ 1.  0. -0.  0. -0. -0.  0. -0.]
 [-0.  1.  0. -0.  0. -0. -0. -0.]
 [-0.  0.  1.  0. -0.  0. -0.  0.]
 [-0. -0. -0.  1.  0. -0.  0. -0.]
 [-0.  0. -0.  0.  1.  0.  0. -0.]
 [-0. -0. -0. -0.  0.  1.  0.  0.]
 [-0.  0. -0. -0.  0. -0.  1.  0.]]

Are the two representations equal? True
```

1.2 Fourier Transform

We can finally approach the harmonic analysis of functions over a group G.

Note that a representation $\rho : G \to \mathbb{R}^{d\times d}$ can be interpreted as a collection of d^2 functions over G, one for each matrix entry of ρ. The **Peter-Weyl theorem** states that the collection of functions in the matrix entries of all irreps $\hat{G}$ of a group G spans the space of all (square-integrable) functions over G.

This result gives us a way to parameterize functions over the group. This is the focus of this section. In particular, this is useful to parameterize functions over groups with infinite elements.

In this section, we will first consider the *dihedral group* D_8 as example. This is the group containing the 8 planar rotations by angles multiple of $\frac{2\pi}{8}$ and *reflection* along the X axis. The group contains in total 16 elements (8 normal rotations and 8 rotations preceeded by the reflection).

[31]:
```
G = dihedral_group(8)
G.order()
```

[31]:
```
16
```

[32]:
```
# element representing the reflection (-) and no rotations
G.reflection
```

[32]:
```
(-, 0[2pi/8])
```

[33]:
```
# element representing a rotation by pi/2 (i.e. 2 * 2pi/8) and no reflections (+)
G.element((0, 2))
```

[33]:
```
(+, 2[2pi/8])
```

[34]:
```
# reflection followed by a rotation by pi/2
print(G.element((0, 2)) @ G.reflection)

# we can also directly generate this element as
print(G.element((1, 2)))
```

```
(-, 2[2pi/8])
(-, 2[2pi/8])
```

[35]:
```
# a rotation by pi/2 followed by a reflection is equivalent to a reclection followed by␣
↪a rotation by 6*2pi/8
G.reflection @ G.element((0, 2))
```

[35]:
```
(-, 6[2pi/8])
```

The list of all elements in the group is obtaied as:

[36]:
```
G.elements
```

[36]:
```
[(+, 0[2pi/8]),
 (+, 1[2pi/8]),
 (+, 2[2pi/8]),
 (+, 3[2pi/8]),
 (+, 4[2pi/8]),
 (+, 5[2pi/8]),
 (+, 6[2pi/8]),
 (+, 7[2pi/8]),
 (-, 0[2pi/8]),
 (-, 1[2pi/8]),
 (-, 2[2pi/8]),
 (-, 3[2pi/8]),
 (-, 4[2pi/8]),
 (-, 5[2pi/8]),
 (-, 6[2pi/8]),
 (-, 7[2pi/8])]
```

Fourier and Inverse Fourier Transform

For most groups, the entries of the irreps don't only span the space of functions but form also a basis (i.e. these functions are mutually orthogonal to each other). Therefore, we can write a function $f : G \to \mathbb{R}$ as

$$f(g) = \sum_{\rho_j \in \hat{G}} \sum_{m,n<d_j} w_{j,m,n} \cdot \sqrt{d_j}[\rho_j(g)]_{mn}$$

where d_j is the dimension of the irrep ρ_j, while m, n index the d_j^2 entries of ρ_j. The coefficients $\{w_{j,m,n} \in \mathbb{R}\}_{j,m,n}$ parameterize the function f on this basis. The $\sqrt{d_j}$ is a scalar factor to ensure the basis is normalized.

We rewrite this expression in a cleaner form by using the following fact. If $A, B \in \mathbb{R}^{d \times d}$, then

$$\text{Tr}(A^T B) = \sum_{m,n<d} A_{mn} B_{mn} \in \mathbb{R} \,.$$

By defininning $\hat{f}(\rho_j) \in \mathbb{R}^{d_j \times d_j}$ as the matrix containing the d_j^2 coefficients $\{w_{j,m,n} \in \mathbb{R}\}_{m,n<d_j}$, we can express the **Inverse Fourier Transform** as:

$$f(g) = \sum_{\rho_j \in \hat{G}} \sqrt{d_j} \text{Tr}\left(\rho_j(g)^T \hat{f}(\rho_j)\right)$$

Similarly, we can project a general function $f : G \to \mathbb{R}$ on an element $\rho_{j,m,n} : G \to \mathbb{R}$ of the basis via:

$$w_{j,m,n} = \frac{1}{|G|} \sum_{g \in G} f(g) \sqrt{d_j} [\rho_j(g)]_{m,n} \, .$$

The projection over all entries of ρ_j can be more cleanly written as follows:

$$\hat{f}(\rho_j) = \frac{1}{|G|} \sum_{g \in G} f(g) \sqrt{d_j} \rho_j(g) \, .$$

which we refer to as **Fourier Transform**.

If the group G is *infinite*, we replace the average over the group elements with an *integral* over them:

$$\hat{f}(\rho_j) = \int_G f(g) \sqrt{d_j} \rho_j(g) dg \, ,$$

For a finite group G, we can access all its irreps by using the `Group.irreps()` method. Let's see an example:

[37]:
```
irreps = G.irreps()
print(f'The dihedral group D8 has {len(irreps)} irreps')
```

```
The dihedral group D8 has 7 irreps
```

[38]:
```
# the first one, is the 1-dimensional trivial representation
print(irreps[0] == G.trivial_representation == G.irrep(0, 0))
```

```
True
```

QUESTION 4

We can now implement the Fourier Transform and the Inverse Fourier Transform for the Dihedral Group D_8. Using the equations above, implement the following methods:

---

[39]:
```
def fourier_transform_D8(f: np.array):
    # the method gets in input a function on the elements of D_8
    # and should return a dictionary mapping each irrep's `id` to the corresponding␣
↪Fourier Transform
    # The i-th element of `f` stores the value of the function on the group element `G.
↪elements[i]`

    G = dihedral_group(8)
    assert f.shape == (16,), f.shape
    ft = {}
```

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```
    ########################
    # INSERT YOUR CODE HERE:

    for rho in G.irreps():
        d = rho.size

        rho_g = np.stack([rho(g) for g in G.elements], axis=0)

        ft[rho.id] = (f.reshape(-1, 1, 1) * rho_g).mean(0) * np.sqrt(d)

    ########################

    return ft
```

[40]:
```
def inverse_fourier_transform_D8(ft: dict):
    # the method gets in input a dictionary mapping each irrep's `id` to the␣
↪corresponding Fourier Transform
    # and should return the function `f` on the elements of D_8
    # The i-th element of `f` stores the value of the function on the group element `G.
↪elements[i]`

    G = dihedral_group(8)
    f = np.zeros(16)

    ########################
    # INSERT YOUR CODE HERE:
    for rho in G.irreps():
        d = rho.size
        for i, g in enumerate(G.elements):
            f[i] += np.sqrt(d) * (ft[rho.id] * rho(g)).sum()
    ########################

    return f
```

We now want to verify that the **Fourier Transform** and the **Inverse Fourier Transform** are inverse of each other:

[41]:
```
f = np.random.randn(16)

ft = fourier_transform_D8(f)

new_f = inverse_fourier_transform_D8(ft)

assert np.allclose(f, new_f)
```

Parameterizing functions over infinite groups

This allows us to also parameterize functions over infinite groups, such as $O(2)$, i.e. the group of all planar rotations and reflections.

[42]:
```
G = o2_group()
```

[43]:
```
# the group has infinite many elements, so the `order` method just returns -1
G.order()
```

[43]:
```
-1
```

The equations remain the same, but this group has an *infinite* number of *irreps*. We can, however, parameterize a function over the group by only considering a finite number of irreps in the sum inside the definition of *Inverse Fourier Transform*. Let $\tilde{G} \subset \hat{G}$ be a finite subset of the irreps of G. We can then write the following transforms within the subspace of functions spanned only by the entries of the irreps in $\tilde{G}$.

Inverse Fourier Transform:

$$f(g) = \sum_{\rho_j \in \tilde{G}} \sqrt{d_j} \text{Tr}\left(\rho_j(g)^T \hat{f}(\rho_j)\right)$$

and **Fourier Transform**:

$$\hat{f}(\rho_j) = \int_G f(g) \sqrt{d_j} \rho_j(g) dg \ ,$$

QUESTION 5

We can now implement the Inverse Fourier Transform for the Orthogonal Group $O(2)$. Since the group has infinite many elements, we can not store the values the function take on each element. Instead, we just sample the function on a particular element of the group:

---

[44]:
```
def inverse_fourier_transform_O2(g: GroupElement, ft: dict):
    # the method gets in input a dictionary mapping each irrep's `id` to the␣
↪corresponding Fourier Transform
    # and a group element `g`
    # The method should return the value of the function evaluated on `g`.

    G = o2_group()
    f = 0

    ########################
    # INSERT YOUR CODE HERE:
    for rho, ft_rho in ft.items():
        rho = G.irrep(*rho)
        d = rho.size
        f += np.sqrt(d) * (ft_rho * rho(g)).sum()
    ########################

    return f
```

Let's plot a function. First we generate a random function by using a few irreps.

[45]:
```
irreps = [G.irrep(0, 0)] + [G.irrep(1, j) for j in range(3)]

ft = {
    rho.id: np.random.randn(rho.size, rho.size)
    for rho in irreps
}
```

Then, we generate a grid on the group where to evaluate the function, i.e. we choose a finite set of element of G. Like the Dihedral group, $O(2)$ contains rotations (parameterized by an angle $\theta \in [0, 2\pi)$) and a reflection followed by any rotation. For example:

[46]:
```
G.sample()
```

[46]:
```
(+, 0.026961821470776897)
```

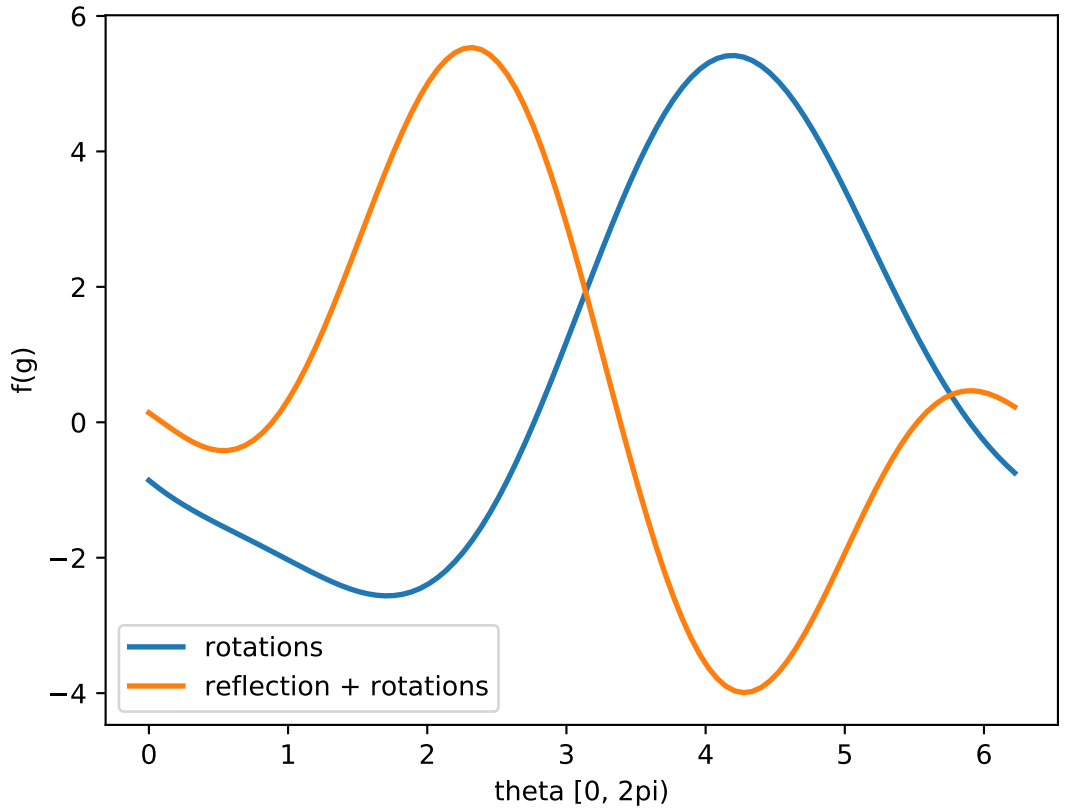
To build our grid, we sample 100 rotations and 100 rotations preceeded by a reflection:

[47]:
```
N = 100
thetas = [i*2*np.pi/N for i in range(N)]
grid_rot = [G.element((0, theta)) for theta in thetas]
grid_refl = [G.element((1, theta)) for theta in thetas]
```

We now evaluate the function over all these elements and, finally, plot it:

[48]:
```
f_rot = [
    inverse_fourier_transform_O2(g, ft) for g in grid_rot
]
f_refl = [
    inverse_fourier_transform_O2(g, ft) for g in grid_refl
]


plt.plot(thetas, f_rot, label='rotations')
plt.plot(thetas, f_refl, label='reflection + rotations')
plt.xlabel('theta [0, 2pi)')
plt.ylabel('f(g)')
plt.legend()
plt.show()
```



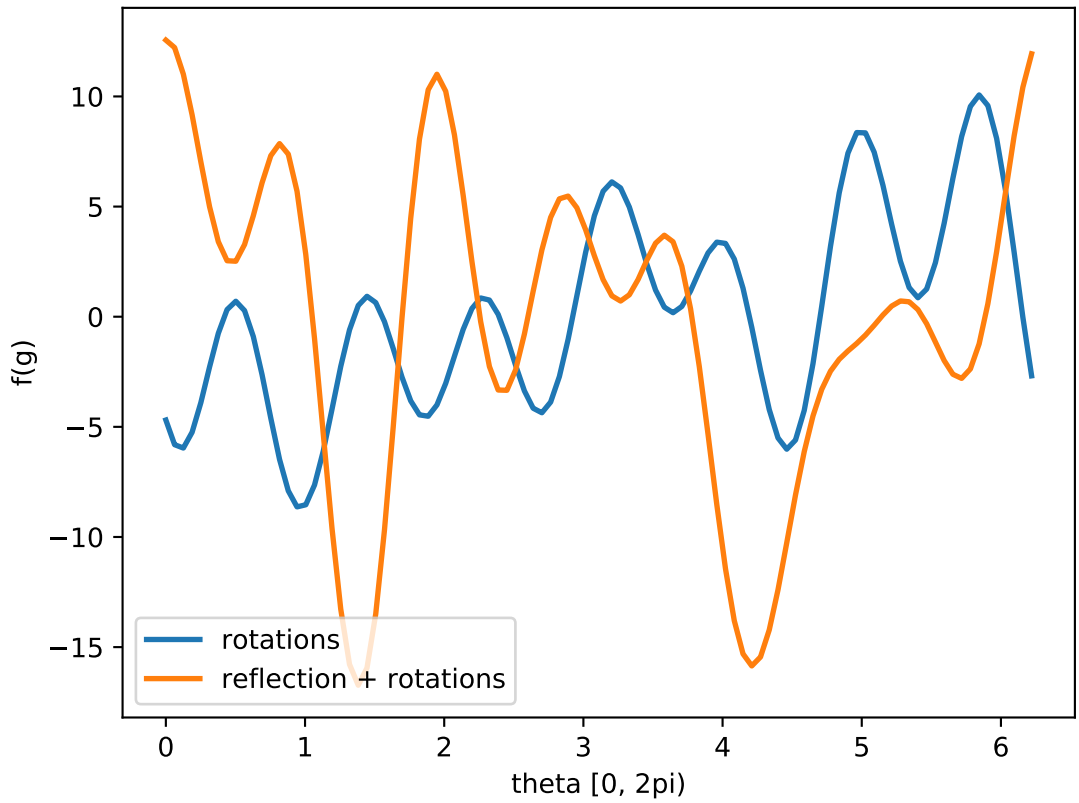
Observe that using more irreps allows one to parameterize more flexible functions. Let's try to add some more:

[49]:
```
irreps = [G.irrep(0, 0)] + [G.irrep(1, j) for j in range(8)]

ft = {
    rho.id: np.random.randn(rho.size, rho.size)
    for rho in irreps
}

f_rot = [
    inverse_fourier_transform_O2(g, ft) for g in grid_rot
]
f_refl = [
    inverse_fourier_transform_O2(g, ft) for g in grid_refl
]


plt.plot(thetas, f_rot, label='rotations')
plt.plot(thetas, f_refl, label='reflection + rotations')
plt.xlabel('theta [0, 2pi)')
plt.ylabel('f(g)')
plt.legend()
plt.show()
```



Fourier Transform of shifted functions

Recall that a group element $g \in G$ can act on a function $f : G \to \mathbb{R}$ as:

$$[g.f](h) = f(g^{-1}h) \; .$$

The Fourier transform defined before has the convenient property that the Fourier transform of f and of $[g.f]$ are related as follows:

$$\widehat{g.f}(\rho_j) = \rho_j(g)\widehat{f}$$

for any irrep ρ_j.

QUESTION 6

Prove the property above.

ANSWER 6

$$\widehat{g.f}(\rho_j) = \int_G [g.f](h)\sqrt{d_j}\rho_j(h)dh \tag{4.1}$$
$$= \int_G f(g^{-1}h)\sqrt{d_j}\rho_j(h)dh \tag{4.2}$$

Define $t = g^{-1}h$ and, therefore, $h = gt$ (4.3)

$$= \int_G f(t)\sqrt{d_j}\rho_j(gt)dt \tag{4.4}$$
$$= \int_G f(t)\sqrt{d_j}\rho_j(g)\rho_j(t)dt \tag{4.5}$$
$$= \rho_j(g)\int_G f(t)\sqrt{d_j}\rho_j(t)dt \tag{4.6}$$
$$= \rho_j(g)\hat{f}(\rho_j) \tag{4.7}$$

We can verify this property visually:

[50]:
```
irreps = [G.irrep(0, 0)] + [G.irrep(1, j) for j in range(8)]

# first, we generate a random function, as earlier
ft = {
    rho.id: np.random.randn(rho.size, rho.size)
    for rho in irreps
}

# second, we sample a random group element `g`
g = G.sample()
print(f'Transforming the function with g={g}')

# finally, we transform the Fourier coefficients as in the equations above:
gft = {
    rho.id: rho(g) @ ft[rho.id]
    for rho in irreps
}

# Let's now visualize the two functions:

f_rot = [
    inverse_fourier_transform_O2(g, ft) for g in grid_rot
]
f_refl = [
    inverse_fourier_transform_O2(g, ft) for g in grid_refl
]

gf_rot = [
    inverse_fourier_transform_O2(g, gft) for g in grid_rot
]
gf_refl = [
```

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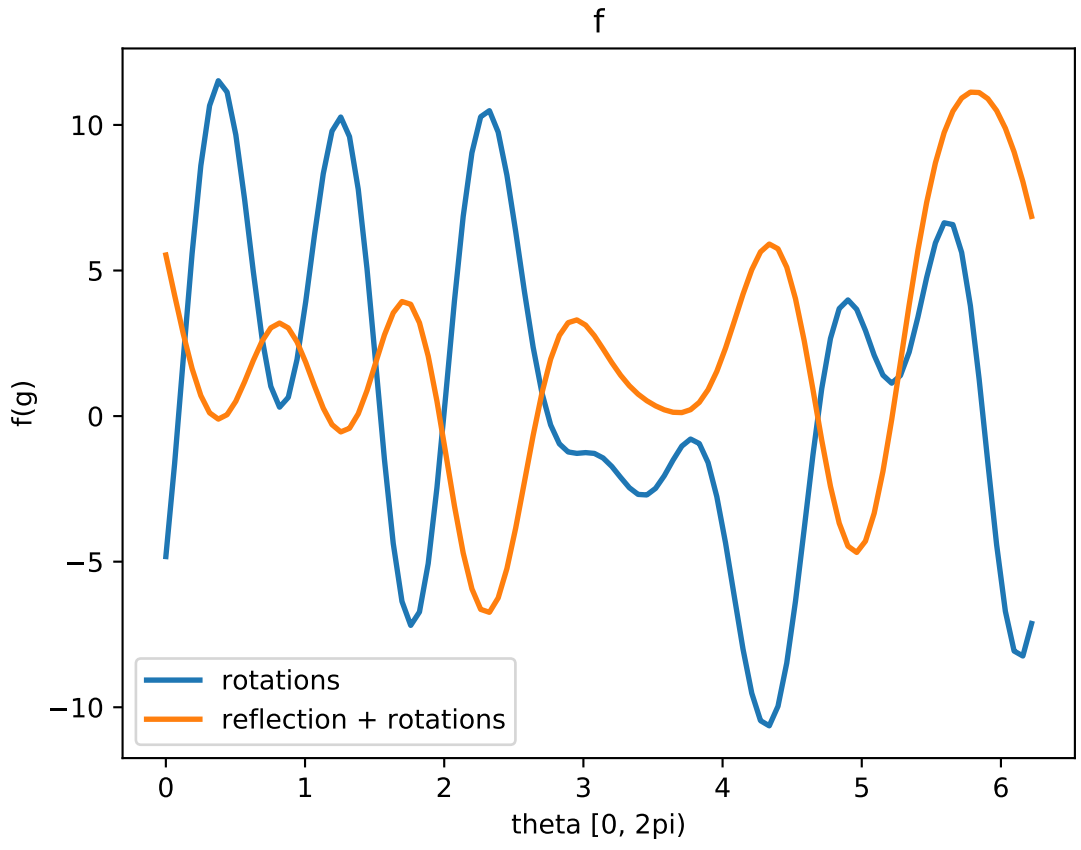
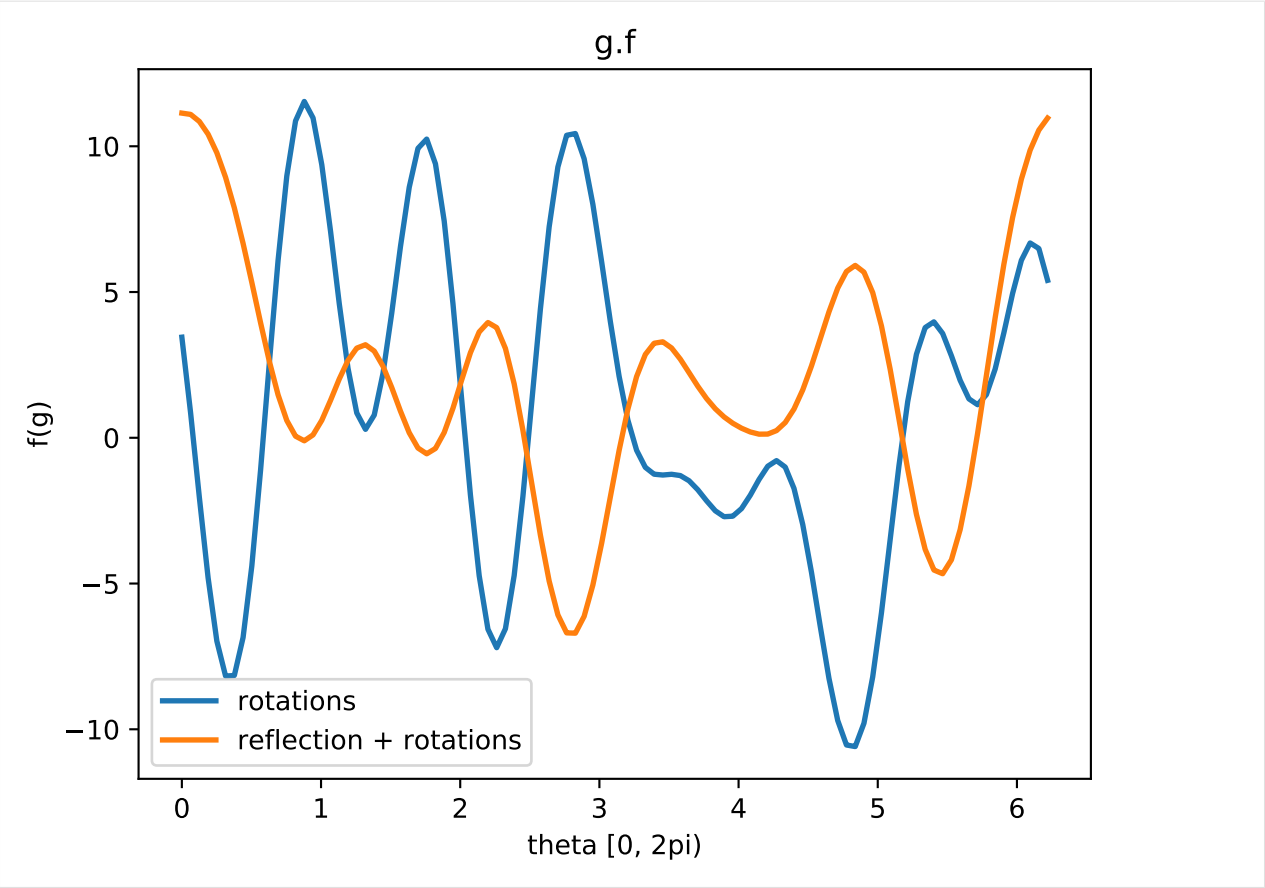
```
    inverse_fourier_transform_02(g, gft) for g in grid_refl
]


plt.plot(thetas, f_rot, label='rotations')
plt.plot(thetas, f_refl, label='reflection + rotations')
plt.xlabel('theta [0, 2pi)')
plt.ylabel('f(g)')
plt.title('f')
plt.legend()
plt.show()

plt.plot(thetas, gf_rot, label='rotations')
plt.plot(thetas, gf_refl, label='reflection + rotations')
plt.xlabel('theta [0, 2pi)')
plt.ylabel('f(g)')
plt.title('g.f')
plt.legend()
plt.show()
```

```
Transforming the function with g=(+, 0.4933335011719361)
```





From the Fourier Transform to the Regular Representation

For simplicity, we can stack all the Fourier coefficients (the output of the Fourier transform, that is, the input of the inverse Fourier transform) into a unique vector. We define the vector $\mathbf{f}$ as the stack of the columns of each Fourier coefficients matrix $f(\rho_j)$.

Let's first introduce some notation. We denote the stack of two vectors $\mathbf{v_1}, \mathbf{v_2}$ as $\mathbf{v_1} \oplus \mathbf{v_2}$. The use of $\oplus$ is not random: if ρ_1 is a representation acting on $\mathbf{v_1}$ and ρ_2 is a representation acting on $\mathbf{v_2}$, then the *direct sum* $\rho_1 \oplus \rho_2$ acts on the concatenated vector $\mathbf{v_1} \oplus \mathbf{v_2}$.

Second, we denote by $\text{vec}(A)$ the vector which is the stack of the columns of a matrix A. In `numpy`, this is written as `A.T.reshape(-1)`, where the transpose is necessary since `numpy` stacks rows by default.

Then, we write:

$$\mathbf{f} = \bigoplus_{\rho_j} \text{vec}(\hat{f}(\rho_j)) \ .$$

Moreover, by using $\widehat{g.f}(\rho_j) = \rho_j(g)\hat{f}(\rho_j)$, we see that the vector containing the coefficients of the function $[g.f]$ will be:

$$\bigoplus_{\rho_j} \text{vec}(\rho_j(g)\hat{f}(\rho_j)) = \bigoplus_{\rho_j} \left(\bigoplus^{d_j} \rho_j(g) \right) \text{vec}(\hat{f}(\rho_j))$$

In other words, the group G is acting on the vector $\mathbf{f}$ with the following representation:

$$\rho(g) = \bigoplus_{\rho_j} \bigoplus^{d_j} \rho_j(g)$$

i.e. $\rho(g)\mathbf{f}$ is the vector containing the Fourier coefficients of the function $[g.f]$.

Note that, essentially, the representation ρ acts on a vector space containing functions over G. This should remind you of the **regular representation** we defined for *finite groups* earlier. Indeed, it turns out that, if G is finite, the representation ρ we have just constructed is **isomorphic** (*equivalent*) to the *regular representation* defined earlier. The change of basis Q is a matrix which performs the Fourier transform, while Q^{-1} performs the inverse Fourier transform. More formally:

$$\rho_{\text{reg}}(g) = Q^{-1} \left(\bigoplus_{\rho_j} \bigoplus^{d_j} \rho_j(g) \right) Q$$

where each irrep ρ_j is repeated d_j times, i.e. a number of times equal to its size.

Intuition: recall that a function $f : G \to \mathbb{R}$ is just a vector living in a vector space. Such vector can be expressed with respect to any basis for this vector space. The first time we introduced the *regular representation* for finite groups, we chose a basis where each axis is associated with a group element; the action of G is realized in this basis by a permutation of all the axes. Here, instead, we defined a basis for the same vector space where G acts indipendently on different subsets of the axes, i.e. the action of G is a block-diagonal matrix (the direct sum of irreps). This is often a more convenient choice of basis as we will see later.

Let verify this equivalence for the Dihdral group D_8:

[51]:
```
G = dihedral_group(8)

rho_irreps = []
for rho_j in G.irreps():
    d_j = rho_j.size
    # repeat each irrep a number of times equal to its size
    rho_irreps += [rho_j]*d_j

rho = directsum(rho_irreps)

print('The representations have the same size:')
print(rho.size, G.regular_representation.size)

print('And contain the same irreps:')
print(rho.irreps)
print(G.regular_representation.irreps)

# Fourier transform matrix:
Q = G.regular_representation.change_of_basis
# inverse Fourier transform matrix:
Qinv = G.regular_representation.change_of_basis_inv

# let's check that the two representations are indeed equivalent
g = G.sample()

rho_g = rho(g)
```

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```
reg_g = G.regular_representation(g)
print()
print('Are the two representations equivalent?', np.allclose(Q @ rho_g @ Qinv, reg_g))
```

```
The representations have the same size:
16 16
And contain the same irreps:
[(0, 0), (1, 0), (1, 1), (1, 1), (1, 2), (1, 2), (1, 3), (1, 3), (1, 4), (0, 4)]
[(0, 0), (1, 0), (1, 1), (1, 1), (1, 2), (1, 2), (1, 3), (1, 3), (1, 4), (0, 4)]

Are the two representations equivalent? True
```

When G is not finite, we can not explicitly store the regular representation ρ_{reg} or the Fourier transform matrix Q, since they are infinite dimensional. Nevertheless, as we have done earlier, we can just consider a subset of all functions, spanned only by a finite number of irreps. We can sample the function on any group element via the Inverse Fourier Transform when needed, without the need to compute the full Inverse Fourier Transform Q^{-1} to store all values.

This is the underlying idea we will exploit later to build GCNNs equivariant to infinite groups.

We can easily generate this representation as (`bl_regular_representation` stands for "band-limited", since only a limited subset of irreps, i.e. frequencies, is used):

[52]:
```
G = o2_group()

rho = G.bl_regular_representation(7)

rho.irreps
```

[52]:
```
[(0, 0),
 (1, 0),
 (1, 1),
 (1, 1),
 (1, 2),
 (1, 2),
 (1, 3),
 (1, 3),
 (1, 4),
 (1, 4),
 (1, 5),
 (1, 5),
 (1, 6),
 (1, 6),
 (1, 7),
 (1, 7)]
```

Irreps with redundant entries: the case of $SO(2)$

We need to conclude with a final note about the Fourier transform. When we introduced it earlier, we said that the entries of the irreps form a **basis** for the functions over *most* groups. Indeed, there exists some groups where the entries of the irreps are partially redundant and, therefore, form an *overcomplete* basis. This is the case, for example, of the group of planar rotations $SO(2)$ (or the group of N discrete rotations C_N). Indeed, an irrep of $SO(2)$ has form:

$$\rho_j(r_\theta) = \begin{bmatrix} \cos(j \cdot \theta) & -\sin(j \cdot \theta) \\ \sin(j \cdot \theta) & \cos(j \cdot \theta) \end{bmatrix}$$

for $\theta \in [0, 2\pi)$, where the integer $j \in \mathbb{N}$ is interpreted as the rotational *frequency*.

You can observe that the two columns of $\rho_j(r_\theta)$ contain redundant elements and span the same 2 dimensional space of functions. It is indeed sufficient to consider only one of the two columns to parameterize functions over $SO(2)$. This also means that the irrep ρ_j appears only once (instead of $d_j = 2$ times) in the regular representation.

We don't generally need to worry much about this, since we can generate the representation as earlier:

[53]:
```
G = so2_group()

rho = G.bl_regular_representation(7)


# observe that each irrep is now repeated only once, even if some are 2-dimensional
rho.irreps
```

[53]:
```
[(0,), (1,), (2,), (3,), (4,), (5,), (6,), (7,)]
```

4.42.3 2. From Group CNNs to Steerable CNNs

We consider a GCNN equivariant to a *semi-direct* product group $\mathbb{R}^n \rtimes G$, with compact group $G \leq O(n)$. This setting covers equivariance to **isometries** (distance preserving transformations) of the Euclidean space $\mathbb{R}^n$; in particular, it includes equivariance to *translations* in $\mathbb{R}^n$ and to a origin-preserving symmetry G (e.g. rotations or reflections in n-dimensions). We call G a **point group**.

If $G = O(n)$, the group of all rotations and reflections in $\mathbb{R}^n$, then $E(n) = \mathbb{R}^n \rtimes O(n)$ is called the **Euclidean group**, and includes all isometries of $\mathbb{R}^n$.

2.1 Feature Fields

In a GCNN, a feature map is a signal $f : \mathbb{R}^n \times G \to \mathbb{R}$. The action of an element $(x, g) \in \mathbb{R}^n \rtimes G$ is:

$$[(x, g).f](y, h) := f(g^{-1}(y - x), g^{-1}h)$$

where $x, y \in \mathbb{R}^n$ and $g, h \in G$.

QUESTION 7

Prove the action has indeed this form.

ANSWER 7

First, recall the group law: for any (x, g) and $(y, h) \in \mathbb{R}^n \rtimes G$

$$(x, g) \cdot (y, h) = (x + g.y, gh)$$

where $x, y, g.y \in \mathbb{R}^n$ and $g, h \in G$. Second, recall the inverse element is $(x, g)^{-1} = (-g^{-1}.x, g^{-1})$. Then:

$$[(x, g).f](y, h) = f((x, g)^{-1} \cdot (y, h)) = f(-g^{-1}.x + g^{-1}.y, g^{-1}h) = f(g^{-1}.(y - x), g^{-1}h)$$

In a GCNN, a feature map f is stored as a multi-dimensional array with an axis for each of the n spatial dimensions and one for the group G.

In a steerable CNN, we replace the G axis with a "Fourier" axis, which contains c Fourier coefficients used to parameterize a function over G, as described in the previous section. Again, let's call $\rho : G \to \mathbb{R}^{c \times c}$ the representation of G acting on these c coefficients. The result is equivalent to a standard GCNN if G is finite (and we have $c = |G|$), but we can now also use infinite G, such as $SO(2)$.

A feature map f can now be interpreted as a vector field on the space $\mathbb{R}^n$, i.e.:

$$f : \mathbb{R}^n \to \mathbb{R}^c$$

which assigns a c-dimensional feature vector $f(x) \in \mathbb{R}^c$ to each spatial position $x \in \mathbb{R}^n$. We call such vector field a **feature vector field**.

The action of $\mathbb{R}^n \rtimes G$ on one such feature vector field is defined as:

$$[(x, g).f](y) := \rho(g) f(g^{-1}(y - x))$$

where $x, y \in \mathbb{R}^n$ and $g \in G$.

QUESTION 8

Prove that this is indeed the right action of $\mathbb{R}^n \rtimes G$ on the feature vector field $f : \mathbb{R}^n \to \mathbb{R}^c$. Recall the action of this group over the functions of the form $\underline{f} : \mathbb{R}^n \rtimes G \to \mathbb{R}$ that we described earlier. Moreover, note that the vector $f(x) \in \mathbb{R}^c$ contains the c Fourier coefficients of the function $\underline{f}(x, \cdot) : G \to \mathbb{R}$ along its G axis, i.e.:

$$f(x) = \bigoplus_{\rho_j} \text{vec}\left(\widehat{\underline{f}(x, \cdot)}(\rho_j)\right)$$

ANSWER 8:

We know from the previous question that

$$[(x,g).\underline{f}](y,h) = \underline{f}(g^{-1}(y-x), g^{-1}h)$$

Recall also that $\rho(g) = \bigoplus_{\rho_j} \bigoplus^{d_j} \rho_j(g) \in \mathbb{R}^{c\times c}$ is the regular representation of G acting on the vector of Fourier coefficients. Then:

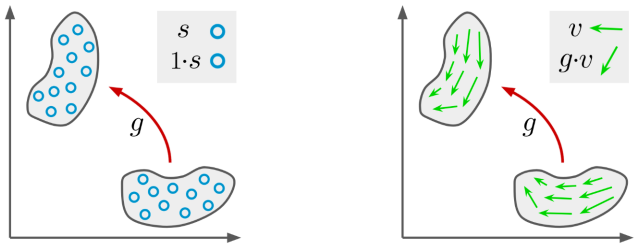
$$\begin{aligned}
[(x,g).f](y) &= \bigoplus_{\rho_j} \text{vec}\left(\left[\widehat{[(x,g).\underline{f}](y,\cdot)}\right](\rho_j)\right) && (4.8)\\
&= \bigoplus_{\rho_j} \text{vec}\left(\left[\underline{f}(g^{-1}\widehat{(y-x)}, g^{-1}\cdot)\right](\rho_j)\right) && (4.9)\\
&= \bigoplus_{\rho_j} \text{vec}\left(\rho_j(g)\left[\underline{f}(g^{-1}\widehat{(y-x)},\cdot)\right](\rho_j)\right) && (4.10)\\
&= \rho(g)f(g^{-1}(y-x)) && (4.11)
\end{aligned}$$

Note that in the equations above, the square brakets in $\widehat{[\cdot]}$ indicate that $\widehat{\cdot}$ covers the whole content of the brackets.

General Steerable CNNs

The framework of Steerable CNNs is actually more general and allows for any representation ρ of G. A different choice of ρ generally require some structural change in the architecture, e.g. by adapting the non-linearity used to ensure equivariance. Anyways, for simplicity, we will stick with the Fourier example in this tutorial.

Throughout the rest of this tutorial, we will assume $n = 2$ for simplicity. That means we will be working for example with planar images and with the isometries of the plane (2D rotations or mirroring). The actions of $g \in G = SO(2)$ on two examples of feature vector fields over $\mathbb{R}^2$ are shown next. On the left, ρ is the trivial representation of $SO(2)$ while, on the right, ρ is the representation of $SO(2)$ as 2×2 rotation matrices.



scalar field vector field

2.2 Defining a Steerable CNN

We can now proceed with building a Steerable CNN. First we import some other useful packages.

[54]:
```
from escnn import group
from escnn import gspaces
from escnn import nn
```

First, we need to choose the group G of point symmetries (reflections and rotations) which are being considered. All of these choices are subgroups $G \leq O(2)$ of the orthogonal group.

For simplicity, we first consider the *finite* group $G = C_4$, which models the 4 *rotations* by angle $\theta \in \{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\}$. Because these are perfect symmetries of the grid, transforming an image with this group does not require any interpolation. We will later extend our examples to an infinite group such as $SO(2)$ or $O(2)$.

Recall that a semi-direct product $\mathbb{R}^2 \rtimes G$ is defined by G but also by the action of G on $\mathbb{R}^2$. We determine both the **point group** G and its **action on the space** $\mathbb{R}^2$ by instantiating a subclass of `gspace.GSpace`. For the rotational action of $G = C_4$ on $\mathbb{R}^2$ this is done by:

[55]:
```
r2_act = gspaces.rot2dOnR2(N=4)
r2_act
```

[55]:
```
C4_on_R2[(None, 4)]
```

[56]:
```
# we can access the group G as
G = r2_act.fibergroup
G
```

[56]:
```
C4
```

Having specified the symmetry transformation on the *base space* $\mathbb{R}^2$, we next need to define the representation $\rho : G \to \mathbb{R}^{c \times c}$ which describes how a **feature vector field** $f : \mathbb{R}^2 \to \mathbb{R}^c$ transforms under the action of G. This transformation law of feature fields is implemented by `nn.FieldType`.

We instantiate the `nn.FieldType` modeling a GCNN feature by passing it the `gspaces.GSpace` instance and the *regular representation* of $G = C_4$. We call a feature field associated with the regular representation ρ_{reg} a **regular feature field**.

[57]:
```
feat_type = nn.FieldType(r2_act, [G.regular_representation])
feat_type
```

[57]:
```
[C4_on_R2[(None, 4)]: {regular (x1)}(4)]
```

Recall that the regular representation of a finite group G built by `G.regular_representation` is a permutation matrix of shape $|G| \times |G|$:

[58]:
```
G.regular_representation(G.sample())
```

[58]:
```
array([[ 1.,  0., -0., -0.],
       [ 0.,  1.,  0., -0.],
       [-0.,  0.,  1.,  0.],
       [-0., -0.,  0.,  1.]])
```

Deep Feature spaces

The deep feature spaces of a GCNN typically comprise multiple channels. Similarly, the feature spaces of a steerable CNN can include multiple independent feature fields. This is achieved via **direc sum**, but stacking multiple copies of ρ.

For example, we can use 3 copies of the regular representation $\rho_{\text{reg}} : G \to \mathbb{R}^{|G|}$. The full feature space is in this case modeled as a *stacked* field $f : \mathbb{R}^2 \to \mathbb{R}^{3|G|}$ which transforms according to the **direct sum** of three regular representations:

$$\rho(r_\theta) = \rho_{\text{reg}}(r_\theta) \oplus \rho_{\text{reg}}(r_\theta) \oplus \rho_{\text{reg}}(r_\theta) = \begin{bmatrix} \rho_{\text{reg}}(\theta) & 0 & 0 \\ 0 & \rho_{\text{reg}}(\theta) & 0 \\ 0 & 0 & \rho_{\text{reg}}(\theta) \end{bmatrix} \in \mathbb{R}^{3|G| \times 3|G|}$$

We instantiate a `nn.FieldType` composed of 3 regular representations by passing the full field representation as a list of three regular representations:

[59]:
```
# Technically, one can also construct the direct-sum representation G.regular_
↪representation + G.regular_representation + G.regular_representation as done
# before. Passing a list containing 3 copies of G.regular_representation allows for more␣
↪efficient implementation of certain operations internally.
feat_type = nn.FieldType(r2_act, [G.regular_representation]*3)
feat_type
```

[59]:
```
[C4_on_R2[(None, 4)]: {regular (x3)}(12)]
```

Input Features

Each hidden layer of a steerable CNN has its own transformation law which the user needs to specify (equivalent to the choice of number of channels in each layer of a conventional CNN). The *input* and *output* of a steerable CNN are also feature fields and their type (i.e. transformation law) is typically determined by the inference task.

The most common example is that of gray-scale input images. A rotation of a gray-scale image is performed by moving each pixel to a new position without changing their intensity values. The invariance of the scalar pixel values under rotations is modeled by the **trivial representation** $\rho_0 : G \to \mathbb{R},\ g \mapsto 1$ of G and identifies them as **scalar fields**. Formally, a scalar field is a function $f : \mathbb{R}^2 \to \mathbb{R}$ mapping to a feature vector with $c = 1$ channels. A rotation $r_\theta \in C_4$ transforms this scalar field as

$$\big[r_\theta \,.f\big](x) \;:=\; \rho_0(r_\theta)\, f\big(r_\theta^{-1}x\big) \;=\; 1 \cdot f\big(r_\theta^{-1}x\big) \;=\; f\big(r_\theta^{-1}x\big)\,.$$

We instantiate the `nn.FieldType` modeling a gray-scale image by passing it the trivial representation of G:

[60]:
```
feat_type_in = nn.FieldType(r2_act, [G.trivial_representation])
feat_type_in
```

[60]:
```
[C4_on_R2[(None, 4)]: {irrep_0 (x1)}(1)]
```

Equivariant Layers

When we build a model **equivariant** to a group G, we require that the output produced by the model transforms consistently when the input transforms under the action of an element $g \in G$. For a function F (e.g. a neural network), the **equivariance constraint** requires:

$$\mathcal{T}_g^{\text{out}}\big[F(x)\big] \;=\; F\big(\mathcal{T}_g^{\text{in}}[x]\big) \quad \forall g \in G$$

where $\mathcal{T}_g^{\text{in}}$ is the transformation of the input by the group element g while $\mathcal{T}_g^{\text{out}}$ is the transformation of the output by the same element. The *field type* `feat_type_in` we have just defined above precisely describes $\mathcal{T}^{\text{in}}$. The transformation law $\mathcal{T}^{\text{out}}$ of the output of the first layer is similarly chosen by defining an instance `feat_type_out` of `nn.FieldType`.

For example, let's use 3 *regular feature fields* in output:

[61]:
```
feat_type_out = nn.FieldType(r2_act, [G.regular_representation]*3)
```

As a shortcut, we can also use:

[62]:
```
feat_type_in = nn.FieldType(r2_act, [r2_act.trivial_repr])
feat_type_out = nn.FieldType(r2_act, [r2_act.regular_repr]*3)
```

Once having defined how the input and output feature spaces should transform, we can build neural network functions as **equivariant modules**. These are implemented as subclasses of an abstract base class `nn.EquivariantModule` which itself inherits from `torch.nn.Module`.

Equivariant Convolution Layer: We start by instantiating a convolutional layer that maps between fields of types `feat_type_in` and `feat_type_out`.

Let $\rho_{\text{in}} : G \to \mathbb{R}^{c_{\text{in}} \times c_{\text{in}}}$ and $\rho_{\text{out}} : G \to \mathbb{R}^{c_{\text{out}} \times c_{\text{out}}}$ be respectively the representations of G associated with `feat_type_in` and `feat_type_out`. Then, an equivariant convolution layer is a standard convolution layer with a filter $k : \mathbb{R}^2 \to \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$ (note the number of input and output channels) which satisfies a particular **steerability constraint**:

$$\forall g \in G, x \in \mathbb{R}^2 \quad k(g.x) = \rho_{\text{out}}(g) k(x) \rho_{\text{in}}(g)^{-1}$$

In particular, the use of convolution guarantees the translation equivariance, while the fact the filters satisfy this steerability constraint guarantees the G-equivairance.

QUESTION 9

Show that if a filter $k : \mathbb{R}^2 \to \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$ satisfies the constraint above, the convolution with it is equivariant to G, i.e. show that

$$f_{\text{out}} = k \star f_{\text{in}} \implies [g.f_{\text{out}}] = k \star [g.f_{\text{in}}]$$

for all $g \in G$.

The action on the features f_{in} and f_{out} is the one previously defined, i.e:

$$[g.f_{\text{in}}](x) = \rho_{\text{in}}(g) f(g^{-1}x)$$

and

$$[g.f_{\text{out}}](x) = \rho_{\text{out}}(g) f(g^{-1}x)$$

while the convolution is defined as

$$f_{\text{out}}(y) = [k \star f_{\text{in}}](y) = \int_{\mathbb{R}^2} k(x-y) f_{\text{in}}(x) dx$$

ANSWER 9

Note that, because k satisfies the steerabile constraint, it follows that $k(x) = \rho_{\text{out}}(g) k(g^{-1}.x) \rho_{\text{in}}(g)^{-1}$. Then:

$$\begin{aligned}
k \star [g.f_{\text{in}}](y) &= \int_{\mathbb{R}^2} k(x-y)[g.f_{\text{in}}](x) dx && (4.12)\\
&= \int_{\mathbb{R}^2} k(x-y) \rho_{\text{in}}(g) f_{\text{in}}(g^{-1}x) dx && (4.13)\\
&= \rho_{\text{out}}(g) \int_{\mathbb{R}^2} k(g^{-1}.(x-y)) f_{\text{in}}(g^{-1}x) dx && (4.14)
\end{aligned}$$

Define $z = g^{-1}.x$ (4.15)

$$\begin{aligned}
&= \rho_{\text{out}}(g) \int_{\mathbb{R}^2} k(z - g^{-1}.y)) f_{\text{in}}(z) dz && (4.16)\\
&= \rho_{\text{out}}(g) f_{\text{out}}(g^{-1}.y) && (4.17)\\
&= [g.f_{\text{out}}](y) && (4.18)
\end{aligned}$$

The steerability constraint restricts the space of possible learnable filters to a smaller space of equivariant filters. Solving this constraint goes beyond the scope of this tutorial; fortunately, the `nn.R2Conv` module takes care of properly parameterizing the filter k such that it satisfies the constraint.

[63]:
```
conv = nn.R2Conv(feat_type_in, feat_type_out, kernel_size=3)
```

Each equivariant module has an input and output type. As a function (`.forward()`), it *requires* its inputs to transform according to its input type and is guaranteed to return feature fields associated with its output type. To prevent the user from accidentally feeding an incorrectly transforming input field into an equivariant module, we perform a dynamic type checking. In order to do so, we define **geometric tensors** as data containers. They are wrapping a *PyTorch* `torch.Tensor` to augment them with an instance of `FieldType`.

Let's build a few random 32x32 gray-scale images and wrap them into an `nn.GeometricTensor`:

[64]:
```
x = torch.randn(4, 1, 32, 32)
# FieldType is a callable object; its call method can be used to wrap PyTorch tensors␣
↪into GeometricTensors
x = feat_type_in(x)

assert isinstance(x.tensor, torch.Tensor)
assert isinstance(x, nn.GeometricTensor)
```

As usually done in *PyTorch*, an image or feature map is stored in a 4-dimensional array of shape BxCxHxW, where B is the batch-size, C is the number of channels and W and H are the spatial dimensions.

We can feed a geometric tensor to an equivariant module as we feed normal tensors in *PyTorch*'s modules:

[65]:
```
y = conv(x)
```

We can verify that the output is indeed associated with the output type of the convolutional layer:

[66]:
```
assert y.type == feat_type_out
```

Lets check whether the output transforms as described by the output type when the input transforms according to the input type. The G-transformation of a geometric tensor is hereby conveniently done by calling `nn.GeometricTensor.transform()`.

[67]:
```
# for each group element
for g in G.elements:
    # transform the input with the current group element according to the input type
    x_transformed = x.transform(g)

    # feed the transformed input in the convolutional layer
    y_from_x_transformed = conv(x_transformed)

    # the result should be equivalent to rotating the output produced in the
    # previous block according to the output type
    y_transformed_from_x = y.transform(g)
    assert torch.allclose(y_from_x_transformed.tensor, y_transformed_from_x.tensor,␣
↪atol=1e-5), g
```

Any network operation is required to be equivariant. `escnn.nn` provides a wide range of equivariant network modules which guarantee this behavior.

Non-Linearities: As an example, we will next apply an *equivariant nonlinearity* to the output feature field of the convolution. Since the regular representations of a finite group G consists of permutation matrices, any pointwise

nonlinearity like *ReLUs* is equivariant. Note that this is *not* the case for many other choices of representations / field types!

We instantiate a `escnn.nn.ReLU`, which, as an `nn.EquivariantModule`, requires to be informed about its input type to be able to perform the type checking. Here we are passing `feat_type_out`, the output of the equivariant convolution layer, as input type. It is not necessary to pass an output type to the nonlinearity since this is here determined by its input type.

[68]:
```
relu = nn.ReLU(feat_type_out)

z = relu(y)
```

We can verify the equivariance again:

[69]:
```
# for each group element
for g in G.elements:
    y_transformed = y.transform(g)
    z_from_y_transformed = relu(y_transformed)

    z_transformed_from_y = z.transform(g)

    assert torch.allclose(z_from_y_transformed.tensor, z_transformed_from_y.tensor,␣
↪atol=1e-5), g
```

Deeper Models: In *deep learning* we usually want to stack multiple layers to build a deep model. As long as each layer is equivariant and consecutive layers are compatible, the equivariance property is preserved by induction.

The compatibility of two consecutive layers requires the output type of the first layer to be equal to the input type of the second layer.

In case we feed an input with the wrong type to a module, an error is raised:

[70]:
```
layer1 = nn.R2Conv(feat_type_in, feat_type_out, kernel_size=3)
layer2 = nn.ReLU(feat_type_in) # the input type of the ReLU should be the output type of␣
↪the convolution

x = feat_type_in(torch.randn(3, 1, 7, 7))

try:
    y = layer2(layer1(x))
except AssertionError as e:
    print(e)
```

```
Error! the type of the input does not match the input type of this module
```

Simple deeper architectures can be built using a **SequentialModule**:

[71]:
```
feat_type_in = nn.FieldType(r2_act, [r2_act.trivial_repr])
feat_type_hid = nn.FieldType(r2_act, 8*[r2_act.regular_repr])
feat_type_out = nn.FieldType(r2_act, 2*[r2_act.regular_repr])

model = nn.SequentialModule(
    nn.R2Conv(feat_type_in, feat_type_hid, kernel_size=3),
    nn.InnerBatchNorm(feat_type_hid),
    nn.ReLU(feat_type_hid, inplace=True),
    nn.R2Conv(feat_type_hid, feat_type_hid, kernel_size=3),
```

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```
    nn.InnerBatchNorm(feat_type_hid),
    nn.ReLU(feat_type_hid, inplace=True),
    nn.R2Conv(feat_type_hid, feat_type_out, kernel_size=3),
).eval()
```

As every layer is equivariant and consecutive layers are compatible, the whole model is equivariant.

[72]:
```
x = torch.randn(1, 1, 17, 17)
x = feat_type_in(x)

y = model(x)

# for each group element
for g in G.elements:
    x_transformed = x.transform(g)
    y_from_x_transformed = model(x_transformed)

    y_transformed_from_x = y.transform(g)

    assert torch.allclose(y_from_x_transformed.tensor, y_transformed_from_x.tensor,␣
↪atol=1e-5), g
```

Invariant Pooling Layer: Usually, at the end of the model we want to produce a single feature vector to use for classification. To do so, it is common to pool over the spatial dimensions, e.g. via average pooling.

This produces (approximatively) translation-invariant feature vectors.

[73]:
```
# average pooling with window size 11
avgpool = nn.PointwiseAvgPool(feat_type_out, 11)

y = avgpool(model(x))

print(y.shape)
```

```
torch.Size([1, 8, 1, 1])
```

In our case, the feature vectors $f(x) \in \mathbb{R}^c$ associated to each point $x \in \mathbb{R}^2$ have a well defined transformation law. The output of the model now transforms according to `feat_type_out` (here two C_4 regular fields, i.e. 8 channels). For our choice of regular representations (which are permutation representations) the channels in the feature vectors associated to each point permute when the input is rotated.

[74]:
```
for g in G.elements:
    print(f'rotation by {g}:', y.transform(g).tensor[0, ...].detach().numpy().squeeze())
```

```
rotation by 0[2pi/4]: [0.508 0.562 0.566 0.59  0.227 0.227 0.224 0.234]
rotation by 1[2pi/4]: [0.59  0.508 0.562 0.566 0.234 0.227 0.227 0.224]
rotation by 2[2pi/4]: [0.566 0.59  0.508 0.562 0.224 0.234 0.227 0.227]
rotation by 3[2pi/4]: [0.562 0.566 0.59  0.508 0.227 0.224 0.234 0.227]
```

Many learning tasks require to build models which are **invariant** under rotations. We can compute invariant features from the output of the model using an **invariant map**. For instance, we can take the maximum value within each regular field. We do so using `nn.GroupPooling`:

[75]:
```
invariant_map = nn.GroupPooling(feat_type_out)

y = invariant_map(avgpool(model(x)))

for g in G.elements:
    print(f'rotation by {g}:', y.transform(g).tensor[0, ...].detach().numpy().squeeze())
```

```
rotation by 0[2pi/4]: [0.59  0.234]
rotation by 1[2pi/4]: [0.59  0.234]
rotation by 2[2pi/4]: [0.59  0.234]
rotation by 3[2pi/4]: [0.59  0.234]
```

[76]:
```
# for each group element
for g in G.elements:
    # rotated the input image
    x_transformed = x.transform(g)
    y_from_x_transformed = invariant_map(avgpool(model(x_transformed)))

    y_transformed_from_x = y # no .transform(g) needed since y should be invariant!

    # check that the output did not change
    # note that here we are not rotating the original output y as before
    assert torch.allclose(y_from_x_transformed.tensor, y_transformed_from_x.tensor,␣
↪atol=1e-6), g
```

2.3 Steerable CNN with infinite group G

We can now repeat the same constructions with G being an infinite group, e.g. the group of all planar rotations $G = SO(2)$.

[77]:
```
# use N=-1 to indicate all rotations
r2_act = gspaces.rot2dOnR2(N=-1)
r2_act
```

[77]:
```
SO(2)_on_R2[(None, -1)]
```

[78]:
```
G = r2_act.fibergroup
G
```

[78]:
```
SO(2)
```

[79]:
```
# For simplicity we take a single-channel gray-scale image in input and we output a␣
↪single-channel gray-scale image, i.e. we use scalar fields in input and output
feat_type_in = nn.FieldType(r2_act, [G.trivial_representation])
feat_type_out = nn.FieldType(r2_act, [G.trivial_representation])
```

As intermidiate feature types, we want to use again the *regular representation*. Because G has an infinite number of elements, we use use the Fourier transform idea described earlier. For example, we will use the first three irreps of $G = SO(2)$, which contains cosines and sines of frequency 0, 1 and 2. Earlier, we built this representation as

```
rho = G.bl_regular_representation(2)
```

To apply a non-linearity, e.g. ELU, we can use the *Inverse Fourier Transform* to sample the function, apply the non-linearity and, finally, compute the *Fourier Transform* to recover the coeffients. Because G has infinite elements, the

Fourier Transform requires an integral over G; this can be **approximated** by a sum over a finite number of samples. The more samples one take, the better the approximation will be, although this also increase the computational cost.

Fortunately, the class `nn.FourierELU` takes care of most of these details. We can just specify which `irreps` to consider (`G.bl_irreps(2)` returns the list of irreps up to frequency 2), the number of `channels` (i.e. copies of the regular representation) and the number `N` of elements of G where to sample the function:

[80]:
```
nonlinearity = nn.FourierELU(r2_act, 16, irreps=G.bl_irreps(2), N=12)
# we do not need to pre-define the feature type: FourierELU will create it internally␣
↪and we can just access it as
feat_type_hid = nonlinearity.in_type

# note also the its input and output types are the same
assert nonlinearity.in_type == nonlinearity.out_type
```

Let's build a simple $G = SO(2)$ equivariant model:

[81]:
```
equivariant_so2_model = nn.SequentialModule(
    nn.R2Conv(feat_type_in, feat_type_hid, kernel_size=7),
    nn.IIDBatchNorm2d(feat_type_hid),
    nonlinearity,
    nn.R2Conv(feat_type_hid, feat_type_hid, kernel_size=7),
    nn.IIDBatchNorm2d(feat_type_hid),
    nonlinearity,
    nn.R2Conv(feat_type_hid, feat_type_out, kernel_size=7),
).eval()
```

and check its equivariance to a few elements of $SO(2)$:

[82]:
```
x = torch.randn(1, 1, 23, 23)
x = feat_type_in(x)

y = equivariant_so2_model(x)

# check equivariance to N=16 rotations
N = 16

try:
    for i in range(N):
        g = G.element(i*2*np.pi/N)
        x_transformed = x.transform(g)
        y_from_x_transformed = equivariant_so2_model(x_transformed)

        y_transformed_from_x = y.transform(g)

        assert torch.allclose(y_from_x_transformed.tensor, y_transformed_from_x.tensor,␣
↪atol=1e-3), g
except:
    print('Error! The model is not equivariant!')
```

```
Error! The model is not equivariant!
```

QUESTION 10

The model is not perfectly equivariant to $G = SO(2)$! Why is this an expected behaviour?

ANSWER 10

The $SO(2)$ group includes all continuous planar rotations. However, when an image is represented on a pixel grid, only the 4 rotations by angles multiple of $\pi/2$ are perfect, while other rotations involve some form of interpolation and generally introduce some noise. This prevents perfect equivariance to all rotations, since rotated versions of the same image inherently include some noise. A similar argument applies to the filters used during convolution: the steerability constraint described before involve a rotation of the filter k itself, but also the filter needs to be represented on discrete grid.

While the model can not be perfectly equivariant, we can compare it with a *conventional CNN* baseline. Let's build a CNN similar to our equivariant model but which is not constrained to be equivariant:

[83]:
```
conventional_model = torch.nn.Sequential(
    torch.nn.Conv2d(feat_type_in.size, feat_type_hid.size, kernel_size=7),
    torch.nn.BatchNorm2d(feat_type_hid.size),
    torch.nn.ELU(),
    torch.nn.Conv2d(feat_type_hid.size, feat_type_hid.size, kernel_size=7),
    torch.nn.BatchNorm2d(feat_type_hid.size),
    torch.nn.ELU(),
    torch.nn.Conv2d(feat_type_hid.size, feat_type_out.size, kernel_size=7),
).eval()
```

To compare the two models, we compute their *equivariance error* for a few elements of G. We define the equivariance error of a model F with respect to a group element $g \in G$ and an input x as:

$$\epsilon_g(F) = \frac{||F(g.X) - g.F(X)||_2}{||F(x)||_2}$$

Note that this is a form of *relative* error. Let's now compute the equivariance error of the two models:

[84]:
```
# let's generate a random image of shape W x W
W = 37
x = torch.randn(1, 1, W, W)

# Because a rotation by an angle smaller than 90 degrees moves pixels outsize the image,␣
↪we mask out all pixels outside the central disk
# We need to do this both for the input and the output

def build_mask(W):
    center_mask = np.zeros((2, W, W))
    center_mask[1, :, :] = np.arange(0, W) - W // 2
    center_mask[0, :, :] = np.arange(0, W) - W // 2
    center_mask[0, :, :] = center_mask[0, :, :].T
    center_mask = center_mask[0, :, :] ** 2 + center_mask[1, :, :] ** 2 < .9*(W // 2) **␣
↪2
    center_mask = torch.tensor(center_mask.reshape(1, 1, W, W), dtype=torch.float)
```

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```
    return center_mask


# create the mask for the input
input_center_mask = build_mask(W)

# mask the input image
x = x * input_center_mask
x = feat_type_in(x)

# compute the output of both models
y_equivariant = equivariant_so2_model(x)
y_conventional = feat_type_out(conventional_model(x.tensor))

# create the mask for the output images
output_center_mask = build_mask(y_equivariant.shape[-1])

# We evaluate the equivariance error on N=100 rotations
N = 100

error_equivariant = []
error_conventional = []

# for each of the N rotations
for i in range(N+1):
    g = G.element(i / N * 2*np.pi)

    # rotate the input
    x_transformed = x.transform(g)
    x_transformed.tensor *= input_center_mask

    # F(g.X)  feed the transformed images in both models
    y_from_x_transformed_equivariant = equivariant_so2_model(x_transformed).tensor
    y_from_x_transformed_conventional = conventional_model(x_transformed.tensor)

    # g.F(x)  transform the output of both models
    y_transformed_from_x_equivariant = y_equivariant.transform(g)
    y_transformed_from_x_conventional = y_conventional.transform(g)

    # mask all the outputs
    y_from_x_transformed_equivariant = y_from_x_transformed_equivariant * output_center_
↪mask
    y_from_x_transformed_conventional = y_from_x_transformed_conventional * output_
↪center_mask
    y_transformed_from_x_equivariant = y_transformed_from_x_equivariant.tensor * output_
↪center_mask
    y_transformed_from_x_conventional = y_transformed_from_x_conventional.tensor *␣
↪output_center_mask

    # compute the relative error of both models
    rel_error_equivariant = torch.norm(y_from_x_transformed_equivariant - y_transformed_
↪from_x_equivariant).item() / torch.norm(y_equivariant.tensor).item()
```

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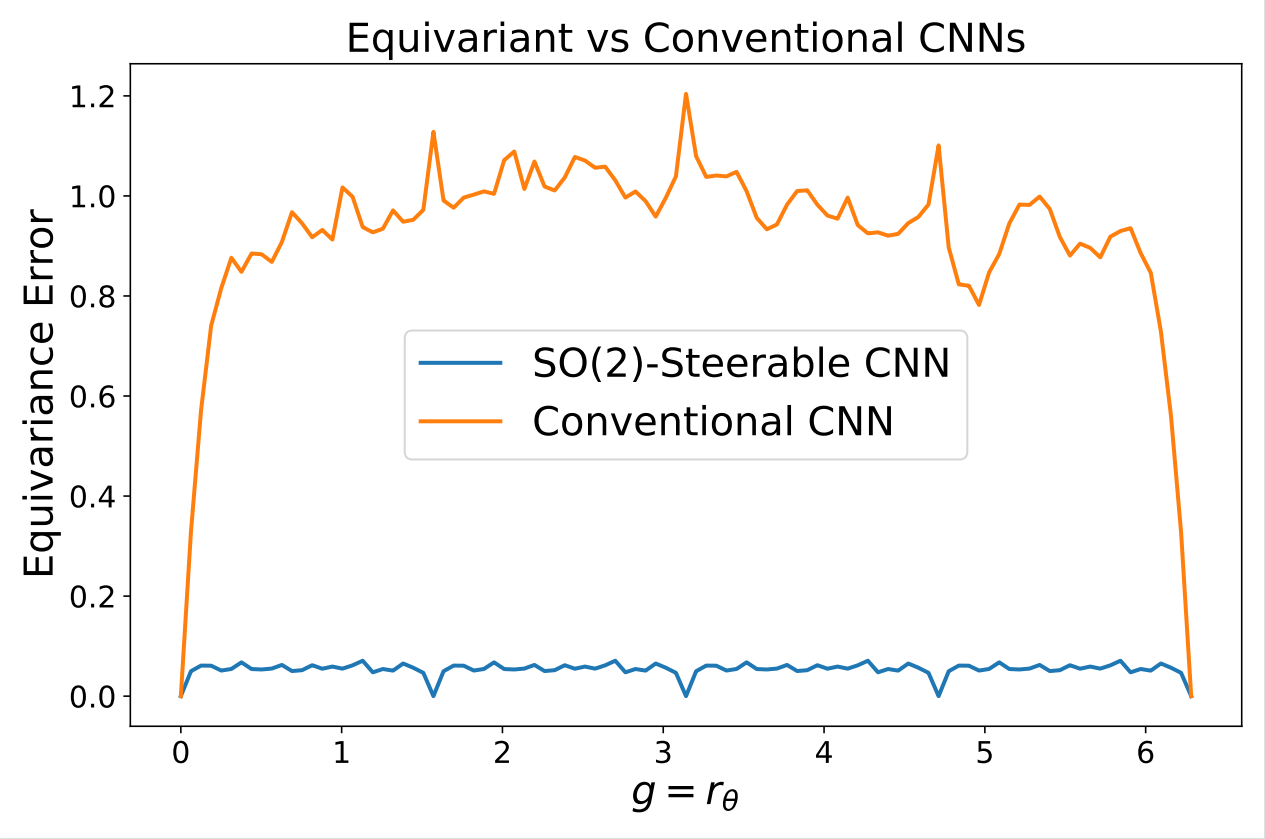
```
    rel_error_conventional = torch.norm(y_from_x_transformed_conventional - y_
↪transformed_from_x_conventional).item() / torch.norm(y_conventional.tensor).item()

    error_equivariant.append(rel_error_equivariant)
    error_conventional.append(rel_error_conventional)

# plot the error of both models as a function of the rotation angle theta
fig, ax = plt.subplots(figsize=(10, 6))

xs = [i*2*np.pi / N for i in range(N+1)]
plt.plot(xs, error_equivariant, label='SO(2)-Steerable CNN')
plt.plot(xs, error_conventional, label='Conventional CNN')
plt.title('Equivariant vs Conventional CNNs', fontsize=20)
plt.xlabel(r'$g = r_\theta$', fontsize=20)
plt.ylabel('Equivariance Error', fontsize=20)
ax.tick_params(axis='both', which='major', labelsize=15)
plt.legend(fontsize=20)
plt.show()
```



4.42.4 3. Build and Train Steerable CNNs

Finally, we will proceed with implementing a **Steerable CNN** and train it on rotated MNIST.

Dataset

We will evaluate the model on the *rotated* MNIST dataset. First, we download the (non-rotated) MNIST 12k data:

[85]:
```
# download the dataset
!wget -nc http://www.iro.umontreal.ca/~lisa/icml2007data/mnist.zip
# uncompress the zip file
!unzip -n mnist.zip -d mnist
```

```
File ‘mnist.zip’ already there; not retrieving.

/bin/bash: unzip: command not found
```

Then, we build the dataset and some utility functions:

[86]:
```
from torch.utils.data import Dataset
from torchvision.transforms import RandomRotation
from torchvision.transforms import Pad
from torchvision.transforms import Resize
from torchvision.transforms import ToTensor
from torchvision.transforms import Compose
from tqdm.auto import tqdm

from PIL import Image

device = 'cuda' if torch.cuda.is_available() else 'cpu'
```

[87]:
```
class MnistDataset(Dataset):

    def __init__(self, mode, rotated: bool = True):
        assert mode in ['train', 'test']

        if mode == "train":
            file = "mnist/mnist_train.amat"
        else:
            file = "mnist/mnist_test.amat"

        data = np.loadtxt(file)

        images = data[:, :-1].reshape(-1, 28, 28).astype(np.float32)

        # images are padded to have shape 29x29.
        # this allows to use odd-size filters with stride 2 when downsampling a feature␣
↪map in the model
        pad = Pad((0, 0, 1, 1), fill=0)

        # to reduce interpolation artifacts (e.g. when testing the model on rotated␣
↪images),
        # we upsample an image by a factor of 3, rotate it and finally downsample it␣
↪again
```

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```
        resize1 = Resize(87) # to upsample
        resize2 = Resize(29) # to downsample

        totensor = ToTensor()

        if rotated:
            self.images = torch.empty((images.shape[0], 1, 29, 29))
            for i in tqdm(range(images.shape[0]), leave=False):
                img = images[i]
                img = Image.fromarray(img, mode='F')
                r = (np.random.rand() * 360.)
                self.images[i] = totensor(resize2(resize1(pad(img)).rotate(r, Image.
↪BILINEAR))).reshape(1, 29, 29)
        else:
            self.images = torch.zeros((images.shape[0], 1, 29, 29))
            self.images[:, :, :28, :28] = torch.tensor(images).reshape(-1, 1, 28, 28)

        self.labels = data[:, -1].astype(np.int64)
        self.num_samples = len(self.labels)

    def __getitem__(self, index):
        image, label = self.images[index], self.labels[index]

        return image, label

    def __len__(self):
        return len(self.labels)
```

[88]:
```
# Set the random seed for reproducibility
np.random.seed(42)

# build the rotated training and test datasets
mnist_train = MnistDataset(mode='train', rotated=True)
train_loader = torch.utils.data.DataLoader(mnist_train, batch_size=64)


mnist_test = MnistDataset(mode='test', rotated=True)
test_loader = torch.utils.data.DataLoader(mnist_test, batch_size=64)

# for testing purpose, we also build a version of the test set with *non*-rotated digits
raw_mnist_test = MnistDataset(mode='test', rotated=False)
```

$SO(2)$ equivariant architecture

We now build an $SO(2)$ equivariant CNN.

Because the inputs are still gray-scale images, the input type of the model is again a *scalar field*. In the intermidiate layers, we will use *regular fields*, such that the models are equivalent to *group-equivariant convolutional neural networks* (GCNNs).

The final classification is performed by a fully connected layer.

[89]:
```
class SO2SteerableCNN(torch.nn.Module):

    def __init__(self, n_classes=10):

        super(SO2SteerableCNN, self).__init__()

        # the model is equivariant under all planar rotations
        self.r2_act = gspaces.rot2dOnR2(N=-1)

        # the group SO(2)
        self.G: SO2 = self.r2_act.fibergroup

        # the input image is a scalar field, corresponding to the trivial representation
        in_type = nn.FieldType(self.r2_act, [self.r2_act.trivial_repr])

        # we store the input type for wrapping the images into a geometric tensor during␣
↪the forward pass
        self.input_type = in_type

        # We need to mask the input image since the corners are moved outside the grid␣
↪under rotations
        self.mask = nn.MaskModule(in_type, 29, margin=1)

        # convolution 1
        # first we build the non-linear layer, which also constructs the right feature␣
↪type
        # we choose 8 feature fields, each transforming under the regular representation␣
↪of SO(2) up to frequency 3
        # When taking the ELU non-linearity, we sample the feature fields on N=16 points
        activation1 = nn.FourierELU(self.r2_act, 8, irreps=G.bl_irreps(3), N=16,␣
↪inplace=True)
        out_type = activation1.in_type
        self.block1 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=7, padding=1, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation1,
        )

        # convolution 2
        # the old output type is the input type to the next layer
        in_type = self.block1.out_type
        # the output type of the second convolution layer are 16 regular feature fields
        activation2 = nn.FourierELU(self.r2_act, 16, irreps=G.bl_irreps(3), N=16,␣
↪inplace=True)
```

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```
        out_type = activation2.in_type
        self.block2 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation2
        )
        # to reduce the downsampling artifacts, we use a Gaussian smoothing filter
        self.pool1 = nn.SequentialModule(
            nn.PointwiseAvgPoolAntialiased(out_type, sigma=0.66, stride=2)
        )

        # convolution 3
        # the old output type is the input type to the next layer
        in_type = self.block2.out_type
        # the output type of the third convolution layer are 32 regular feature fields
        activation3 = nn.FourierELU(self.r2_act, 32, irreps=G.bl_irreps(3), N=16,␣
↪inplace=True)
        out_type = activation3.in_type
        self.block3 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation3
        )

        # convolution 4
        # the old output type is the input type to the next layer
        in_type = self.block3.out_type
        # the output type of the fourth convolution layer are 64 regular feature fields
        activation4 = nn.FourierELU(self.r2_act, 32, irreps=G.bl_irreps(3), N=16,␣
↪inplace=True)
        out_type = activation4.in_type
        self.block4 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation4
        )
        self.pool2 = nn.SequentialModule(
            nn.PointwiseAvgPoolAntialiased(out_type, sigma=0.66, stride=2)
        )

        # convolution 5
        # the old output type is the input type to the next layer
        in_type = self.block4.out_type
        # the output type of the fifth convolution layer are 96 regular feature fields
        activation5 = nn.FourierELU(self.r2_act, 64, irreps=G.bl_irreps(3), N=16,␣
↪inplace=True)
        out_type = activation5.in_type
        self.block5 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation5
        )
```

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```
        # convolution 6
        # the old output type is the input type to the next layer
        in_type = self.block5.out_type
        # the output type of the sixth convolution layer are 64 regular feature fields
        activation6 = nn.FourierELU(self.r2_act, 64, irreps=G.bl_irreps(3), N=16,␣
↪inplace=True)
        out_type = activation6.in_type
        self.block6 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=1, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation6
        )
        self.pool3 = nn.PointwiseAvgPoolAntialiased(out_type, sigma=0.66, stride=1,␣
↪padding=0)

        # number of output invariant channels
        c = 64

        # last 1x1 convolution layer, which maps the regular fields to c=64 invariant␣
↪scalar fields
        # this is essential to provide *invariant* features in the final classification␣
↪layer
        output_invariant_type = nn.FieldType(self.r2_act, c*[self.r2_act.trivial_repr])
        self.invariant_map = nn.R2Conv(out_type, output_invariant_type, kernel_size=1,␣
↪bias=False)

        # Fully Connected classifier
        self.fully_net = torch.nn.Sequential(
            torch.nn.BatchNorm1d(c),
            torch.nn.ELU(inplace=True),
            torch.nn.Linear(c, n_classes),
        )

    def forward(self, input: torch.Tensor):
        # wrap the input tensor in a GeometricTensor
        # (associate it with the input type)
        x = self.input_type(input)

        # mask out the corners of the input image
        x = self.mask(x)

        # apply each equivariant block

        # Each layer has an input and an output type
        # A layer takes a GeometricTensor in input.
        # This tensor needs to be associated with the same representation of the layer's␣
↪input type
        #
        # Each layer outputs a new GeometricTensor, associated with the layer's output␣
↪type.
        # As a result, consecutive layers need to have matching input/output types
```

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```
        x = self.block1(x)
        x = self.block2(x)
        x = self.pool1(x)

        x = self.block3(x)
        x = self.block4(x)
        x = self.pool2(x)

        x = self.block5(x)
        x = self.block6(x)

        # pool over the spatial dimensions
        x = self.pool3(x)

        # extract invariant features
        x = self.invariant_map(x)

        # unwrap the output GeometricTensor
        # (take the Pytorch tensor and discard the associated representation)
        x = x.tensor

        # classify with the final fully connected layer
        x = self.fully_net(x.reshape(x.shape[0], -1))

        return x
```

Equivariance Test before training

Let's instantiate the model:

[90]:
```
model = SO2SteerableCNN().to(device)
```

The model is now randomly initialized. Therefore, we do not expect it to produce the right class probabilities.

However, the model should still produce the same output for rotated versions of the same image. This is true for rotations by multiples of $\frac{\pi}{2}$, but is only approximate for other rotations.

Let's test it on a random test image: we feed $N = 20$ rotated versions of the first image in the test set and print the output logits of the model for each of them.

[91]:
```
def test_model_single_image(model: torch.nn.Module, x: torch.Tensor, N: int = 8):
    np.set_printoptions(linewidth=10000)

    x = Image.fromarray(x.cpu().numpy()[0], mode='F')


    # to reduce interpolation artifacts (e.g. when testing the model on rotated images),
    # we upsample an image by a factor of 3, rotate it and finally downsample it again
    resize1 = Resize(87) # to upsample
    resize2 = Resize(29) # to downsample

    totensor = ToTensor()
```

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```
    x = resize1(x)

    # evaluate the `model` on N rotated versions of the input image `x`
    model.eval()

    print()
    print('##########################################################################################
↪############')
    header = 'angle  |  ' + '  '.join(["{:5d}".format(d) for d in range(10)])
    print(header)
    with torch.no_grad():
        for r in range(N):
            x_transformed = totensor(resize2(x.rotate(r*360./N, Image.BILINEAR))).
↪reshape(1, 1, 29, 29)
            x_transformed = x_transformed.to(device)

            y = model(x_transformed)
            y = y.to('cpu').numpy().squeeze()

            angle = r * 360. / N
            print("{:6.1f} : {}".format(angle, y))
    print('##########################################################################################
↪############')
    print()
```

[92]:
```
# retrieve the first image from the test set
x, y = next(iter(raw_mnist_test))

# evaluate the model
test_model_single_image(model, x, N=20)
```

```
##########################################################################################
↪#
angle  |      0      1      2      3      4      5      6      7      8      9
   0.0 : [ 0.106  1.08  -1.623 -0.825  1.574 -0.265 -0.12   1.242  0.219  1.639]
  18.0 : [ 0.093  1.087 -1.643 -0.828  1.574 -0.27  -0.117  1.255  0.213  1.631]
  36.0 : [ 0.094  1.072 -1.632 -0.833  1.562 -0.272 -0.121  1.257  0.194  1.602]
  54.0 : [ 0.091  1.068 -1.615 -0.833  1.568 -0.262 -0.131  1.236  0.209  1.59 ]
  72.0 : [ 0.108  1.081 -1.623 -0.829  1.573 -0.261 -0.129  1.227  0.231  1.628]
  90.0 : [ 0.106  1.08  -1.623 -0.825  1.574 -0.265 -0.12   1.242  0.219  1.639]
 108.0 : [ 0.093  1.087 -1.643 -0.828  1.574 -0.27  -0.117  1.255  0.213  1.631]
 126.0 : [ 0.094  1.072 -1.632 -0.833  1.562 -0.272 -0.121  1.257  0.194  1.602]
 144.0 : [ 0.091  1.068 -1.615 -0.833  1.568 -0.262 -0.131  1.236  0.209  1.59 ]
 162.0 : [ 0.108  1.081 -1.623 -0.829  1.573 -0.261 -0.129  1.227  0.231  1.628]
 180.0 : [ 0.106  1.08  -1.623 -0.825  1.574 -0.265 -0.12   1.242  0.219  1.639]
 198.0 : [ 0.093  1.087 -1.643 -0.828  1.574 -0.27  -0.117  1.255  0.213  1.631]
 216.0 : [ 0.094  1.072 -1.632 -0.833  1.562 -0.272 -0.121  1.257  0.194  1.602]
 234.0 : [ 0.091  1.068 -1.615 -0.833  1.568 -0.262 -0.131  1.236  0.209  1.59 ]
 252.0 : [ 0.108  1.081 -1.623 -0.829  1.573 -0.261 -0.129  1.227  0.231  1.628]
```

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```
 270.0 : [ 0.106  1.08  -1.623 -0.825  1.574 -0.265 -0.12   1.242  0.219  1.639]
 288.0 : [ 0.093  1.087 -1.643 -0.828  1.574 -0.27  -0.117  1.255  0.213  1.631]
 306.0 : [ 0.094  1.072 -1.632 -0.833  1.562 -0.272 -0.121  1.257  0.194  1.602]
 324.0 : [ 0.091  1.068 -1.615 -0.833  1.568 -0.262 -0.131  1.236  0.209  1.59 ]
 342.0 : [ 0.108  1.081 -1.623 -0.829  1.573 -0.261 -0.129  1.227  0.231  1.628]
##########################################################################################
↪#
```

The output of the model is already almost invariant but we observe small fluctuations in the outputs. This is the effect of the discretization artifacts (e.g. the pixel grid can not be perfectly rotated by any angle without interpolation) and can not be completely removed.

Training the model

Let's train the model now. The procedure is the same used to train a normal *PyTorch* architecture:

[93]:
```
# build the training and test function

def test(model: torch.nn.Module):
    # test over the full rotated test set
    total = 0
    correct = 0

    with torch.no_grad():
        model.eval()
        for i, (x, t) in enumerate(test_loader):
            x = x.to(device)
            t = t.to(device)

            y = model(x)

            _, prediction = torch.max(y.data, 1)
            total += t.shape[0]
            correct += (prediction == t).sum().item()
    return correct/total*100.


def train(model: torch.nn.Module, lr=1e-4, wd=1e-4, checkpoint_path: str = None):
    if checkpoint_path is not None:
        checkpoint_path = os.path.join(CHECKPOINT_PATH, checkpoint_path)

    if checkpoint_path is not None and os.path.isfile(checkpoint_path):
        model.load_state_dict(torch.load(checkpoint_path))
        model.eval()
        return

    loss_function = torch.nn.CrossEntropyLoss()
    optimizer = torch.optim.Adam(model.parameters(), lr=lr, weight_decay=wd)

    for epoch in tqdm(range(21)):
```

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```
        model.train()
        for i, (x, t) in enumerate(train_loader):
            optimizer.zero_grad()

            x = x.to(device)
            t = t.to(device)

            y = model(x)

            loss = loss_function(y, t)

            loss.backward()

            optimizer.step()
            del x, y, t, loss

        if epoch % 10 == 0:
            accuracy = test(model)
            print(f"epoch {epoch} | test accuracy: {accuracy}")

    if checkpoint_path is not None:
        torch.save(model.state_dict(), checkpoint_path)
```

Finally, train the $SO(2)$ equivariant model:

[94]:
```
# set the seed manually for reproducibility
torch.manual_seed(42)
model = SO2SteerableCNN().to(device)

train(model, checkpoint_path="steerable_so2-pretrained.ckpt")

accuracy = test(model)
print(f"Test accuracy: {accuracy}")
```

```
Test accuracy: 94.98400000000001
```

[95]:
```
def test_model_rotations(model: torch.nn.Module, N: int = 24, M: int = 2000, checkpoint_
↪path: str = None):
    # evaluate the `model` on N rotated versions of the first M images in the test set

    if checkpoint_path is not None:
        checkpoint_path = os.path.join(CHECKPOINT_PATH, checkpoint_path)

    if checkpoint_path is not None and os.path.isfile(checkpoint_path):
        accuracies = np.load(checkpoint_path)
        return accuracies.tolist()

    model.eval()

    # to reduce interpolation artifacts (e.g. when testing the model on rotated images),
    # we upsample an image by a factor of 3, rotate it and finally downsample it again
    resize1 = Resize(87) # to upsample
```

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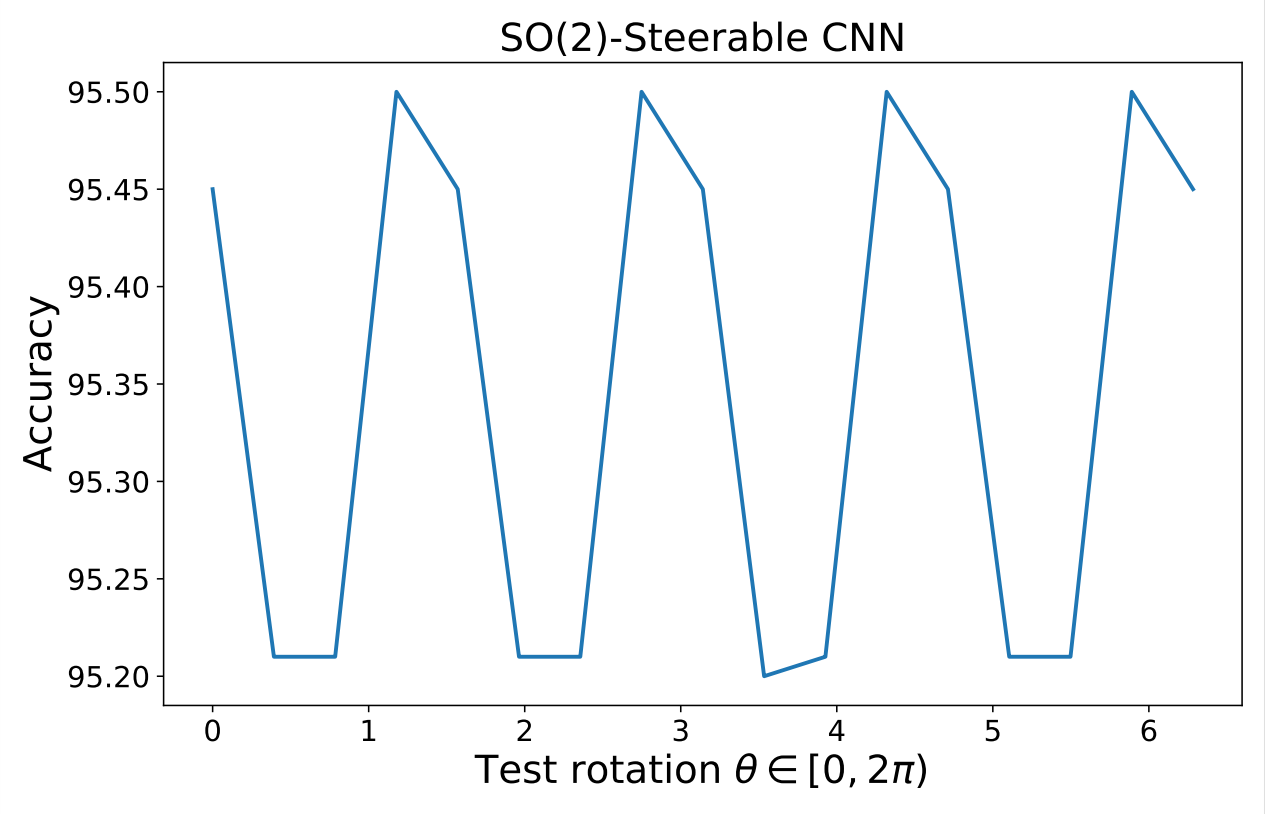
```
    resize2 = Resize(29) # to downsample

    totensor = ToTensor()

    accuracies = []
    with torch.no_grad():
        model.eval()

        for r in tqdm(range(N)):
            total = 0
            correct = 0

            for i in range(M):
                x, t = raw_mnist_test[i]

                x = Image.fromarray(x.numpy()[0], mode='F')

                x = totensor(resize2(resize1(x).rotate(r*360./N, Image.BILINEAR))).
↪reshape(1, 1, 29, 29).to(device)

                x = x.to(device)

                y = model(x)

                _, prediction = torch.max(y.data, 1)
                total += 1
                correct += (prediction == t).sum().item()

            accuracies.append(correct/total*100.)

    if checkpoint_path is not None:
        np.save(checkpoint_path, np.array(accuracies))

    return accuracies
```

[96]:
```
accs_so2 = test_model_rotations(model, 16, 10000, checkpoint_path="steerable_so2-
↪accuracies.npy")
```

[97]:
```
# plot the accuracy of as a function of the rotation angle theta applied to the test set
fig, ax = plt.subplots(figsize=(10, 6))

N = 16

xs = [i*2*np.pi / N for i in range(N+1)]
plt.plot(xs, accs_so2 + [accs_so2[0]])
plt.title('SO(2)-Steerable CNN', fontsize=20)
plt.xlabel(r'Test rotation $\theta \in [0, 2\pi)$', fontsize=20)
plt.ylabel('Accuracy', fontsize=20)
ax.tick_params(axis='both', which='major', labelsize=15)
plt.show()
```



Even after training, the model is not perfectly $SO(2)$ equivariant, but we observe the accuracy is rather stable to rotations.

C_4 equivariant architecture

For comparison, let's build a similar architecture equivariant only to $N = 4$ rotations.

[98]:
```
class CNSteerableCNN(torch.nn.Module):

    def __init__(self, n_classes=10):

        super(CNSteerableCNN, self).__init__()

        # the model is equivariant to rotations by multiples of 2pi/N
        self.r2_act = gspaces.rot2dOnR2(N=4)

        # the input image is a scalar field, corresponding to the trivial representation
        in_type = nn.FieldType(self.r2_act, [self.r2_act.trivial_repr])

        # we store the input type for wrapping the images into a geometric tensor during␣
↪the forward pass
        self.input_type = in_type

        # We need to mask the input image since the corners are moved outside the grid␣
↪under rotations
        self.mask = nn.MaskModule(in_type, 29, margin=1)
```

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```
        # convolution 1
        # first we build the non-linear layer, which also constructs the right feature␣
↪type
        # we choose 8 feature fields, each transforming under the regular representation␣
↪of C_4
        activation1 = nn.ELU(nn.FieldType(self.r2_act, 8*[self.r2_act.regular_repr]),␣
↪inplace=True)
        out_type = activation1.in_type
        self.block1 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=7, padding=1, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation1,
        )

        # convolution 2
        # the old output type is the input type to the next layer
        in_type = self.block1.out_type
        # the output type of the second convolution layer are 16 regular feature fields
        activation2 = nn.ELU(nn.FieldType(self.r2_act, 16*[self.r2_act.regular_repr]),␣
↪inplace=True)
        out_type = activation2.in_type
        self.block2 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation2
        )
        self.pool1 = nn.SequentialModule(
            nn.PointwiseAvgPoolAntialiased(out_type, sigma=0.66, stride=2)
        )

        # convolution 3
        # the old output type is the input type to the next layer
        in_type = self.block2.out_type
        # the output type of the third convolution layer are 32 regular feature fields
        activation3 = nn.ELU(nn.FieldType(self.r2_act, 32*[self.r2_act.regular_repr]),␣
↪inplace=True)
        out_type = activation3.in_type
        self.block3 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation3
        )

        # convolution 4
        # the old output type is the input type to the next layer
        in_type = self.block3.out_type
        # the output type of the fourth convolution layer are 32 regular feature fields
        activation4 = nn.ELU(nn.FieldType(self.r2_act, 32*[self.r2_act.regular_repr]),␣
↪inplace=True)
        out_type = activation4.in_type
        self.block4 = nn.SequentialModule(
```

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```
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation4
        )
        self.pool2 = nn.SequentialModule(
            nn.PointwiseAvgPoolAntialiased(out_type, sigma=0.66, stride=2)
        )

        # convolution 5
        # the old output type is the input type to the next layer
        in_type = self.block4.out_type
        # the output type of the fifth convolution layer are 64 regular feature fields
        activation5 = nn.ELU(nn.FieldType(self.r2_act, 64*[self.r2_act.regular_repr]),␣
↪inplace=True)
        out_type = activation5.in_type
        self.block5 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=2, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation5
        )

        # convolution 6
        # the old output type is the input type to the next layer
        in_type = self.block5.out_type
        # the output type of the sixth convolution layer are 64 regular feature fields
        activation6 = nn.ELU(nn.FieldType(self.r2_act, 64*[self.r2_act.regular_repr]),␣
↪inplace=True)
        out_type = activation6.in_type
        self.block6 = nn.SequentialModule(
            nn.R2Conv(in_type, out_type, kernel_size=5, padding=1, bias=False),
            nn.IIDBatchNorm2d(out_type),
            activation6
        )
        self.pool3 = nn.PointwiseAvgPoolAntialiased(out_type, sigma=0.66, stride=1,␣
↪padding=0)

        # number of output invariant channels
        c = 64

        output_invariant_type = nn.FieldType(self.r2_act, c*[self.r2_act.trivial_repr])
        self.invariant_map = nn.R2Conv(out_type, output_invariant_type, kernel_size=1,␣
↪bias=False)


        # Fully Connected classifier
        self.fully_net = torch.nn.Sequential(
            torch.nn.BatchNorm1d(c),
            torch.nn.ELU(inplace=True),
            torch.nn.Linear(c, n_classes),
        )

    def forward(self, input: torch.Tensor):
```

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```
        # wrap the input tensor in a GeometricTensor
        # (associate it with the input type)
        x = self.input_type(input)

        # mask out the corners of the input image
        x = self.mask(x)

        # apply each equivariant block

        # Each layer has an input and an output type
        # A layer takes a GeometricTensor in input.
        # This tensor needs to be associated with the same representation of the layer's␣
↪input type
        #
        # Each layer outputs a new GeometricTensor, associated with the layer's output␣
↪type.
        # As a result, consecutive layers need to have matching input/output types
        x = self.block1(x)
        x = self.block2(x)
        x = self.pool1(x)

        x = self.block3(x)
        x = self.block4(x)
        x = self.pool2(x)

        x = self.block5(x)
        x = self.block6(x)

        # pool over the spatial dimensions
        x = self.pool3(x)

        # extract invariant features
        x = self.invariant_map(x)

        # unwrap the output GeometricTensor
        # (take the Pytorch tensor and discard the associated representation)
        x = x.tensor

        # classify with the final fully connected layer
        x = self.fully_net(x.reshape(x.shape[0], -1))

        return x
```

Instantiate and train the C_4 equivariant model:

[99]:
```
torch.manual_seed(42)
model_c4 = CNSteerableCNN().to(device)
train(model_c4, checkpoint_path="steerable_c4-pretrained.ckpt")

accuracy = test(model_c4)
print(f"Test accuracy: {accuracy}")
```

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```
accs_c4 = test_model_rotations(model_c4, 16, 10000, checkpoint_path="steerable_c4-
↪accuracies.npy")
```

```
Test accuracy: 93.84
```

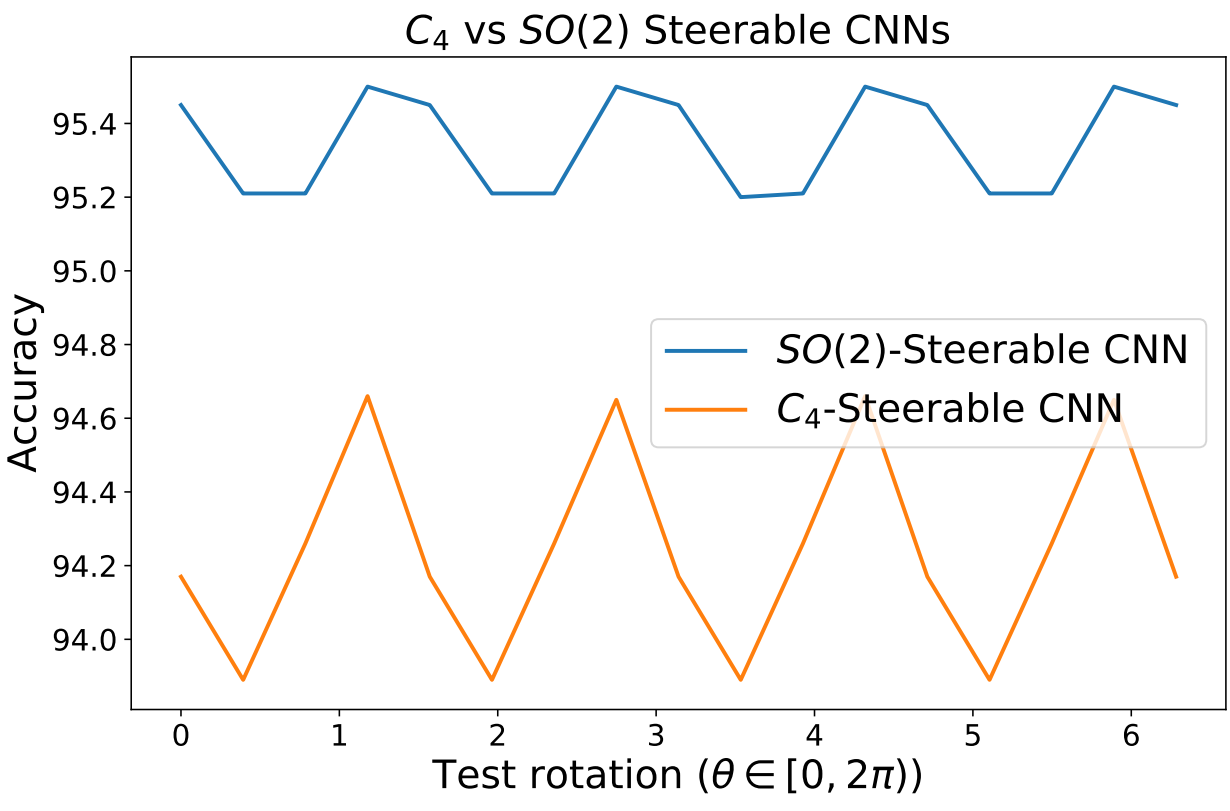
Finally, let's compare the performance of both models on the rotated test sets:

[100]:
```
# plot the accuracy of as a function of the rotation angle theta applied to the test set
fig, ax = plt.subplots(figsize=(10, 6))

N=16

xs = [i*2*np.pi / N for i in range(N+1)]
plt.plot(xs, accs_so2 + [accs_so2[0]], label=r'$SO(2)$-Steerable CNN')
plt.plot(xs, accs_c4 + [accs_c4[0]], label=r'$C_4$-Steerable CNN')
plt.title(r'$C_4$ vs $SO(2)$ Steerable CNNs', fontsize=20)

plt.xlabel(r'Test rotation ($\theta \in [0, 2\pi)$)', fontsize=20)
plt.ylabel('Accuracy', fontsize=20)
ax.tick_params(axis='both', which='major', labelsize=15)
plt.legend(fontsize=20)
plt.show()
```



While perfect equivariance to $SO(2)$ is not achievable due to the discretizations, the $SO(2)$ equivariant architecture is more stable over the rotations of the test set than the C_4 model. Moreover, since C_4 is the only perfect symmetry of the pixel grid and since $C_4 < SO(2)$, the $SO(2)$ equivariant architecture is also perfectly equivariant to rotations by multiples of $\pi/2$.

4.42.5 Conclusion

In this tutorial, you first leart about *group representation theory* and the *Fourier Transform* over compact groups. These are the mathematical tools used to formalize Steerable CNNs.

In the second part of this tutorial, you learnt about *steerable feature fields* and *steerable CNNs*. In particular, the previously defined Fourier transform allowed us to build a steerable CNN which is equivalent to a Group-Convolutional Neural Network (GCNN) equivariant to translations and the continuous group $G = SO(2)$ of rotations.

In our steerable CNNs, we mostly leveraged the *regular representation* of the group G, but the framework of steerable CNNs allows for a variety of representations. If you are interested in knowing more about steerable CNNs, this is a (non-exhaustive) list of relevant works you can check out:

- Steerable CNNs
- Harmonic Networks: Deep Translation and Rotation Equivariance
- 3D Steerable CNNs
- Tensor Field Networks
- A General Theory of Equivariant CNNs on Homogeneous Spaces
- Cormorant: Covariant Molecular Neural Networks
- General E(2)-Equivariant Steerable CNNs
- A Program to Build E(N)-Equivariant Steerable CNNs

4.43 DPM1 - Deep Probabilistic Models I

Filled notebook:
Recordings: Lecture 1.1 & Lecture 1.2
Authors: Wilker Aziz & Bryan Eikema

4.43.1 0. General notes

This notebook illustrates the concepts discussed in the module **Deep probabilistic models I** offered within DL2.

The examples in the notebook are based on NLP datasets, but the concepts are general enough that you can apply them in any domain. At the end of the notebook, we invite you to try your favourite dataset (as long as you can design an encoder for the data type you are interested in, transferring ideas from this notebook should be fairly simple).

The notebook starts with modelling univariate response variables conditionally, given a high-dimensional and structured input. We look into a nominal response variable and then into a numerical one. Next, we look into a structured response variable.

0.1 ILOs

- Prescribe joint distributions using PyTorch
- Estimate the parameters of the model via maximum likelihood estimation
- Implement a decision rule

0.2 Setting up

[1]:
```
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0

import random
import numpy as np
import torch

try:
    import nltk
    import sklearn
except ModuleNotFoundError: # Install nltk and sklearn if necessary
    !pip install --quiet nltk, sklearn
    import nltk

def seed_all(seed=42):
    np.random.seed(seed)
    random.seed(seed)
    torch.manual_seed(seed)

seed_all()
```

4.43.2 1. Data

In this tutorial we will design conditional models involving structured data. We use text as an example and design

1. a classifier
2. an ordinal regressor
3. a sequence labeller

At the end of the tutorial you are encouraged to design similar models for a different type of data (for example, consider a different modality of data).

[2]:
```
nltk.download('treebank')
nltk.download('brown')
nltk.download('punkt')
nltk.download('universal_tagset')
```

```
[nltk_data] Downloading package treebank to /home/phillip/nltk_data...
[nltk_data]   Package treebank is already up-to-date!
[nltk_data] Downloading package brown to /home/phillip/nltk_data...
[nltk_data]   Unzipping corpora/brown.zip.
[nltk_data] Downloading package punkt to /home/phillip/nltk_data...
[nltk_data]   Package punkt is already up-to-date!
[nltk_data] Downloading package universal_tagset to
[nltk_data]     /home/phillip/nltk_data...
[nltk_data]   Package universal_tagset is already up-to-date!
```

[2]:
```
True
```

1.1 Sentiment

[3]:
```
from nltk.corpus import treebank, brown
```

The brown corpus contains texts organized into 15 genres.

[4]:
```
brown.categories()
```

[4]:
```
['adventure',
 'belles_lettres',
 'editorial',
 'fiction',
 'government',
 'hobbies',
 'humor',
 'learned',
 'lore',
 'mystery',
 'news',
 'religion',
 'reviews',
 'romance',
 'science_fiction']
```

The dataset is already preprocessed for us:

[5]:
```
print("'fiction' examples")
for i, x in zip(range(3), brown.sents(categories=['fiction'])):
    print(i, x)
print()
print("'religion' examples")
for i, x in zip(range(3), brown.sents(categories=['religion'])):
    print(i, x)
print()
print("'learned' examples")
for i, x in zip(range(3), brown.sents(categories=['learned'])):
    print(i, x)
```

```
'fiction' examples
0 ['Thirty-three']
1 ['Scotty', 'did', 'not', 'go', 'back', 'to', 'school', '.']
```

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```
2 ['His', 'parents', 'talked', 'seriously', 'and', 'lengthily', 'to', 'their', 'own',
↪'doctor', 'and', 'to', 'a', 'specialist', 'at', 'the', 'University', 'Hospital', '--',
↪'Mr.', 'McKinley', 'was', 'entitled', 'to', 'a', 'discount', 'for', 'members', 'of',
↪'his', 'family', '--', 'and', 'it', 'was', 'decided', 'it', 'would', 'be', 'best', 'for
↪', 'him', 'to', 'take', 'the', 'remainder', 'of', 'the', 'term', 'off', ',', 'spend',
↪'a', 'lot', 'of', 'time', 'in', 'bed', 'and', ',', 'for', 'the', 'rest', ',', 'do',
↪'pretty', 'much', 'as', 'he', 'chose', '--', 'provided', ',', 'of', 'course', ',', 'he
↪', 'chose', 'to', 'do', 'nothing', 'too', 'exciting', 'or', 'too', 'debilitating', '.']

'religion' examples
0 ['As', 'a', 'result', ',', 'although', 'we', 'still', 'make', 'use', 'of', 'this',
↪'distinction', ',', 'there', 'is', 'much', 'confusion', 'as', 'to', 'the', 'meaning',
↪'of', 'the', 'basic', 'terms', 'employed', '.']
1 ['Just', 'what', 'is', 'meant', 'by', '``', 'spirit', "''", 'and', 'by', '``', 'matter
↪', "''", '?', '?']
2 ['The', 'terms', 'are', 'generally', 'taken', 'for', 'granted', 'as', 'though', 'they',
↪ 'referred', 'to', 'direct', 'and', 'axiomatic', 'elements', 'in', 'the', 'common',
↪'experience', 'of', 'all', '.']

'learned' examples
0 ['1', '.']
1 ['Introduction']
2 ['It', 'has', 'recently', 'become', 'practical', 'to', 'use', 'the', 'radio', 'emission
↪', 'of', 'the', 'moon', 'and', 'planets', 'as', 'a', 'new', 'source', 'of',
↪'information', 'about', 'these', 'bodies', 'and', 'their', 'atmospheres', '.']
```

[6]:
```
def split_nltk_categorised_corpus(corpus, categories, max_length=30, num_heldout=100):
    """
    Shuffle and split a corpus.
    corpus: a corpus of tagged sequences, each sequence is a pair, each pair is a token␣
↪and a tag.
    max_length: discard sentences longer than this

    Return:
        (training word sequences, training tag sequences),
        (dev word sequences, dev tag sequences),
        (test word sequences, test tag sequences),
    """

    sentences = []
    labels = []
    for k, c in enumerate(categories):
        seqs = corpus.sents(categories=[c])
        sentences.extend(seqs)
        labels.extend(len(seqs) * [k])
    # do not change the seed in here
    order = np.random.RandomState(42).permutation(np.arange(len(sentences)))
    shuffled_sentences = [[w for w in sentences[i]] for i in order if len(sentences[i])
↪<= max_length]
    shuffled_labels = [labels[i] for i in order if len(sentences[i]) <= max_length]
    return (shuffled_sentences[2*num_heldout:], shuffled_labels[2*num_heldout:]),␣
↪(shuffled_sentences[num_heldout:2*num_heldout], shuffled_labels[num_heldout:2*num_
↪heldout]), (shuffled_sentences[:num_heldout], shuffled_labels[:num_heldout])
```

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[7]:
```
%%time
(cat_training_x, cat_training_y), (cat_dev_x, cat_dev_y), (cat_test_x, cat_test_y) =␣
↪split_nltk_categorised_corpus(brown, brown.categories(), num_heldout=1000)
print(f"Number of sentences: training={len(cat_training_x)} dev={len(cat_dev_x)} test=
↪{len(cat_test_x)}")
```

```
Number of sentences: training=44685 dev=1000 test=1000
CPU times: user 3.07 s, sys: 59.2 ms, total: 3.13 s
Wall time: 3.13 s
```

[8]:
```
len(cat_training_x), len(cat_dev_x), len(cat_test_x)
```

[8]:
```
(44685, 1000, 1000)
```

[9]:
```
cat_training_y[0], cat_training_x[0]
```

[9]:
```
(1,
 ['That',
  'is',
  'why',
  'the',
  'members',
  'of',
  'the',
  'beat',
  'generation',
  'proudly',
  'assume',
  'the',
  'title',
  'of',
  'the',
  'holy',
  'barbarians',
  ';',
  ';'])
```

1.2 Age

Schler et al (2006) collected a dataset of blog posts annotated for the age of the author, we will use a subset of that dataset. The complete dataset can be found on Kaggle.

Warning: we will use this dataset to illustrate Poisson regression, but note that in general age may be a protected attribute in certain applications, and one should carefully consider the implications of designing and deploying an age detection system.

[10]:
```
# Download the data
!wget https://surfdrive.surf.nl/files/index.php/s/2xWdFxnewjN9gsq/download -O blog-
↪authorship.json.gz
!gzip -d blog-authorship.json.gz
```

```
--2022-04-05 17:42:50--  https://surfdrive.surf.nl/files/index.php/s/2xWdFxnewjN9gsq/
↪download
Resolving surfdrive.surf.nl (surfdrive.surf.nl)... 145.100.27.67, 2001:610:108:203b:0:
↪a11:da7a:5afe
Connecting to surfdrive.surf.nl (surfdrive.surf.nl)|145.100.27.67|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 25699440 (25M) [application/gzip]
Saving to: 'blog-authorship.json.gz'

blog-authorship.jso 100%[===================>]  24.51M  16.1MB/s    in 1.5s

2022-04-05 17:42:52 (16.1 MB/s) - 'blog-authorship.json.gz' saved [25699440/25699440]
```

[11]:
```
import json

with open("blog-authorship.json") as f:
    blog_data = json.load(f)
```

[12]:
```
blog_data.keys()
```

[12]:
```
dict_keys(['source', 'ack', 'subset', 'format', 'training', 'dev', 'test'])
```

[13]:
```
blog_data['source'], blog_data['ack']
```

[13]:
```
('[Blog authorship corpus](https://www.kaggle.com/rtatman/blog-authorship-corpus)',
 '[Schler et al (2006)](http://www.cs.biu.ac.il/~schlerj/schler_springsymp06.pdf)')
```

We already have a training/dev/test split, each data point is a pair and the text is not preprocessed for us:

[14]:
```
len(blog_data['training']), len(blog_data['dev']), len(blog_data['test'])
```

[14]:
```
(200000, 40000, 49174)
```

[15]:
```
blog_data['training'][0]
```

[15]:
```
['I hate exams considering I just failed one. Yippee', 16]
```

We need to tokenize the data for use in deep learning. We will use the NLTK word tokenizer for this. We also lowercase the inputs and shuffle the training data. This will take some 3 minutes.

[16]:
```
%%time
from nltk.tokenize import word_tokenize

# Tokenize and shuffle the data.
order = np.random.RandomState(42).permutation(np.arange(len(blog_data["training"])))
blog_training_x = [word_tokenize(blog_data["training"][i][0].lower()) for i in order]
blog_training_y = [[blog_data["training"][i][1]] for i in order]
blog_dev_x = [word_tokenize(x[0].lower()) for x in blog_data["dev"]]
blog_dev_y = [[x[1]] for x in blog_data["dev"]]
blog_test_x = [word_tokenize(x[0].lower()) for x in blog_data["test"]]
blog_test_y = [[x[1]] for x in blog_data["test"]]
```

```
CPU times: user 1min 10s, sys: 306 ms, total: 1min 11s
Wall time: 1min 11s
```

[17]:
```
# Example pre-processed data point
print(f"input: {blog_training_x[0]}")
print(f"age of author: {blog_training_y[0]}")
```

```
input: ['urllink', 'this', 'is', 'my', 'friend', 'sam', '.', 'he', "'s", 'a', 'little',
↪'weird', '.', 'he', "'s", 'nice', 'though', '.', 'but', 'weird', '.']
age of author: [17]
```

1.3 Syntactic categories

From NLTK, we will also take the `treebank` corpus where words are annotated with their syntactic categories (parts of speech, or POS tags).

The method `tagged_sents` will give us a view of tokenized sentences with their token lag tag annotation:

[18]:
```
example = treebank.tagged_sents(tagset='universal')[0]  # 'universal' here refers to the␣
↪style of tags
example
```

[18]:
```
[('Pierre', 'NOUN'),
 ('Vinken', 'NOUN'),
 (',', '.'),
 ('61', 'NUM'),
 ('years', 'NOUN'),
 ('old', 'ADJ'),
 (',', '.'),
 ('will', 'VERB'),
 ('join', 'VERB'),
 ('the', 'DET'),
 ('board', 'NOUN'),
 ('as', 'ADP'),
 ('a', 'DET'),
 ('nonexecutive', 'ADJ'),
 ('director', 'NOUN'),
 ('Nov.', 'NOUN'),
 ('29', 'NUM'),
 ('.', '.')]
```

[19]:
```
def split_nltk_tagged_corpus(corpus, max_length=30, num_heldout=100):
    """
    Shuffle and split a corpus.
    corpus: a corpus of tagged sequences, each sequence is a pair, each pair is a token␣
↪and a tag.
    max_length: discard sentences longer than this

    Return:
        (training word sequences, training tag sequences),
        (dev word sequences, dev tag sequences),
        (test word sequences, test tag sequences),
    """
    tagged_sentences = corpus.tagged_sents(tagset='universal')
    # do not change the seed in here
    order = np.random.RandomState(42).permutation(np.arange(len(tagged_sentences)))
```

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```
    word_sequences = [[w.lower() for w, t in tagged_sentences[i]] for i in order if␣
↪len(tagged_sentences[i]) <= max_length]
    tag_sequences = [[t for w, t in tagged_sentences[i]] for i in order if len(tagged_
↪sentences[i]) <= max_length]
    return (word_sequences[2*num_heldout:], tag_sequences[2*num_heldout:]), (word_
↪sequences[num_heldout:2*num_heldout], tag_sequences[num_heldout:2*num_heldout]), (word_
↪sequences[:num_heldout], tag_sequences[:num_heldout])
```

For `treebank` this will take about 10 seconds.

[20]:
```
%%time
(tagger_training_x, tagger_training_y), (tagger_dev_x, tagger_dev_y), (tagger_test_x,␣
↪tagger_test_y) = split_nltk_tagged_corpus(treebank, num_heldout=100)
print(f"Number of sentences: training={len(tagger_training_x)} dev={len(tagger_dev_x)}␣
↪test={len(tagger_test_x)}")
```

```
Number of sentences: training=2486 dev=100 test=100
CPU times: user 2.38 s, sys: 116 ms, total: 2.5 s
Wall time: 2.52 s
```

[21]:
```
print("# A few training sentences\n")
for n in range(3):
    print(f"x_{n} = {tagger_training_x[n]}")
    print(f"y_{n} = {tagger_training_y[n]}")
    print()
```

```
# A few training sentences

x_0 = ['they', 'know', '0', 'he', 'is', 'generally', 'opposed', 'to', 'cop-killer',
↪'bullets', ',', 'but', 'that', 'he', 'had', 'some', 'reservations', 'about', 'the',
↪'language', 'in', 'the', 'legislation', '.', "'"]
y_0 = ['PRON', 'VERB', 'X', 'PRON', 'VERB', 'ADV', 'VERB', 'PRT', 'ADJ', 'NOUN', '.',
↪'CONJ', 'ADP', 'PRON', 'VERB', 'DET', 'NOUN', 'ADP', 'DET', 'NOUN', 'ADP', 'DET', 'NOUN
↪', '.', '.']

x_1 = ['california', "'s", 'education', 'department', 'suspects', 'adult',
↪'responsibility', 'for', 'erasures', 'at', '40', 'schools', 'that', '*t*-85', 'changed
↪', 'wrong', 'answers', 'to', 'right', 'ones', 'on', 'a', 'statewide', 'test', '.']
y_1 = ['NOUN', 'PRT', 'NOUN', 'NOUN', 'VERB', 'NOUN', 'NOUN', 'ADP', 'NOUN', 'ADP', 'NUM
↪', 'NOUN', 'DET', 'X', 'VERB', 'ADJ', 'NOUN', 'PRT', 'ADJ', 'NOUN', 'ADP', 'DET', 'ADJ
↪', 'NOUN', '.']

x_2 = ['the', 'loan', 'may', 'be', 'extended', '*-1', 'by', 'the', 'mcalpine', 'group',
↪'for', 'an', 'additional', 'year', 'with', 'an', 'increase', 'in', 'the', 'conversion',
↪ 'price', 'to', '$', '2.50', '*u*', 'a', 'share', '.']
y_2 = ['DET', 'NOUN', 'VERB', 'VERB', 'VERB', 'X', 'ADP', 'DET', 'NOUN', 'NOUN', 'ADP',
↪'DET', 'ADJ', 'NOUN', 'ADP', 'DET', 'NOUN', 'ADP', 'DET', 'NOUN', 'NOUN', 'PRT', '.',
↪'NUM', 'X', 'DET', 'NOUN', '.']
```

1.4 Vocabulary

As always when dealing with NLP models, we need an object to maintain our vocabulary of known tokens. We will rely on word-tokenization.

Our vocabulary class will maintain the set of known tokens, and a dictionary to convert tokens to codes and codes back to tokens. The class will also take care of some special symbols (e.g., BOS, EOS, UNK, PAD).

Finally, if later on you test your model on sentences that are not word tokenized, you can use `nlt.tokenize.word_tokenize` or any other tokenizer you like (as long as the level of tokenization is similar to the one you used for training your model.

This class will be used for maintaining both the vocabulary of known tokens and the set of known tags for the tagger data.

[22]:
```
import numpy as np
from itertools import chain
from collections import Counter, OrderedDict

class Vocab:

    def __init__(self, corpus: list, min_freq=1):
        """
        corpus: list of documents, each document is a list of tokens, each token is a␣
↪string
        min_freq: words that occur less than this value are discarded
        """

        # Count word occurrences
        counter = Counter(chain(*corpus))

        # Sort them by frequency
        sorted_by_freq_tuples = sorted(counter.items(), key=lambda pair: pair[1],␣
↪reverse=True)

        # Special tokens
        self.pad_token = "-PAD-" # used to fill sequences in a batch to maximum sequence␣
↪length
        self.bos_token = "-BOS-" # begin of sequence
        self.eos_token = "-EOS-" # end of sequence
        self.unk_token = "-UNK-" # unknown symbol
        self.pad_id = 0
        self.bos_id = 1
        self.eos_id = 2
        self.unk_id = 3

        self.known_symbols = [self.pad_token, self.bos_token, self.eos_token, self.unk_
↪token]
        self.counts = [0, 0]

        # Vocabulary
        self.word2id = OrderedDict()
        self.word2id[self.pad_token] = self.pad_id
        self.word2id[self.bos_token] = self.bos_id
        self.word2id[self.eos_token] = self.eos_id
```

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```
        self.word2id[self.unk_token] = self.unk_id
        self.min_freq = min_freq
        for w, n in sorted_by_freq_tuples:
            if n >= min_freq: # discard infrequent words
                self.word2id[w] = len(self.known_symbols)
                self.known_symbols.append(w)
                self.counts.append(n)

        # Store the counts as well
        self.counts = np.array(self.counts)

    def __len__(self):
        return len(self.known_symbols)

    def __getitem__(self, word: str):
        """
        Return the id (int) of a word (str)
        """
        return self.word2id.get(word, self.unk_id)

    def encode(self, doc: list, add_bos=False, add_eos=False, pad_right=0):
        """
        Transform a document into a numpy array of integer token identifiers.
        doc: list of tokens, each token is a string
        add_bos: whether to add the BOS token
        add_eos: whether to add the EOS token
        pad_right: number of suffix padding tokens

        Return: a list of codes (possibly with BOS and EOS added as well as padding)
        """
        return [self.word2id.get(w, self.unk_id) for w in chain([self.bos_token] *␣
↪int(add_bos), doc, [self.eos_token] * int(add_eos), [self.pad_token] * pad_right)]

    def batch_encode(self, docs: list, add_bos=False, add_eos=False):
        """
        Transform a batch of documents into a numpy array of integer token identifiers.
        This will pad the shorter documents to the length of the longest document.
        docs: a list of documents
        add_bos: whether to add the BOS token
        add_eos: whether to add the EOS token
        pad_right: number of suffix padding tokens

        Return: numpy array with shape [len(docs), longest_doc + add_bos + add_eos]
        """
        max_len = max(len(doc) for doc in docs)
        return np.array([self.encode(doc, add_bos=add_bos, add_eos=add_eos, pad_
↪right=max_len-len(doc)) for doc in docs])

    def decode(self, ids, strip_pad=False):
        """
        Transform a np.array document into a list of tokens.
        ids: np.array with shape [num_tokens]
```

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```
        strip_pad: whether PAD tokens should be deleted from the output

        Return: list of strings with size [num_tokens - num_padding]
        """
        if strip_pad:
            return [self.known_symbols[id] for id in ids if id != self.pad_id]
        else:
            return [self.known_symbols[id] for id in ids]

    def batch_decode(self, docs, strip_pad=False):
        """
        Transform a np.array collection of documents into a collection of lists of␣
↪tokens.
        ids: np.array with shape [num_docs, max_length]
        strip_pad: whether PAD tokens should be deleted from the output

        Return: list of documents, each a list of tokens, each token a string
        """
        return [self.decode(doc, strip_pad=strip_pad) for doc in docs]
```

Let's see how this works on the tagger corpus:

[23]:
```
# We get a vocabulary for words
word_vocab = Vocab(tagger_training_x, min_freq=2)
# and a vocabulary for tags
tag_vocab = Vocab(tagger_training_y, min_freq=1)
# You can see their sizes V and C:
len(word_vocab), len(tag_vocab)
```

[23]:
```
(3358, 16)
```

The encode method turns a sequence of (str) symbols into a sequence of (int) codes:

We can also have encode add some special symbols for us (but remember to be consistent, you should always have token sequences and tag sequences that match in length):

We can also encode and decode entire batches of sequences. This will use pad symbols/codes to make the sequences in the same batch have the same length:

[24]:
```
word_vocab.batch_encode(tagger_training_x[:3], add_bos=False, add_eos=True)
```

[24]:
```
array([[  45,  907,   13,   36,   18,  600, 1078,    8, 1651, 1652,    6,
          41,   19,   36,   66,   71, 2194,   55,    5, 2195,   10,    5,
         487,    4,   21,    2,    0,    0,    0],
       [ 488,   14, 1309,  156, 2196,    3,    3,   16,    3,   31,  449,
         908,   19,    3,  601,  909,  772,    8,  343,  910,   26,    9,
        2197,  344,    4,    2,    0,    0,    0],
       [   5,  542,  129,   40, 2198,   12,   34,    5, 1310,  264,   16,
          44,  378,   54,   37,   44,  324,   10,    5, 2199,  186,    8,
          25, 1311,   23,    9,  111,    4,    2]])
```

[25]:
```
word_vocab.batch_decode(word_vocab.batch_encode(tagger_training_x[:3], add_bos=False,␣
↪add_eos=True), strip_pad=True)
```

[25]:
```
[['they',
  'know',
  '0',
  'he',
  'is',
  'generally',
  'opposed',
  'to',
  'cop-killer',
  'bullets',
  ',',
  'but',
  'that',
  'he',
  'had',
  'some',
  'reservations',
  'about',
  'the',
  'language',
  'in',
  'the',
  'legislation',
  '.',
  "'",
  '-EOS-'],
 ['california',
  "'s",
  'education',
  'department',
  'suspects',
  '-UNK-',
  '-UNK-',
  'for',
  '-UNK-',
  'at',
  '40',
  'schools',
  'that',
  '-UNK-',
  'changed',
  'wrong',
  'answers',
  'to',
  'right',
  'ones',
  'on',
  'a',
  'statewide',
  'test',
  '.',
  '-EOS-'],
 ['the',
```

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```
 'loan',
 'may',
 'be',
 'extended',
 '*-1',
 'by',
 'the',
 'mcalpine',
 'group',
 'for',
 'an',
 'additional',
 'year',
 'with',
 'an',
 'increase',
 'in',
 'the',
 'conversion',
 'price',
 'to',
 '$',
 '2.50',
 '*u*',
 'a',
 'share',
 '.',
 '-EOS-']]
```

1.5 Corpus and Data Loader

We will be developing our models in torch, thus we need to wrap our corpus into a `Dataset` and a `DataLoader`:

[26]:
```
import torch
from torch.utils.data import Dataset, DataLoader

class TextRegressionCorpus(Dataset):
    """
    Use this to give torch access to a corpus of documents annotated with a simple␣
↪response variable (e.g., category or real number)
    This class will also know the vocab objects for tokens
    and it will take care of coding strings into integers consistently.
    """

    def __init__(self, corpus_x, corpus_y, vocab_x: Vocab):
        """
        In PyTorch we better always manipulate numerical codes, rather than text.
        So, our Corpus object will contain a vocab that converts words to codes.

        corpus_x: token sequences
        corpus_y: response values
```

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```
        vocab_x: vocabulary of input symbols
        """
        self.corpus_x = list(corpus_x)
        self.corpus_y = list(corpus_y)
        if len(self.corpus_x) != len(self.corpus_y):
            raise ValueError("I need pairs")
        self.vocab_x = vocab_x

    def __len__(self):
        """Size of the corpus in number of sequence pairs"""
        return len(self.corpus_x)

    def __getitem__(self, idx):
        """Return corpus_x[idx] and corpus_y[idx] converted to codes and with the EOS␣
↪code in the end"""
        x = self.vocab_x.encode(self.corpus_x[idx], add_bos=False, add_eos=True)
        y = self.corpus_y[idx]
        return x, y

    def pad_to_longest(self, pairs, pad_id=0):
        """
        Take a list of coded sequences and returns a torch tensor where
        every sentence has the same length (by means of using PAD tokens)
        """
        longest = max(len(x) for x, y in pairs)
        batch_x = torch.tensor([x + [self.vocab_x.pad_id] * (longest - len(x)) for x, y␣
↪in pairs])
        batch_y = torch.tensor([y for x, y in pairs])
        return batch_x, batch_y


class ParallelCorpus(Dataset):
    """
    Use this to give torch access to a corpus of sequence pairs.
    This class will also know the vocab objects for the two streams.
    and it will take care of coding strings into integers consistently.
    """

    def __init__(self, corpus_x, corpus_y, vocab_x: Vocab, vocab_y: Vocab):
        """
        In PyTorch we better always manipulate numerical codes, rather than text.
        So, our Corpus object will contain a vocab that converts words to codes.

        corpus_x: token sequences
        corpus_y: tag sequences
        vocab_x: vocabulary for token sequences
        vocab_y: vocabulary for tag sequences
        """
        self.corpus_x = list(corpus_x)
        self.corpus_y = list(corpus_y)
        assert len(self.corpus_x) == len(self.corpus_y), "I need sequence pairs"
        self.vocab_x = vocab_x
```

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```
        self.vocab_y = vocab_y

    def __len__(self):
        """Size of the corpus in number of sequence pairs"""
        return len(self.corpus_x)

    def __getitem__(self, idx):
        """
        Return corpus_x[idx] and corpus_y[idx] converted to codes
        the latter has the EOS code in the end
        """
        x = self.vocab_x.encode(self.corpus_x[idx], add_bos=False, add_eos=True)
        y = self.vocab_y.encode(self.corpus_y[idx], add_bos=False, add_eos=True)
        return x, y

    def pad_to_longest(self, pairs, pad_id=0):
        """
        Take a list of coded sequences and returns a torch tensor where
        every sentence has the same length (by means of using PAD tokens)
        """
        longest_x = max(len(x) for x, y in pairs)
        longest_y = max(len(y) for x, y in pairs)
        batch_x = torch.tensor([x + [self.vocab_x.pad_id] * (longest_x - len(x)) for x,␣
↪y in pairs])
        batch_y = torch.tensor([y + [self.vocab_y.pad_id] * (longest_y - len(y)) for x,␣
↪y in pairs])
        return batch_x, batch_y


class TaggedCorpus(ParallelCorpus):
    """
    Use this to give torch access to a corpus of tagged sequences.
    This class will also know the vocab objects for tokens and tags,
    and it will take care of coding strings into integers consistently.
    """

    def __init__(self, corpus_x, corpus_y, vocab_x: Vocab, vocab_y: Vocab):
        """
        In PyTorch we better always manipulate numerical codes, rather than text.
        So, our Corpus object will contain a vocab that converts words to codes.

        corpus_x: token sequences
        corpus_y: tag sequences
        vocab_x: vocabulary for token sequences
        vocab_y: vocabulary for tag sequences
        """
        super().__init__(corpus_x, corpus_y, vocab_x, vocab_y)
        assert all(len(x) == len(y) for x, y in zip(corpus_x, corpus_y)), "A sequence␣
↪pair should match in number of steps"
```

We join our input and output data into torch `Dataset` objects for training, development and testing. Note that training, development and testing data share the same vocabularies, which were constructed using the training set alone. We can wrap the tagger data around a `Dataset` object as:

[27]:
```
tagger_training = TaggedCorpus(tagger_training_x, tagger_training_y, word_vocab, tag_
↪vocab)
```

Here's an example of how we get a `DataLoader` for a corpus, we simply choose the `Dataset` object we want (training/dev/test), the batch size we want, whether we need shuffling (e.g., for training batches in SGD), and how we "glue" data points of different length together (i.e., a function such as `pad_to_longest` which `TextRegressionCorpus` and `TaggedCorpus` provide for us).

[28]:
```
batcher = DataLoader(tagger_training, batch_size=3, shuffle=True, collate_fn=tagger_
↪training.pad_to_longest)
for batch_x, batch_y in batcher:
    print("# This is how the tagged sequences in a batch come out of the data loader\n")
    for x, y in zip(batch_x, batch_y):
        print(x)
        print(y)
        print()

    print("# And we can always decode them for inspection\n")
    # stripping padding makes it easier to read the examples
    for x, y in zip(word_vocab.batch_decode(batch_x, strip_pad=True), tag_vocab.batch_
↪decode(batch_y, strip_pad=True)):
        print(x)
        print(y)
        print()
    break
```

```
# This is how the tagged sequences in a batch come out of the data loader

tensor([  77, 2535,    5,  318,    6,   43,  776,    4,    2,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0])
tensor([14,  5,  8,  4,  6, 14,  4,  6,  2,  0,  0,  0,  0,  0,  0,  0,  0,  0,
         0,  0,  0,  0,  0,  0])

tensor([   3,    3,   11,    3,   98,   13,   45,   29,    3,    7,  101,  918,
         175,   34, 1491,   15,    8,    3,   49,    3,  748,  213,    4,    2])
tensor([ 4,  4, 15,  4,  5, 10, 14,  5,  9,  7,  8,  4, 10,  7,  4, 10, 13,  5,
        15,  5,  4,  4,  6,  2])

tensor([ 46, 882,  69,   2,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,
          0,   0,   0,   0,   0,   0,   0,   0,   0,   0])
tensor([4, 4, 6, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0])

# And we can always decode them for inspection

['i', 'loved', 'the', 'school', ',', 'its', 'history', '.', '-EOS-']
['PRON', 'VERB', 'DET', 'NOUN', '.', 'PRON', 'NOUN', '.', '-EOS-']

['-UNK-', '-UNK-', 'and', '-UNK-', 'say', '0', 'they', 'are', '-UNK-', 'of', 'any',
↪'efforts', '*ich*-1', 'by', 'mcgraw-hill', '*', 'to', '-UNK-', 'or', '-UNK-', 'scoring
↪', 'high', '.', '-EOS-']
['NOUN', 'NOUN', 'CONJ', 'NOUN', 'VERB', 'X', 'PRON', 'VERB', 'ADJ', 'ADP', 'DET', 'NOUN
↪', 'X', 'ADP', 'NOUN', 'X', 'PRT', 'VERB', 'CONJ', 'VERB', 'NOUN', 'NOUN', '.', '-EOS-
↪']
```

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```
['new', 'account', ':', '-EOS-']
['NOUN', 'NOUN', '.', '-EOS-']
```

4.43.3 2. Text encoders

In NLP applications, we often have to *encode* a piece of text. For example, that is the case in text classification and regression, as well as in sequence labelling.

Assume for example, a text classifier that takes a document $x_{1:l} = \langle x_1, \ldots, x_l \rangle$, where each token $x_i \in \mathcal{W}$ is from a finite vocabulary of V tokens and predicts a distribution over C classes from a set $\mathcal{T} = \{1, \ldots, C\}$. An encoding function can map $x_{1:l}$ to a D-dimensional vector $\mathbf{u}$, which we can then transform to a C-dimensional vector of scores using an affine transformation, which in turn we can constrain to the probability simplex via softmax:

$$Y|X_{1:l} = x_{1:l} \sim \text{Categorical}(\mathbf{g}(x_{1:l}; \theta)) \tag{4.19}$$

$$\mathbf{u} = \text{encode}_D(x_{1:l}; \theta_{\text{enc}}) \tag{4.20}$$

$$\mathbf{s} = \text{affine}_C(\mathbf{u}; \theta_{\text{out}}) \tag{4.21}$$

$$\mathbf{g}(x_{1:l}; \theta) = \text{softmax}(\mathbf{s}) \tag{4.22}$$

Here I use a subscript to indicate the dimensionality of the output of the function, the named parameters after ; are the trainable parameters of the function.

Generally text encoders may return a single output vector per document, or one vector per word in the document.

[29]:
```
import torch
import torch.nn as nn
import torch.nn.functional as F


class Encoder(nn.Module):

    def __init__(self, output_dim):
        super().__init__()
        self._output_dim = output_dim

    @property
    def output_dim(self):
        return self._output_dim

    def forward(self, x):
        """
        x: [batch_size, max_length]

        Return a tensor of shape [batch_size, max_length, output_dim] or
            [batch_size, output_dim]
        """
        raise NotImplementedError("Implement me!")
```

We develop a very basic text encoder based on a bidirectional LSTM. In principle, any powerful encoder (including pretrained encoders) can be used, we go ahead with the BiLSTM to keep the tutorial lightweight.

[30]:
```
class TextEncoder(Encoder):
    """
    Given a predictor x this NN parameterises the pdf of the random variable Y|X=x.
    In other words, it predicts the conditional distribution P(Y|X=x).
    When reduce_mean is True the forward will return a single output vector per document.
    When reduce_mean is False one vector per word in the document is returned instead.
    """

    def __init__(self, vocab_size: int, word_embed_dim: int, hidden_size: int, reduce_
↪mean=False, pad_id=0, p_drop=0.):
        super().__init__(2 * hidden_size)
        self.pad_id = pad_id
        self.word_embed_dim = word_embed_dim
        self.hidden_size = hidden_size
        self.vocab_size = vocab_size
        self.word_embed = nn.Embedding(self.vocab_size, embedding_dim=word_embed_dim)
        self.encoder = nn.LSTM(
            input_size=word_embed_dim,
            hidden_size=hidden_size,
            num_layers=1,
            batch_first=True,
            bidirectional=True,
        )
        self.reduce_mean = reduce_mean

    def forward(self, x):
        """
        x: [batch_size, max_length]
        """
        # We begin by embedding the tokens
        # [batch_size, max_length, embed_dim]
        h = self.word_embed(x)
        # [batch_size, max_length, 2*hidden_size*num_layers]
        h, _ = self.encoder(h)
        if self.reduce_mean: # average pooling
            h = torch.where((x == self.pad_id).unsqueeze(-1), torch.zeros_like(h), h)
            h = torch.sum(h, axis=-2) / torch.sum((x != self.pad_id).float(), -1,␣
↪keepdims=True)
        return h
```

4.43.4 3. Probabilistic model

A probabilistic model prescribes the probability measure of a random experiment, in this tutorial we will design models by explicitly parameterising a probability density function (pdf using NNs. When our random variables (rvs) are multivariate or structured we will pick a factorisation of the joint pdf, decide on the statistical family of each factor, and parameterise the factors using NNs.

Generically, we will be modelling the distribution of some random variable Y (univariate, multivariate, structured) conditioned on an assignment of some random variable $X = x$ (typically structured).

For example, x may be a piece of text or an image. The response variable may be a category, a numerical measurement, a vector of attributes/measurements, a data structure (e.g., sequence, tree, graph).

For us, a probabilistic model can at the very least * assign probability density to an assignment $Y = y$ given $X = x$ * sample an assignment of Y given $X = x$ and we will use the forward method of a PyTorch Module to parameterise the relevant conditional probability distributions.

Occasionally, we will be able to support other operations such as finding the median, mean, mode, etc.

[31]:
```
class Model(nn.Module):
    """
    A probabilistic model predicts the probability measure of a random experiment.
    We will predict the distribution of the random variable Y conditioned on
    an assignment to the random variable X=x.

    As a modelling mechanism we will use pmfs and pdfs, hence predicting
    the distribution P(Y|X=x) requires mapping from x to the parameters of a
    pmf/pdf for Y, or, in case of multivariate/structured data, a joint pdf
    whose factorisation we decide upon.

    For us, a model needs to satisfy the following desiderata:
    * parameterising the pdf is tractable
    * assessing the pdf for a given outcome Y=y|X=x is tractable
    * drawing samples from P(Y|X=x) is tractable
    * the pdf p(y|x) is differentiable with respect to the parameters of the
      NN that predicts its parameter(s)


    The only aspects of the Model's API that is fixed are:
    * log_prob(x, y) -> tensor of floats, one value per instance in the batch
    * sample(x, sample_size) -> batch of samples
    * forward(...) -> a torch.distribution object
        the signature of the forward method may vary in subclasses

    """

    def __init__(self, event_shape=tuple()):
        """
        The event_shape is the shape of the outcome of the rv Y.
        """
        super().__init__()
        self._event_shape = event_shape

    @property
    def event_shape(self):
        return self._event_shape

    def num_parameters(self):
        return sum(np.prod(theta.shape) for theta in self.parameters())

    def forward(self, x):
        """
        x: [batch_size, ...]
        """
        raise NotImplementedError("Each type of model will have a different␣
↪implementation here")
```

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```
    def sample(self, x, sample_size=tuple()):
        """
        x: [batch_size, ...]
        Return a batch of samples from Y|X=x
        """
        raise NotImplementedError("Each type of model will have a different␣
↪implementation here")

    def log_prob(self, x, y):
        """
        Computes the log pdf for Y=y|X=x for each pair in the batch.

        x: batch_shape + event_shape_x
        y: batch_shape + event_shape
        """

        # Predict the conditional probability distribution using the forward function.
        # This will return one such probability distribution per batch element.
        cpds = self(x=x)

        # Computer the log probability of each element in the batch.
        logp = cpds.log_prob(y) # [batch_size]

        return logp
```

4.43.5 4. Parameter estimation

We will estimate parameters using maximum likelihood estimation (MLE), via gradient-based search. This means we need to assess the model's likelihood given a dataset (or batch) of observations and the likelihood function must be tractable and differentiable with respect to the NN parameters.

[32]:
```
def loss(self, x, y):
    """
    No matter the probabilistic model, the loss is the negative log likelihood
    of the parameters estimated on a single batch:
        - 1/batch_size * \sum_{s} log P(y[s]|x[s], theta)

    x: batch_shape + event_shape_x
    y: batch_shape + event_shape
    """
    return -self.log_prob(x=x, y=y).mean(0)
```

[33]:
```
def distortion(model, dl, device):
    """
    Wrapper for estimating distortion using all data points in a data loader.
    """
    total_log_prob = 0.
    data_size = 0
    with torch.no_grad():
        for batch_x, batch_y in dl:
```

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```
            total_log_prob = total_log_prob + model.log_prob(batch_x.to(device), batch_y.
↪to(device)).sum()
            data_size += batch_x.shape[0]
    return - total_log_prob / data_size
```

4.43.6 5. Decision rules

A rational decision maker chooses her actions to maximise expected utility.

Let $u(y, c)$ quantify the benefit in choosing $c \in \mathcal{Y}$ when y is the truth. When deciding under uncertainty, we solve

$$y^\star = \arg\max_{c \in \mathcal{Y}} \mathbb{E}[u(Y, c)|X = x] \tag{4.23}$$

where the expectation is with respect to the pdf $p_{Y|X=x}$.

For certain utility functions and pdf combinations, this can be solved in closed form. In many cases there is not tractable algorithm for this decision problem, then approximations are needed.

When the utility function is $u(y, c) = [y = c]$ (which evaluates to 1 if y and c are the same, and 0 otherwise), $y^\star$ corresponds to the mode of $p_{Y|X=x}$.

In structure prediction, utility functions may reward partial/structural similarity between y and c. For example, a utility function for strings may be based on Levenshtein distance/similarity.

[34]:
```
class DecisionRule:

    def __init__(self):
        super().__init__()

    def __call__(self, model, x):
        """
        This function should map from a model and input, and the resulting predicted␣
↪probability distribution,
        to a single outcome.
        """
        raise NotImplementedError("Implement me!")


class ExactMode(DecisionRule):
    """
    This decision rule returns the most probable outcome under the predicted probability␣
↪distribution, assuming
    a unimodal or discrete probability distribution.
    """

    def __call__(self, model, x):
        return model.mode(x)
```

We have some helper code for predictions using the batches in a data loader:

[35]:
```
def predict(model, rule, dl, device, return_targets=False, strip_pad=True):
    """
    Wrapper for predictions using a decision rule.

    model: one of our taggers
    dl: a data loader for the heldout data
    device: the PyTorch device where the model is stored
    return_targets: also return the targets from the data loader
        you can use this when the actual targets are in the dataloader (e.g., for dev␣
↪set)

    Return
        * a list of predictions, each a sequence of tags (already decoded)
        * if return_targets=True, additionally return a list of targets, each a sequence␣
↪of tags (already decoded)
    """
    all_preds = []
    all_targets = []
    with torch.no_grad():
        for batch_x, batch_y in dl:
            preds = rule(model, batch_x.to(device))
            all_preds.extend(preds.cpu().numpy())
            all_targets.extend(batch_y.cpu().numpy())

    if return_targets:
        return all_preds, all_targets
    else:
        return all_preds
```

4.43.7 6. Training procedure

The training procedure is always the exact same, no matter the model, so we abstract it for you.

[36]:
```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.distributions as td
import torch.optim as opt
from tqdm.notebook import tqdm
import matplotlib.pyplot as plt
```

[37]:
```
from sklearn.metrics import classification_report, mean_squared_error, mean_absolute_
↪error, median_absolute_error
from collections import defaultdict
from itertools import chain


def flatten(seq):
    """flattens a python list"""
    return list(chain.from_iterable(seq))
```

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```
def report_regression(y_true, y_pred):
    return {"MSE": mean_squared_error(y_true, y_pred), "MAE": mean_absolute_error(y_true,
↪ y_pred), "MdAE": median_absolute_error(y_true, y_pred)}

def report_classification(y_true, y_pred):
    return classification_report(y_true, y_pred, output_dict=True, zero_division=0)

def report_tagging(y_true, y_pred, score_pad=False, pad_id=0):
    if not score_pad:
        pairs = [(t, p) for t, p in zip(flatten(y_true), flatten(y_pred)) if t != pad_id]
        y_true = [t for t, p in pairs]
        y_pred = [p for t, p in pairs]
    return classification_report(y_true, y_pred, output_dict=True, zero_division=0)
```

[38]:
```
def train_neural_model(model: Model, optimiser, decision_rule: DecisionRule,
    training_data, dev_data,
    batch_size=200, num_epochs=10, check_every=10,
    report_fn=None, report_metrics=[],
    device=torch.device('cuda:0')
    ):
    """
    model: pytorch model
    optimiser: pytorch optimiser
    training_corpus: a TaggedCorpus for trianing
    dev_corpus: a TaggedCorpus for dev
    batch_size: use more if you have more memory
    num_epochs: use more for improved convergence
    check_every: use less to check performance on dev set more often
    device: where we run the experiment

    Return a log of quantities computed during training (for plotting)
    """
    # We use the training data in random order for parameter estimation
    batcher = DataLoader(training_data, batch_size=batch_size, shuffle=True, collate_
↪fn=training_data.pad_to_longest)
    # We use the dev data for evaluation during training (no need for randomisation here)
    dev_batcher = DataLoader(dev_data, batch_size=batch_size, shuffle=False, collate_
↪fn=dev_data.pad_to_longest)

    total_steps = num_epochs * len(batcher)
    log = defaultdict(list)

    model.eval()
    log['D'].append(distortion(model, dev_batcher, device=device).item())

    if report_fn:
        preds, targets = predict(
            model,
            decision_rule,
            dev_batcher,
            device=device,
            return_targets=True
```

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```
        )
        report = report_fn(targets, preds)
        for metric in report_metrics:
            log[metric].append(report[metric])

    step = 0

    with tqdm(range(total_steps)) as bar:
        for epoch in range(num_epochs):
            for batch_x, batch_y in batcher:
                model.train()
                optimiser.zero_grad()

                L = loss(model, batch_x.to(device), batch_y.to(device))

                L.backward()
                optimiser.step()

                bar_dict = OrderedDict()
                bar_dict['loss'] = f"{L.item():.2f}"
                bar_dict['D'] =  f"{log['D'][-1]:.2f}"
                for metric in report_metrics:
                    bar_dict[metric] =  "{:.2f}".format(log[metric][-1])
                bar.set_postfix(bar_dict)
                bar.update()

                log['loss'].append(L.item())

                if step % check_every == 0:
                    model.eval()
                    log['D'].append(distortion(model, dev_batcher, device=device).item())

                    if report_fn:
                        preds, targets = predict(
                            model,
                            decision_rule,
                            dev_batcher,
                            device=device,
                            return_targets=True
                        )
                        report = report_fn(targets, preds)
                        for metric in report_metrics:
                            log[metric].append(report[metric])

                step += 1

    model.eval()
    log['D'].append(distortion(model, dev_batcher, device=device).item())

    if report_fn:
        preds, targets = predict(
            model,
```

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```
            decision_rule,
            dev_batcher,
            device=device,
            return_targets=True
        )
        report = report_fn(targets, preds)
        for metric in report_metrics:
            log[metric].append(report[metric])

    return log
```

4.43.8 7. Examples

7.1 Categorical

Here we design a probabilistic model for a Categorical response variable Y given a document x:

$$Y|X = x \sim \text{Categorical}(\mathbf{g}(x;\theta)) \tag{4.24}$$
$$\mathbf{u} = \text{encode}_D(x;\theta_{\text{enc}}) \tag{4.25}$$
$$\mathbf{s} = \text{affine}_C(\mathbf{u};\theta_{\text{out}}) \tag{4.26}$$
$$\mathbf{g}(x;\theta) = \text{softmax}(\mathbf{s}) \tag{4.27}$$

[39]:
```
class CategoricalModel(Model):
    """
    Given a predictor x this NN parameterises the pdf of the random variable Y|X=x,
    where Y is Categorically distributed.
    In other words, it predicts the conditional distribution P(Y|X=x).
    """

    def __init__(self, support_size, hidden_size: int, encoder: Encoder, p_drop=0.):
        super().__init__(tuple())
        self.encoder = encoder
        self.support_size = support_size
        self.hidden_size = hidden_size

        # We have a simple neural network that maps from the text encodings to
        # logits for the Categorical distribution.
        self.logits_predictor = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(encoder.output_dim, hidden_size),
            nn.ReLU(),
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, support_size)
        )

    def forward(self, x):

        # We begin by encoding the tokens
```

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```
        h = self.encoder(x) # batch_shape, (enc_dim,)

        # We use the logit predictor network to transform those into logits.
        logits = self.logits_predictor(h) # batch_shape, (support_size,)

        # We return a Categorical distribution with the predicted logits as its␣
↪parameters.
        return td.Categorical(logits=logits)

    def sample(self, x, sample_size=tuple()):
        with torch.no_grad():
            cpd = self(x=x)
            return cpd.sample(sample_size)

    def mode(self, x):
        with torch.no_grad():
            # Predict the Categorical distribution of P(Y|X=x)
            cpd = self(x=x)

            # We can easily obtain the exact mode by taking the argmax over logits.
            mode = torch.argmax(cpd.logits, -1)

            return mode
```

Let's sanity check our implementation by doing a forwards pass through a randomly initialized text encoder and Categorical model:

[40]:
```
encoder = TextEncoder(len(word_vocab), 7, 5, True)
cat_model = CategoricalModel(3, 12, encoder)
for batch_x, batch_y in batcher:
    print(batch_x.shape)
    print(cat_model(batch_x).logits)
    print(cat_model.mode(batch_x))
    print(cat_model.sample(batch_x))
    break
```

```
torch.Size([3, 28])
tensor([[-1.2122, -1.1352, -0.9647],
        [-1.1917, -1.1365, -0.9799],
        [-1.2199, -1.1338, -0.9599]], grad_fn=<SubBackward0>)
tensor([2, 2, 2])
tensor([1, 2, 1])
```

[41]:
```
# We already set up the data at the start of this notebook. We are only left to␣
↪construct the word vocabulary.
cat_vocab = Vocab(cat_training_x, min_freq=2)
print(len(cat_vocab))
```

```
22734
```

[42]:
```
# Now let's train a model on this data.

# First, reset random number generators
```

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```
seed_all()

# Use GPU acceleration
my_device = torch.device('cuda:0')

# Create the model
model = CategoricalModel(
    support_size=len(brown.categories()),
    hidden_size=32,
    encoder=TextEncoder(
        vocab_size=len(cat_vocab),
        word_embed_dim=100,
        hidden_size=64,
        reduce_mean=True,
        pad_id=cat_vocab.pad_id
    ),
    p_drop=0.1
).to(my_device)

# Construct an Adam optimiser
optimiser = opt.Adam(model.parameters(), lr=5e-3)

print("Model")
print(model)

# Report number of parameters
print(f"Model size: {model.num_parameters():,} parameters")

# Train the model
log = train_neural_model(
    model, optimiser,
    decision_rule=ExactMode(),
    training_data=TextRegressionCorpus(cat_training_x, cat_training_y, cat_vocab),
    dev_data=TextRegressionCorpus(cat_dev_x, cat_dev_y, cat_vocab),
    report_fn=report_classification,
    report_metrics=['accuracy'],
    batch_size=500, num_epochs=20, check_every=100,
    device=my_device
)

# Plot loss and validation checks
fig, axs = plt.subplots(1, 3, sharey=False, figsize=(12, 4))
_ = axs[0].plot(np.arange(len(log['loss'])), log['loss'])
_ = axs[0].set_xlabel('steps')
_ = axs[0].set_ylabel('training loss')
_ = axs[1].plot(np.arange(len(log['D'])), log['D'])
_ = axs[1].set_xlabel('steps (in 100s)')
_ = axs[1].set_ylabel('D given dev')
_ = axs[2].plot(np.arange(len(log['accuracy'])), log['accuracy'])
_ = axs[2].set_xlabel('steps (in 10s)')
_ = axs[2].set_ylabel('dev acc')
_ = fig.tight_layout(h_pad=2, w_pad=2)
```

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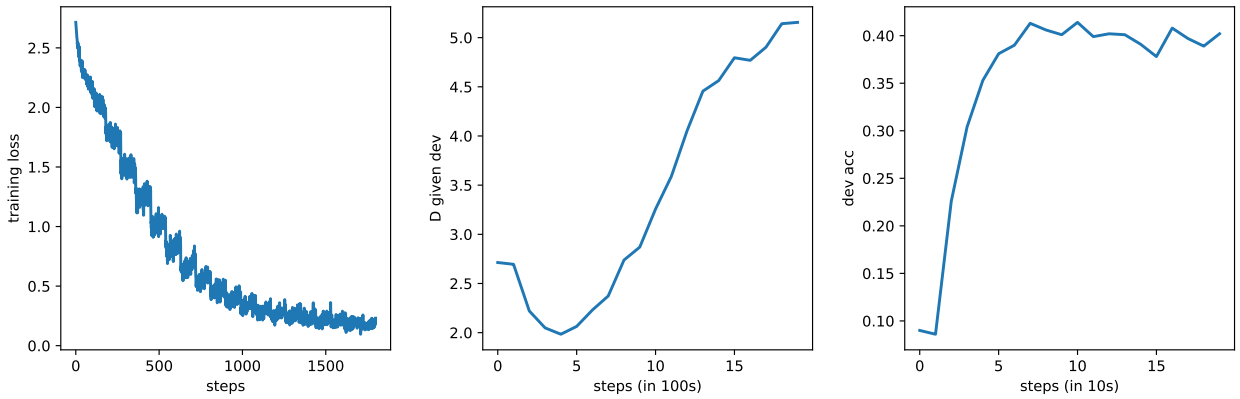
```
plt.show()
```

```
Model
CategoricalModel(
  (encoder): TextEncoder(
    (word_embed): Embedding(22734, 100)
    (encoder): LSTM(100, 64, batch_first=True, bidirectional=True)
  )
  (logits_predictor): Sequential(
    (0): Dropout(p=0.1, inplace=False)
    (1): Linear(in_features=128, out_features=32, bias=True)
    (2): ReLU()
    (3): Dropout(p=0.1, inplace=False)
    (4): Linear(in_features=32, out_features=15, bias=True)
  )
)
Model size: 2,363,015 parameters
```

```
  0%|          | 0/1800 [00:00<?, ?it/s]
```



Let's use the model for some predictions.

[43]:
```
# Set up the test dataloader
cat_test_corpus = TextRegressionCorpus(cat_test_x, cat_test_y, cat_vocab)
cat_test_dl = DataLoader(cat_test_corpus, batch_size=3, shuffle=True, collate_fn=cat_
↪test_corpus.pad_to_longest)
batch_x, batch_y = next(iter(cat_test_dl))

# Use the mode to form predictions.
decision_rule = ExactMode()
predictions = decision_rule(model, batch_x.to(my_device))

for x, pred, truth in zip(batch_x, batch_y, predictions):
    print(f"input: {' '.join(cat_vocab.decode(x, strip_pad=True))}")
    print(f"prediction: {brown.categories()[pred]}")
    print(f"truth: {brown.categories()[truth]}")
    print()
```

```
input: Have you examined this problem of increasing consumer sophistication from the␣
↪standpoint of your own company ? ? -EOS-
```

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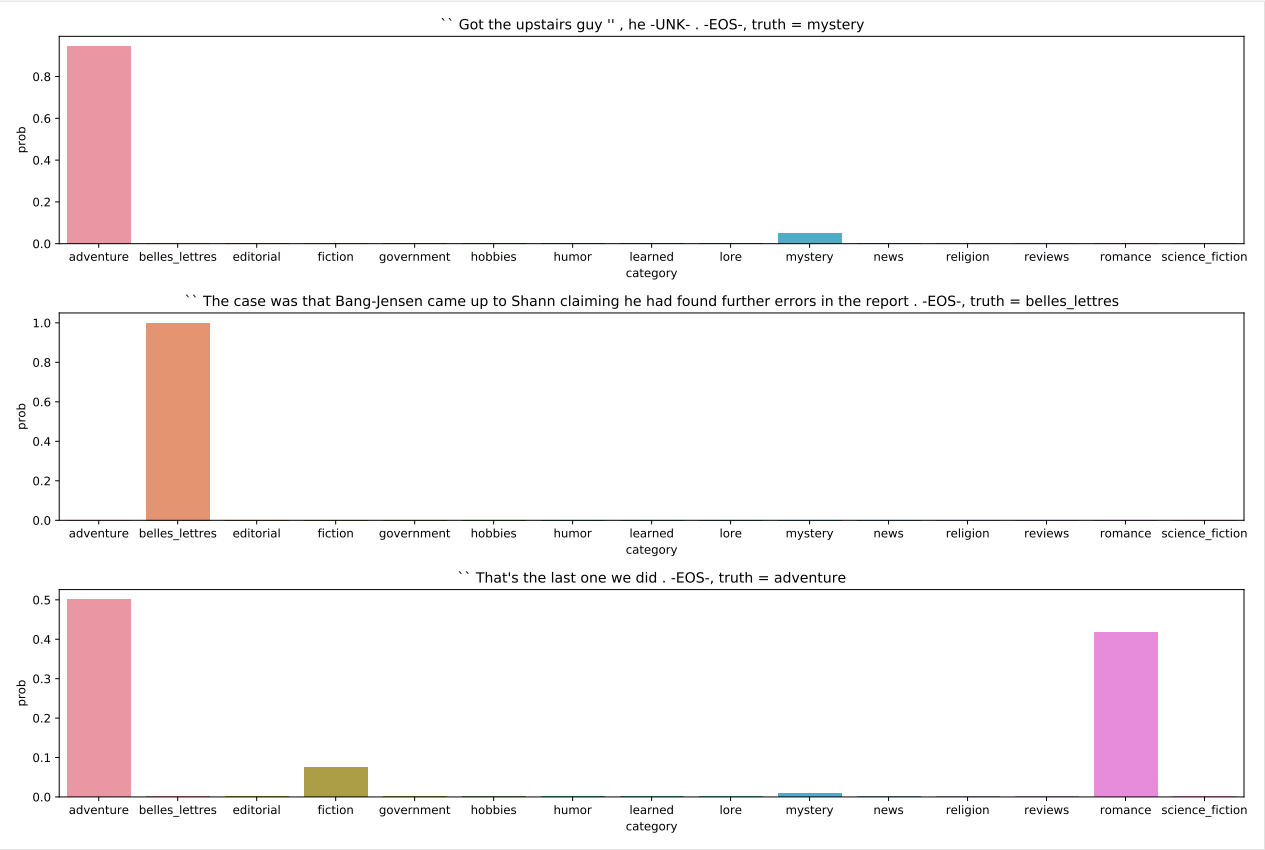
```
prediction: hobbies
truth: lore

input: Some have plenty of money -- some have very little money . -EOS-
prediction: lore
truth: mystery

input: Thus far the advances made have been almost entirely along functional lines . -
↪EOS-
prediction: belles_lettres
truth: learned
```

[44]:
```
# We can also visualize the predicted Categoricals and use them for sampling or input
# to any arbitrary decision rule.
import seaborn as sns
import pandas as pd

with torch.no_grad():
    batch_x, batch_y = next(iter(cat_test_dl))
    cpds = model(batch_x.to(my_device))

fig, axes = plt.subplots(3, 1, figsize=(15, 10))
for ax, x, y, predicted_probs in zip(axes, batch_x, batch_y, cpds.probs):
    sns.barplot(data=pd.DataFrame({"category": brown.categories(), "prob": predicted_
↪probs.cpu()}),
                x="category", y="prob", ax=ax)
    ax.set_title(f"{' '.join(cat_vocab.decode(x, strip_pad=True))}, truth = {brown.
↪categories()[y]}")

plt.tight_layout()
plt.show()
```



7.2 Poisson

Here we design a probabilistic model for an ordinal response variable Y given a document x, for which we choose to model with a Poisson pmf:

$$Y|X = x \sim \text{Poisson}(g(x;\theta)) \tag{4.28}$$
$$\mathbf{u} = \text{encode}_D(x;\theta_{\text{enc}}) \tag{4.29}$$
$$s = \text{affine}_1(\mathbf{u};\theta_{\text{out}}) \tag{4.30}$$
$$g(x;\theta) = \text{softplus}(s) \tag{4.31}$$

The Poisson rate parameter must be strictly positive, thus we use a softplus output.

[45]:
```
class PoissonModel(Model):
    """
    This model predicts a conditional Poisson distribution Y|X=x for ordinal data.
    """

    def __init__(self, hidden_size: int, encoder: Encoder, p_drop=0.):
        super().__init__(tuple())
        self.encoder = encoder
        self.hidden_size = hidden_size
```

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```
        # The poisson distribution has 1 parameter: its rate. This needs to be a␣
↪positive real number.
        self.rate_predictor = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(encoder.output_dim, hidden_size),
            nn.ReLU(),
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, 1),
            nn.Softplus()
        )

    def forward(self, x):
        h = self.encoder(x)
        rate = self.rate_predictor(h)
        return td.Poisson(rate=rate)

    def sample(self, x, sample_size=tuple()):
        with torch.no_grad():
            cpd = self(x=x)
            return cpd.sample(sample_size)

    def mode(self, x):
        with torch.no_grad():
            cpd = self(x=x)
            rate = cpd.rate
            return torch.floor(rate)
```

[46]:
```
# Let's train on the age data using a conditional Poisson model.

# We need to construct the vocabulary for this data.
blog_vocab = Vocab(blog_training_x, min_freq=2)
print(f"{len(cat_vocab):,} words in the vocabulary.")

# Reset the random seeds
seed_all()

# Use GPU acceleration
my_device = torch.device('cuda:0')

# Create a similar model as before, but predicting a Poisson distribution instead.
model = PoissonModel(
    hidden_size=32,
    encoder=TextEncoder(
        vocab_size=len(blog_vocab),
        word_embed_dim=100,
        hidden_size=64,
        reduce_mean=True,
        pad_id=blog_vocab.pad_id
    ),
    p_drop=0.1
).to(my_device)
```

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```
# construct an Adam optimiser
optimiser = opt.Adam(model.parameters(), lr=5e-3)

print("Model")
print(model)

# Report number of parameters
print(f"Model size: {model.num_parameters():,} parameters")

# Train the model
log = train_neural_model(
    model, optimiser,
    decision_rule=ExactMode(),
    training_data=TextRegressionCorpus(blog_training_x, blog_training_y, blog_vocab),
    dev_data=TextRegressionCorpus(blog_dev_x, blog_dev_y, blog_vocab),
    report_fn=report_regression,
    report_metrics=["MSE", "MAE", "MdAE"],
    batch_size=500, num_epochs=1, check_every=100,
    device=my_device
)

# Plot loss and validation checks
fig, axs = plt.subplots(1, 4, sharey=False, figsize=(16, 4))
_ = axs[0].plot(np.arange(len(log['loss'])), log['loss'])
_ = axs[0].set_xlabel('steps')
_ = axs[0].set_ylabel('training loss')
_ = axs[1].plot(np.arange(len(log['D'])), log['D'])
_ = axs[1].set_xlabel('steps (in 100s)')
_ = axs[1].set_ylabel('D given dev')
_ = axs[2].plot(np.arange(len(log['MAE'])), log['MAE'])
_ = axs[2].set_xlabel('steps (in 10s)')
_ = axs[2].set_ylabel('dev mean absolute error')
_ = axs[3].plot(np.arange(len(log['MdAE'])), log['MdAE'])
_ = axs[3].set_xlabel('steps (in 10s)')
_ = axs[3].set_ylabel('dev median absolute error')
_ = fig.tight_layout(h_pad=2, w_pad=2)
plt.show()
```

```
22,734 words in the vocabulary.
Model
PoissonModel(
  (encoder): TextEncoder(
    (word_embed): Embedding(83532, 100)
    (encoder): LSTM(100, 64, batch_first=True, bidirectional=True)
  )
  (rate_predictor): Sequential(
    (0): Dropout(p=0.1, inplace=False)
    (1): Linear(in_features=128, out_features=32, bias=True)
    (2): ReLU()
    (3): Dropout(p=0.1, inplace=False)
    (4): Linear(in_features=32, out_features=1, bias=True)
    (5): Softplus(beta=1, threshold=20)
```

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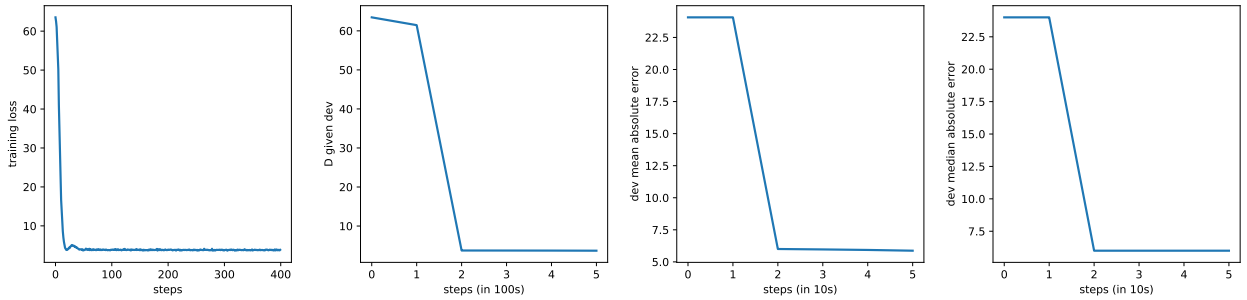
```
  )
)
Model size: 8,442,353 parameters
```

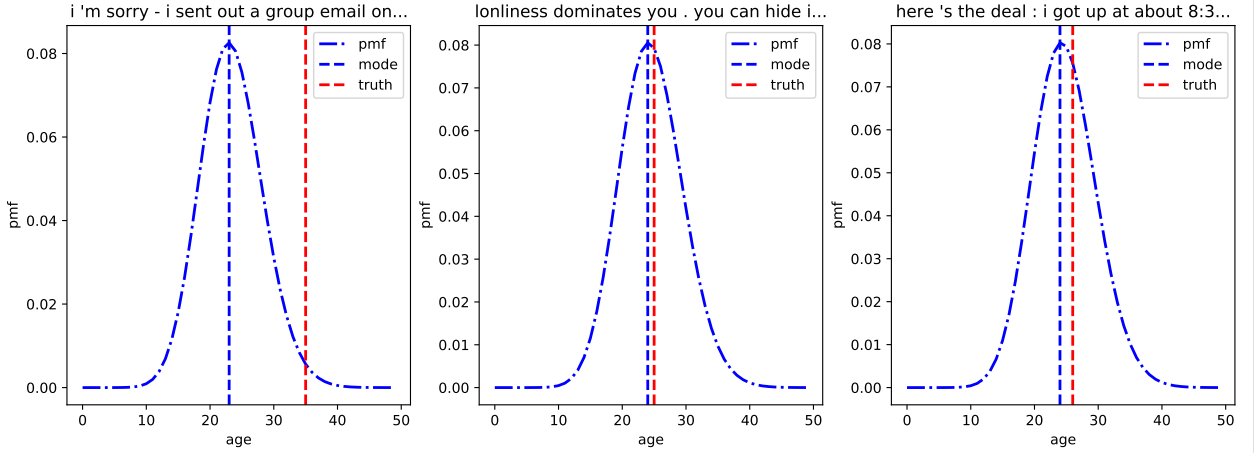
```
  0%|          | 0/400 [00:00<?, ?it/s]
```



[47]:
```
# Set up the test dataloader
blog_test_corpus = TextRegressionCorpus(blog_test_x, blog_test_y, blog_vocab)
blog_test_dl = DataLoader(blog_test_corpus, batch_size=3, shuffle=True, collate_fn=blog_
↪test_corpus.pad_to_longest)
batch_x, batch_y = next(iter(blog_test_dl))

# We can use the mode again to form predictions.
decision_rule = ExactMode()
predictions = decision_rule(model, batch_x.to(my_device))

for x, pred, truth in zip(batch_x, batch_y, predictions):
    print(f"input: {' '.join(blog_vocab.decode(x, strip_pad=True))}")
    print(f"prediction: {pred.item()}")
    print(f"truth: {truth.item()}")
    print()
```

```
input: every day deserves a good urllink insult . but , no one insults like shakespeare␣
↪... : drunkenness is his best virtue , for he will be swine drunk , and in his sleep␣
↪he does little harm , save to his -UNK- about him . -EOS-
prediction: 26
truth: 24.0

input: here 's something i never thought i 'd never see : an epa ad mocking the idea of␣
↪good fuel -UNK- in cars . urllink http : -UNK- maybe the appliance department should␣
↪talk to the transportation department and get everyone on the same page . -EOS-
prediction: 17
truth: 24.0

input: i ca n't tolerate bitches ... im just allergic to them . they have no quality in␣
↪starting a conversation and worse of all , a disgrace to women around the world . its␣
↪in me ... i ca n't tolerate them . heard of a saying , respect yourself ... before␣
↪others respect you .. very the true ... -EOS-
prediction: 24
truth: 24.0
```

[48]:
```
# We can also visualize the pmf of the predicted conditional Poisson distributions.
with torch.no_grad():
    batch_x, batch_y = next(iter(blog_test_dl))
    cpds = model(batch_x.to(my_device))
    mode = model.mode(batch_x.to(my_device))

x = torch.arange(0, 50).repeat(3, 1)
pmf = cpds.log_prob(x.to(my_device)).exp()

fig, axes = plt.subplots(1, 3, figsize=(15, 5))
for i in range(3):
    axes[i].plot(x[i].cpu(), pmf[i].cpu().numpy(), ls='-.', color='b', label='pmf')
    axes[i].axvline(mode[i].cpu().numpy(), ls="--", color='b', label='mode')
    axes[i].axvline(batch_y[i].numpy(), color='r', ls='--', label='truth')
    axes[i].set_xlabel("age")
    axes[i].set_ylabel("pmf")
    axes[i].set_title(f"{' '.join(blog_vocab.decode(batch_x[i], strip_pad=True))[:40]}...
↪")
    axes[i].legend()
```



7.3 Sequence labelling

In sequence labelling we have two sequences of equal length: a word sequence $x_{1:l}$ and a tag sequence $y_{1:l}$.

The word sequence $x_{1:l} = \langle x_1, \ldots, x_l \rangle$, where l is the sequence length, is such that token x_i belongs to a vocabulary $\mathcal{W}$ of V known words.

The tag sequence $y_{1:l} = \langle y_1, \ldots, y_l \rangle$, where l is the same length as the document $x_{1:l}$, is such that each tag y_i belongs to a vocabulary $\mathcal{T}$ of C known tags.

As always, our models are probability distributions, but this time we need a distribution over a space of sequences. A sequence is a finite length object, but it cannot be seen as a fixed dimensional vector (a multivariate random variable), for its length is not at all fixed. A sequence is best seen as a data structure. To prescribe a distribution over a general data structure, we can decompose this structure into parts, prescribe distributions for the parts, and combine them into a single pdf.

Chain rule allows us to re-express a pdf over an arbitrary sample space (with multivariate or structured outcomes) as a product of pdfs, each over a simpler space space (e.g., with univariate outcomes):

$$p(y_{1:l}|x_{1:l},\theta) = \prod_{i=1}^{l} p(y_i|x_{1:l}, y_1^{i-1}, \theta) \tag{4.32}$$

$$= \prod_{i=1}^{l} \text{Categorical}(y_i|\mathbf{g}(x_{1:l}, y_1^{i-1}; \theta)) \tag{4.33}$$

where, on the right-hand side of the first equation, we have pdfs (or pfms) for each step of the sequence. In the second row, we use a Categorical pmf since each step of the sequence is a simple categorical variable. Each pmf is parameterised in context using some trainable function $\mathbf{g}$ with parameters θ.

The above is a *factorisation* of the joint pdf. This is one valid factorisation, and this one does not make any conditional independence assumptions (i.e., it conditions on all parts of the structure already generated). We could simplify the factorisation by making such conditional independence (or Markov) assumptions. For example, we might use only $x_{1:l}$ and the previous step y_{i-1} when parameterising the distribution of Y_i. These assumptions are justified on a case by case basis depending on application domain.

[49]:
```
class Tagger(Model):

    def __init__(self, vocab_size: int, tagset_size: int, pad_id=0, bos_id=1, eos_id=2):
        super().__init__()
        self._vocab_size = vocab_size
        self._tagset_size = tagset_size
        self._pad = pad_id
        self._bos = bos_id
        self._eos = eos_id

    @property
    def vocab_size(self):
        return self._vocab_size

    @property
    def tagset_size(self):
        return self._tagset_size

    @property
    def pad(self):
        return self._pad

    @property
    def bos(self):
        return self._bos

    @property
    def eos(self):
        return self._eos

    def num_parameters(self):
        return sum(np.prod(theta.shape) for theta in self.parameters())

    def forward(self, x, y_in):
        """
        To predict the distribution of Y[i], an autoregressive model conditions
```

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```
         on both x and y[:i]. Normally, y_in is prepended with some BOS code so
         that both sequences have the same length.

        x: [batch_size, max_length]
        y_in: [batch_size, max_length]

        Return a batch of cpds, one per step.
        """
        raise NotImplementedError("Each type of tagger will have a different␣
↪implementation here")

    def log_prob(self, x, y):
        """
        Computes the log conditional probability of each tag sequence in a batch.

        x: [batch_size, max_length]
        y: [batch_size, max_length]
        """
        # shift the output sequence and prepend the BOS code
        # (after all, we do not want to condition on what we need to predict)
        batch_size, max_len = y.shape
        bos = torch.full((batch_size, 1), self.bos, device=y.device)
        y_in = torch.cat([bos, y], 1)[:,:-1]

        # one C-dimensional Categorical cpd for each token in the batch
        cpds = self(x=x, y_in=y_in)
        # [batch_size, max_length]
        logp = cpds.log_prob(y)
        # [batch_size]
        logp = torch.where(y != self.pad, logp, torch.zeros_like(logp)).sum(-1)
        return logp

    def greedy(self, x):
        """
        For each cpd Y[i]|X=x, predicts the mode of the cpd.
        x: [batch_size, max_length]

        Return: tag sequences [batch_size, max_length]
        """
        raise NotImplementedError("Each type of tagger differs here")

    def sample(self, x, sample_size=tuple()):
        """
        Per word sequence in the batch, draws a number of samples from the model, each␣
↪sample is a complete tag sequence.

        x: [batch_size, max_len]

        Return: tag sequences with shape [batch_size, max_len] if sample_size is None
            else with shape [sample_size, batch_size, max_len]
        """
        raise NotImplementedError("Each type of tagger differs here")
```

[50]:
```
# we get a vocabulary for words
word_vocab = Vocab(tagger_training_x, min_freq=2)
# and a vocabulary for tags
tag_vocab = Vocab(tagger_training_y, min_freq=1)
# you can see their sizes V and C:
len(word_vocab), len(tag_vocab)
```

[50]:
```
(3358, 16)
```

7.3.1 Independent C-way classification

Our first tagger is in fact just a C-way classifier that we use to predict a distribution over C tags for different positions of an input sequence conditioned on the entire input sequence.

Here is the model of the ith tag given $x_{1:l}$:

$$Y_i|S = x_{1:l} \sim \text{Categorical}(\mathbf{g}(i, x_{1:l}; \theta)) \tag{4.34}$$

where $\mathbf{g}$ is a neural network. For example:

$$\mathbf{e}_j = \text{embed}_D(x_j; \theta_{\text{in}}) \qquad j \in \{1, \ldots, l\} \tag{4.35}$$
$$\mathbf{u}_{1:l} = \text{birnn}_{2K}(\mathbf{e}_{1:l}; \theta_{\text{bienc}}) \tag{4.36}$$
$$\mathbf{s}_i = \text{affine}_C(\mathbf{u}_i; \theta_{\text{out}}) \tag{4.37}$$
$$\mathbf{g}(i, x_{1:l}) = \text{softmax}(\mathbf{s}_i) \tag{4.38}$$

The bidirection RNN layer concatenates the states of two independent RNN layers, one that processes the sequence from left-to-right, another that processes it from right-to-left.

Note how this model ignores every other tag in the sequence.

[51]:
```
class BasicTagger(Tagger):

    def __init__(self, vocab_size, tagset_size, word_embed_dim: int, hidden_size: int, p_
↪drop=0, pad_id=0, bos_id=1, eos_id=2):
        """
        vocab_size: number of known words
        tagset_size: number of known tags
        word_embed_dim: dimensionality of word embeddings
        hidden_size: dimensionality of hidden layers
        recurrent_encoder: enable recurrent encoder
        bidirectional_encoder: for a recurrent encoder, make it bidirectional
        """
        super().__init__(vocab_size=vocab_size, tagset_size=tagset_size, pad_id=pad_id,␣
↪bos_id=bos_id, eos_id=eos_id)
        self.word_embed_dim = word_embed_dim
        self.hidden_size = hidden_size
        self.encoder = TextEncoder(
            vocab_size=vocab_size,
            word_embed_dim=word_embed_dim,
            hidden_size=hidden_size,
            reduce_mean=False,
            pad_id=pad_id,
```

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```
            p_drop=p_drop
        )
        # the bidirectional LSTM encoder produces outputs of size 2*hidden_size
        # thus our linear layer must take 2*hidden_size inputs
        self.logits_predictor = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(self.encoder.output_dim, self.tagset_size)
        )

    def forward(self, x, y_in=None):
        """
        Parameterise the conditional distributions over Y[i] given the entire word␣
↪sequence x.

        x: [batch_size, max_length]
        y: not used by this class

        Return: a batch of C-dimensional Categorical distributions, one per step of the␣
↪sequence.
        """
        # We begin by encoding the tokens
        # [batch_size, max_length, enc_dim]
        h = self.encoder(x)
        # finally, per step of the sequence we predict logits for the possible tags
        # [batch_size, max_length, tagset_size]
        s = self.logits_predictor(h)
        # and convert those logits to Categorical distributions
        return td.Categorical(logits=s)

    def greedy(self, x):
        """
        For each cpd Y[i]|X=x, predicts the mode of the cpd.
        x: [batch_size, max_length]

        Return: tag sequences [batch_size, max_length]
        """
        batch_size = x.shape[0]
        max_length = x.shape[1]
        with torch.no_grad():
            cpds = self(x)
            # [batch_size, max_length]
            y_pred = torch.argmax(cpds.probs, -1)
            # if a position in x is padded, it should be padded in y
            y_pred = torch.where(x != self.pad, y_pred, torch.zeros_like(y_pred) + self.
↪pad)
            return y_pred

    def mode(self, x):
        return self.greedy(x)

    def sample(self, x, sample_size=None):
        """
```

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```
        Per word sequence in the batch, draws a number of samples from the model, each␣
↪sample is a complete tag sequence.

        x: [batch_size, max_len]

        Return: tag sequences with shape [batch_size, max_len] if sample_size is None
            else with shape [sample_size, batch_size, max_len]
        """
        batch_size = x.shape[0]
        max_length = x.shape[1]
        with torch.no_grad():
            cpds = self(x)
            if sample_size is None:
                shape = (1,)
            else:
                shape = (sample_size,)
            # [sample_size, batch_size, max_length]
            y_pred = cpds.sample(shape)
            # if a position in x is padding, it must be padded in y too
            y_pred = torch.where(x.unsqueeze(0) != self.pad, y_pred, torch.zeros_like(y_
↪pred) + self.pad)
            # takes care of output shape
            if sample_size is None:
                return y_pred.squeeze(0)
            else:
                return y_pred
```

[52]:
```
def test_basic_tagger(training_x, training_y, vocab_x, vocab_y):
    seed_all()
    toy_uni_tagger = BasicTagger(
        vocab_size=len(vocab_x),
        tagset_size=len(vocab_y),
        word_embed_dim=32,
        hidden_size=32
    )

    assert type(toy_uni_tagger(torch.from_numpy(vocab_x.batch_encode(training_x[:2]))))␣
↪is td.Categorical

    assert toy_uni_tagger.log_prob(
            torch.from_numpy(vocab_x.batch_encode(training_x[:2])),
            torch.from_numpy(vocab_y.batch_encode(training_y[:2]))
        ).shape == (2,)

    assert loss(toy_uni_tagger,
            torch.from_numpy(vocab_x.batch_encode(training_x[:2])),
            torch.from_numpy(vocab_y.batch_encode(training_y[:2]))
        ).shape == tuple()

    assert toy_uni_tagger.sample(torch.from_numpy(vocab_x.batch_encode(training_x[:2]))).
↪shape == vocab_x.batch_encode(training_x[:2]).shape
```

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```
    assert toy_uni_tagger.sample(torch.from_numpy(vocab_x.batch_encode(training_x[:2])),␣
↪3).shape == (3,) + vocab_x.batch_encode(training_x[:2]).shape

    assert toy_uni_tagger.greedy(torch.from_numpy(vocab_x.batch_encode(training_x[:2]))).
↪shape == vocab_x.batch_encode(training_x[:2]).shape


test_basic_tagger(tagger_training_x, tagger_training_y, word_vocab, tag_vocab)
```

7.3.2 Autoregressive tagger

When predicting the distribution of Y_i, an autoregressive tagger conditions on the tag sequence already generated thus far, hence it makes no Markov assumption. This is the model of the ith tag:

$$Y_i|S = x_{1:l}, H = y_1^{i-1} \sim \text{Categorical}(\mathbf{g}(i, x_{1:l}, y_1^{i-1}; \theta)) \tag{4.39}$$

where $\mathbf{g}$ is a neural network. For example:

$$\begin{aligned}
\mathbf{e}_j &= \text{embed}_{D_1}(x_j; \theta_{\text{words}}) && j \in \{1, \dots, l\} && (4.40)\\
\mathbf{t}_k &= \text{embed}_{D_2}(y_k; \theta_{\text{tags}}) && k < i && (4.41)\\
\mathbf{u}_{1:l} &= \text{birnn}_{2K}(\mathbf{e}_{1:l}; \theta_{\text{bienc}}) && && (4.42)\\
\mathbf{v}_i &= \text{rnnstep}_K(\mathbf{v}_{i-1}, \mathbf{t}_{i-1}; \theta_{\text{dec}}) && && (4.43)\\
\mathbf{s}_i &= \text{ffnn}_C(\text{concat}(\mathbf{u}_i, \mathbf{v}_i); \theta_{\text{out}}) && && (4.44)\\
\mathbf{g}(i, x_{1:l}) &= \text{softmax}(\mathbf{s}_i) && && (4.45)
\end{aligned}$$

Again, we have two different embedding layers, one for words and one for tags. Again, we use a bidirectional rnn to encode the whole document. Now, for the ith position, we use an RNN generator/decoder cell to encode the complete history of previous tags. We then predict the logits by using an FFNN to combine the history encoding with the document encoding for position i.

There's yet another way to parameterise this model, in which we let the RNN decoder compose the features of the history with the features of the document:

$$\begin{aligned}
\mathbf{e}_j &= \text{embed}_{D_1}(x_j; \theta_{\text{words}}) && j \in \{1, \dots, l\} && (4.46)\\
\mathbf{t}_k &= \text{embed}_{D_2}(y_k; \theta_{\text{tags}}) && k < i && (4.47)\\
\mathbf{u}_{1:l} &= \text{birnn}_{2K}(\mathbf{e}_{1:l}; \theta_{\text{bienc}}) && && (4.48)\\
\mathbf{v}_i &= \text{rnnstep}_K(\mathbf{v}_{i-1}, \text{concat}(\mathbf{u}_i, \mathbf{t}_{i-1}); \theta_{\text{dec}}) && && (4.49)\\
\mathbf{s}_i &= \text{affine}_C(\mathbf{v}_i; \theta_{\text{out}}) && && (4.50)\\
\mathbf{g}(i, x_{1:l}) &= \text{softmax}(\mathbf{s}_i) && && (4.51)
\end{aligned}$$

Both are very good options.

[53]:
```
class AutoregressiveTagger(Tagger):

    def __init__(self, vocab_size: int, tagset_size: int, word_embed_dim: int, tag_embed_
↪dim: int, hidden_size: int, p_drop=0., pad_id=0, bos_id=1, eos_id=2):
        """
        ngram_size: longest ngram (for tag sequence)
        vocab_size: number of known words
        tagset_size: number of known tags
        word_embed_dim: dimensionality of word embeddings
        tag_embed_dim: dimensionality of tag embeddings (needed to encode the history of␣
↪ngram_size-1 tags)
        hidden_size: dimensionality of hidden layers
        """
        super().__init__(vocab_size=vocab_size, tagset_size=tagset_size, pad_id=pad_id,␣
↪bos_id=bos_id, eos_id=eos_id)
        self.word_embed_dim = word_embed_dim
        self.tag_embed_dim = tag_embed_dim
        self.hidden_size = hidden_size

        self.encoder = TextEncoder(
            vocab_size=vocab_size,
            word_embed_dim=word_embed_dim,
            hidden_size=hidden_size,
            reduce_mean=False,
            pad_id=pad_id
        )
        # we need to embed tags in the history
        self.tag_embed = nn.Embedding(tagset_size, embedding_dim=tag_embed_dim)

        self.decoder = nn.LSTM(
            input_size=tag_embed_dim,
            hidden_size=hidden_size,
            num_layers=1,
            batch_first=True,
            bidirectional=False
        )
        # for each position i, we need to combine the encoding of x[i] in context
        # as well as the history of ngram_size-1 tags
        # so we use a FFNN for that:
        self.logits_predictor = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(self.encoder.output_dim + hidden_size, hidden_size),
            nn.ReLU(),
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, tagset_size),
        )

        self.init_state = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(self.encoder.output_dim, hidden_size),
            nn.Tanh()
        )
        self.init_cell = nn.Sequential(
```

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```
            nn.Dropout(p_drop),
            nn.Linear(self.encoder.output_dim, hidden_size),
            nn.Tanh()
        )

    def forward(self, x, y_in):
        """
        Parameterise the conditional distributions over Y[i] given history y[:i] and all␣
↪of x.

        This procedure takes care that the ith output distribution conditions only on␣
↪the n-1 observations before y[i].
        It also takes care of padding to the left with BOS symbols.

        x: word sequences [batch_size, max_length]
        y_in: history of tag sequences  [batch_size, max_length]

        Return: a batch of V-dimensional Categorical distributions, one per step of the␣
↪sequence.
        """

        # Let's start by encoding the conditioning sequences
        # [batch_size, max_length, enc_dim]
        u = self.encoder(x)

        # here we pad the tag sequence with BOS on the left
        # [batch_size, max_len, tag_emb_dim]
        t_in = self.tag_embed(y_in)

        # encode the histories
        # [batch_size, max_len, hidden_size]
        v, _ = self.decoder(t_in)

        # Now we can combine the encodings of x and the encodings of histories, we do so␣
↪via concatenation
        # since there's a fixed number of such encodings per step of the sequence
        # [batch_size, max_length, 3*hidden_size]
        u = torch.cat([u, v], -1)
        # We are now ready to map the state of each step of the sequence to a C-
↪dimensional vector of logits
        # we do so using our FFNN
        # [batch_size, max_length, tagset_size]
        s = self.logits_predictor(u)

        return td.Categorical(logits=s)

    def greedy(self,x):
        """
        Draws a number of samples from the model, each sample is a complete sequence.
        We impose a maximum number of steps, to avoid infinite loops.
        This procedure takes care of mapping sampled symbols to pad after the EOS symbol␣
↪is generated.
```

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```
        """
        batch_size = x.shape[0]
        max_length = x.shape[1]

        with torch.no_grad():
            # add the beginning we do not know the tag sequence
            # but NNs work with fixed dimensional tensors,
            # so we allocate a tensor full of BOS codes
            y = torch.full((batch_size, max_length + 1), self.bos, device=self.tag_embed.
↪weight.device)
            # Per step
            for i in range(max_length):
                # we parameterise a cpd for Y[i]|X=x
                # note that the forward method takes care of not conditioning on y[i]␣
↪itself
                # and only using the ngram_size-1 previous tags
                # at this point, the tag y[i] is a dummy code
                # the forward method recomputes all cds in the batch, this will include␣
↪the cpd for Y[i]
                # [batch_size, max_len, C]
                cpds = self(x=x, y_in=y[:,:-1])
                # we get their modes via argmax
                # [batch_size, max_len]
                modes = torch.argmax(cpds.probs, -1)

                # Here we update the current token to the freshly obtained mode
                #  and also replace the token by 0 (pad) in case the sentence is already␣
↪complete
                y[:, i+1] = modes[:, i]
            # discard the BOS token
            y = y[:,1:]
            # where we had a PAD token in x, we change the y token to PAD too
            y = torch.where(x != self.pad, y, torch.zeros_like(y) + self.pad)

            return y

    def mode(self, x):
        raise NotImplementedError("The search for the mode of the autoregressive tagger␣
↪is intractable, consider using `greedy` or a sampling-based approximation. ")

    def _sample(self, x):
        """
        Draws a number of samples from the model, each sample is a complete sequence.
        We impose a maximum number of steps, to avoid infinite loops.
        This procedure takes care of mapping sampled symbols to pad after the EOS symbol␣
↪is generated.
        """
        batch_size = x.shape[0]
        max_length = x.shape[1]

        with torch.no_grad():
            # add the beginning we do not know the tag sequence
```

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```
            # but NNs work with fixed dimensional tensors,
            # so we allocate a tensor full of BOS codes
            y = torch.full((batch_size, max_length + 1), self.bos, device=self.tag_embed.
↪weight.device)

            # Per step
            for i in range(max_length):
                # we parameterise a cpd for Y[i]|X=x
                # note that the forward method takes care of not conditioning on y[i]␣
↪itself
                # and only using the ngram_size-1 previous tags
                # at this point, the tag y[i] is a dummy code
                # the forward method recomputes all cds in the batch, this will include␣
↪the cpd for Y[i]
                # we get their modes via argmax
                # [batch_size, max_len, C]
                cpds = self(x=x, y_in=y[:,:-1])
                # [batch_size, max_len]
                samples = cpds.sample()

                # Here we update the current token to the freshly obtained mode
                #  and also replace the token by 0 (pad) in case the sentence is already␣
↪complete
                y[:, i+1] = samples[:,i]
            # discard the BOS token
            y = y[:,1:]
            # where we had a PAD token in x, we change the y token to PAD too
            y = torch.where(x != self.pad, y, torch.zeros_like(y) + self.pad)

            return y

    def sample(self, x, sample_size=None):
        """
        Draws a number of samples from the model, each sample is a complete sequence.
        We impose a maximum number of steps, to avoid infinite loops.
        This procedure takes care of mapping sampled symbols to pad after the EOS symbol␣
↪is generated.
        """
        if sample_size is None:
            return self._sample(x)
        else:
            samples = [self._sample(x) for _ in range(sample_size)]
            return torch.stack(samples)
```

[54]:
```
def test_autoreg_tagger(training_x, training_y, vocab_x, vocab_y):
    seed_all()
    toy_ar_tagger = AutoregressiveTagger(
        vocab_size=len(vocab_x),
        tagset_size=len(vocab_y),
        word_embed_dim=32,
        tag_embed_dim=16,
        hidden_size=32
```

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```
    )

    assert type(toy_ar_tagger(
        torch.from_numpy(vocab_x.batch_encode(training_x[:2])),
        torch.from_numpy(vocab_y.batch_encode(training_y[:2])))
    ) is td.Categorical

    assert toy_ar_tagger.log_prob(
            torch.from_numpy(vocab_x.batch_encode(training_x[:2])),
            torch.from_numpy(vocab_y.batch_encode(training_y[:2]))
        ).shape == (2,)

    assert loss(toy_ar_tagger,
            torch.from_numpy(vocab_x.batch_encode(training_x[:2])),
            torch.from_numpy(vocab_y.batch_encode(training_y[:2]))
        ).shape == tuple()

    assert toy_ar_tagger.sample(torch.from_numpy(vocab_x.batch_encode(training_x[:2]))).
↪shape == vocab_x.batch_encode(training_x[:2]).shape

    assert toy_ar_tagger.sample(torch.from_numpy(vocab_x.batch_encode(training_x[:2])),␣
↪3).shape == (3,) + vocab_x.batch_encode(training_x[:2]).shape

    assert toy_ar_tagger.greedy(torch.from_numpy(vocab_x.batch_encode(training_x[:2]))).
↪shape == vocab_x.batch_encode(training_x[:2]).shape


test_autoreg_tagger(tagger_training_x, tagger_training_y, word_vocab, tag_vocab)
```

Because labelling is a chain of classification decisions, we can also evaluate our tagger in terms of accuracy of its decisions. For that we need a decision rule. Normally, in NLP, we use the most probable tag sequence as a decision. That is, given a sentence $x_{1:l}$ we search in the space $\{1, \dots, C\}^l$ of all tag sequences of length l, for the one sequence that the model assigns highest probability to (i.e., the *mode* of the conditional distribution):

$$y^\star = \arg \max_{c_{1:l} \in \{1,\dots,C\}^l} \log P(G = c_{1:l} | S = x_{1:l}) \tag{4.52}$$

This search is defined over an extremely large space and is generally not tractable. For some types of tagger, because of their conditional independence assumptions, this search may be doable in polynomial time (as a function of sequence length), for others this is not at all possible.

For the basic tagger, which treats the tags as independent given the sentence, this search can be done exactly, because greedily maximising each step independently is equivalently to maximising the joint assignment of the entire sequence for that model.

Search for the unigram tagger

We search for the best tag in each position, which takes time $\mathcal{O}(C)$ per position,

$$y_i^\star = \arg \max_{c \in \{1,\dots,C\}} \log P(Y_i = c | S = x_{1:l}) \tag{4.53}$$

and put them together in a sequence. The total operation takes time $\mathcal{O}(l \times C)$.

Search for the autoregressive tagger

The autoregressive tagger makes no conditional independence assumptions, and the search problem is genuinely intractable for this model. Being intractable means there is not efficient algorithm known to be able to handle it. In fact, the current hypothesis is that an efficient (by efficient we mean that it runs in polynomial time as a function of l) is actually impossible in standard computer architectures. Problems of this kind are called NP-complete.

For this tutorial, we will again use the greedy approximation:

$$\hat{y}_i = \arg \max_{c \in \{1,\ldots,C\}} \log P(Y_i = c | S = x_{1:l}, H = \hat{y}_1^{i-1}) \tag{4.54}$$

where we solve the argmax locally per position in order from left-to-right. For each step Y_i we condition on the already predicted argmax for all the preceding steps.

Once we have a search algorithm in place to make predictions we can compute accuracy and/or other metrics common for classification.

[55]:
```
class GreedyMode(DecisionRule):

    def __call__(self, model, x):
        return model.greedy(x)
```

On GPU, this should take just about 2 minutes:

[56]:
```
seed_all() # reset random number generators before creating your model and training it

my_device = torch.device('cuda:0')

tagger = BasicTagger(
    vocab_size=len(word_vocab),
    tagset_size=len(tag_vocab),
    word_embed_dim=4,
    hidden_size=8,
).to(my_device)


# construct an Adam optimiser
optimiser = opt.Adam(tagger.parameters(), lr=5e-3)

print("Model")
print(tagger)

# report number of parameters
print(f"Model size: {tagger.num_parameters():,} parameters")

# Train the model
log = train_neural_model(
    tagger, optimiser,
    decision_rule=ExactMode(),
    training_data=TaggedCorpus(tagger_training_x, tagger_training_y, word_vocab, tag_
↪vocab),
    dev_data=TaggedCorpus(tagger_dev_x, tagger_dev_y, word_vocab, tag_vocab),
```

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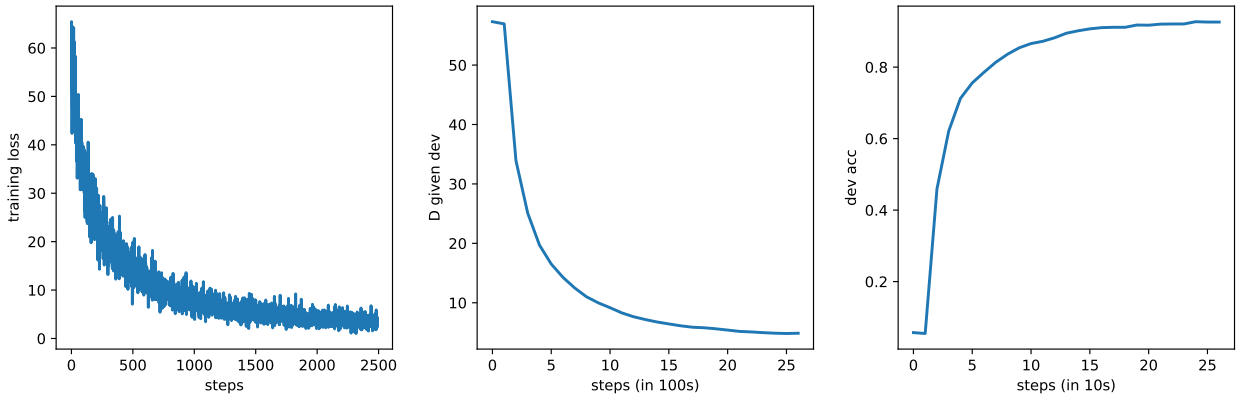
```
    report_fn=report_tagging, report_metrics=['accuracy'],
    batch_size=10, num_epochs=10, check_every=100,
    device=my_device
)

# Plot loss and validation checks
fig, axs = plt.subplots(1, 3, figsize=(12, 4))
_ = axs[0].plot(np.arange(len(log['loss'])), log['loss'])
_ = axs[0].set_xlabel('steps')
_ = axs[0].set_ylabel('training loss')
_ = axs[1].plot(np.arange(len(log['D'])), log['D'])
_ = axs[1].set_xlabel('steps (in 100s)')
_ = axs[1].set_ylabel('D given dev')
_ = axs[2].plot(np.arange(len(log['accuracy'])), log['accuracy'])
_ = axs[2].set_xlabel('steps (in 10s)')
_ = axs[2].set_ylabel('dev acc')
_ = fig.tight_layout(h_pad=2, w_pad=2)
plt.show()
```

```
Model
BasicTagger(
  (encoder): TextEncoder(
    (word_embed): Embedding(3358, 4)
    (encoder): LSTM(4, 8, batch_first=True, bidirectional=True)
  )
  (logits_predictor): Sequential(
    (0): Dropout(p=0, inplace=False)
    (1): Linear(in_features=16, out_features=16, bias=True)
  )
)
Model size: 14,600 parameters
```

```
  0%|          | 0/2490 [00:00<?, ?it/s]
```



[57]:
```
seed_all() # reset random number generators before creating your model and training it

my_device = torch.device('cuda:0')

ar_tagger = AutoregressiveTagger(
```

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```
    vocab_size=len(word_vocab),
    tagset_size=len(tag_vocab),
    word_embed_dim=4,
    tag_embed_dim=4,
    hidden_size=8,
).to(my_device)


# construct an Adam optimiser
optimiser = opt.Adam(ar_tagger.parameters(), lr=5e-3)

print("Model")
print(ar_tagger)

# report number of parameters
print(f"Model size: {ar_tagger.num_parameters():,} parameters")

# Train the model
log = train_neural_model(
    ar_tagger, optimiser,
    decision_rule=GreedyMode(),
    training_data=TaggedCorpus(tagger_training_x, tagger_training_y, word_vocab, tag_
↪vocab),
    dev_data=TaggedCorpus(tagger_dev_x, tagger_dev_y, word_vocab, tag_vocab),
    report_fn=report_tagging, report_metrics=['accuracy'],
    batch_size=10, num_epochs=10, check_every=100,
    device=my_device
)

# Plot loss and validation checks
fig, axs = plt.subplots(1, 3, figsize=(12, 4))
_ = axs[0].plot(np.arange(len(log['loss'])), log['loss'])
_ = axs[0].set_xlabel('steps')
_ = axs[0].set_ylabel('training loss')
_ = axs[1].plot(np.arange(len(log['D'])), log['D'])
_ = axs[1].set_xlabel('steps (in 100s)')
_ = axs[1].set_ylabel('D given dev')
_ = axs[2].plot(np.arange(len(log['accuracy'])), log['accuracy'])
_ = axs[2].set_xlabel('steps (in 10s)')
_ = axs[2].set_ylabel('dev acc')
_ = fig.tight_layout(h_pad=2, w_pad=2)
plt.show()
```

```
Model
AutoregressiveTagger(
  (encoder): TextEncoder(
    (word_embed): Embedding(3358, 4)
    (encoder): LSTM(4, 8, batch_first=True, bidirectional=True)
  )
  (tag_embed): Embedding(16, 4)
  (decoder): LSTM(4, 8, batch_first=True)
  (logits_predictor): Sequential(
```

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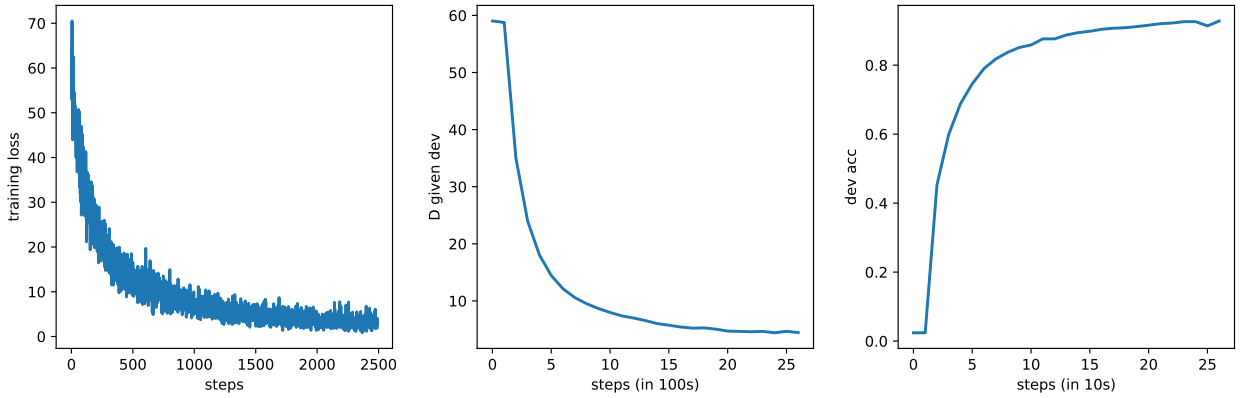
```
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=24, out_features=8, bias=True)
    (2): ReLU()
    (3): Dropout(p=0.0, inplace=False)
    (4): Linear(in_features=8, out_features=16, bias=True)
  )
  (init_state): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=16, out_features=8, bias=True)
    (2): Tanh()
  )
  (init_cell): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=16, out_features=8, bias=True)
    (2): Tanh()
  )
)
Model size: 15,456 parameters
```

```
  0%|          | 0/2490 [00:00<?, ?it/s]
```



[58]:
```
tagger_dev_data = TaggedCorpus(tagger_dev_x, tagger_dev_y, word_vocab, tag_vocab)
tagger_dev_dl = DataLoader(tagger_dev_data, batch_size=1, shuffle=False, collate_
↪fn=tagger_dev_data.pad_to_longest)
for batch_x, batch_y in tagger_dev_dl:
    print("Sample")
    y_out = ar_tagger.sample(batch_x.to(my_device))

    for x, y in zip(word_vocab.batch_decode(batch_x, strip_pad=True), tag_vocab.batch_
↪decode(y_out, strip_pad=False)):
        print(" ".join(f"{w}/{t}" for w, t in zip(x, y)))

    print("\nGreedy")

    y_out = ar_tagger.greedy(batch_x.to(my_device))

    for x, y in zip(word_vocab.batch_decode(batch_x, strip_pad=True), tag_vocab.batch_
↪decode(y_out, strip_pad=False)):
        print(" ".join(f"{w}/{t}" for w, t in zip(x, y)))
```

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```
    break
```

```
Sample
-UNK-/NOUN ,/. a/DET -UNK-/NOUN -UNK-/VERB the/DET -UNK-/NOUN of/ADP -UNK-/ADJ -UNK-/
↪NOUN ,/. is/VERB marketed/VERB *-1/X as/ADP a/DET $/. -UNK-/NUM *u*/X -UNK-/VERB for/
↪ADP -UNK-/ADJ -UNK-/NOUN ./. -EOS-/-EOS-

Greedy
-UNK-/NOUN ,/. a/DET -UNK-/NOUN -UNK-/VERB the/DET -UNK-/NOUN of/ADP -UNK-/ADJ -UNK-/
↪NOUN ,/. is/VERB marketed/VERB *-1/X as/ADP a/DET $/. -UNK-/NUM *u*/X -UNK-/VERB for/
↪ADP -UNK-/NOUN -UNK-/NOUN ./. -EOS-/-EOS-
```

4.43.9 8. Exercise: design your own deep probabilistic model (optional, non-graded)

Now it's time to design your own probabilistic model. The objective is to find a dataset and design a probabilistic model for it, parameterised by a neural network. Be conscious about the distributions you choose to model your data with, make sure they are appropriate for the data! Use maximum likelihood estimation for estimating neural network parameters. Also, be conscious about the decision rule you use. Can you obtain the mode exactly and is it appropriate under your model? Is there perhaps another criterion more sensible? Can you think of a way to use maximisation of expected utility for your model? As we have already provided many helper classes for learning features from text data, we encourage you to look into textual datasets, but note the data you are modelling can still be of any domain: ordinal, real numbers, discrete, structured, etc. Some good places to look for such data are:

- NLTK: https://www.nltk.org/nltk_data/
- HuggingFace: https://huggingface.co/datasets
- Kaggle: https://www.kaggle.com/datasets

Remarks on other types of data:

- some structured data are fixed-dimensional (e.g., an image of size HxWxC), some models are built upon a chain rule factorisation just like the sequence labeller above, but their parameterisation might exploit the fact that the dimensionality is fixed (a good example is a MADE, you can ask Wilker more about those);
- some structured data are made of continuous parts (e.g., a time series in the finance domain, or in medical applications), in those cases your conditional factors are from a numerical family (e.g., Poisson, Normal, Gamma, etc), sometimes you need a distribution more powerful than the typical unimodal exponential family, in those cases you can use a mixture Model (we discuss those in the second module in the series) or a normalising flow (you can ask Wilker more about those, but note that Stratis will discuss NFs along with other advanced generative models)

4.44 DPM2 - Variational inference for deep discrete latent variable models

Filled notebook:
Recordings: Lecture 1.3, Lecture 1.4 & Lecture 1.5
Authors: Wilker Aziz

4.44.1 0. Intended Learning Outcomes

After this tutorial the student should be able to

- parameterise a latent variable model with discrete latent variables
- estimate parameters using exact log-likelihood function (when tractable)
- estimate parameters using neural variational inference

0.1 Setting up

[1]:
```
import torch
import numpy as np
import random
import matplotlib.pyplot as plt
import torch.nn as nn
import torch.nn.functional as F
import torch.distributions as td

from itertools import chain
from collections import defaultdict, OrderedDict
from tqdm.auto import tqdm

from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For having SVG graphics
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0

%matplotlib inline
```

[2]:
```
def seed_all(seed=42):
    np.random.seed(seed)
    random.seed(seed)
    torch.manual_seed(seed)

seed_all()
```

4.44.2 1. Data

We are going to use toy image datasets for this notebook. These are fixed-dimensional observations for which encoder and decoders are relatively easy to design. This way we can focus on the aspects that are probabilistic in nature.

[3]:
```
from torchvision.datasets import FashionMNIST
from torchvision import transforms
from torchvision.transforms import ToTensor
from torch.utils.data import random_split, Dataset
from torch.utils.data.dataloader import DataLoader
from torchvision.utils import make_grid
import torch.optim as opt

DATASET_PATH = "../../data"
my_device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
```

A helper to binarize datasets:

[4]:
```
class Binarizer(Dataset):

    def __init__(self, ds, threshold=0.5):
        self._ds = ds
        self._threshold = threshold

    def __len__(self):
        """Size of the corpus in number of sequence pairs"""
        return len(self._ds)

    def __getitem__(self, idx):
        """
        Return corpus_x[idx] and corpus_y[idx] converted to codes
        the latter has the EOS code in the end
        """
        x, y = self._ds[idx]
        return (x >= self._threshold).float(), y
```

FashionMNIST

[5]:
```
dataset = FashionMNIST(root=DATASET_PATH, train=True, download=True,
                       transform=transforms.Compose([transforms.Resize(64), transforms.
↪ToTensor()]))
```

[6]:
```
img_shape = dataset[0][0].shape
print("Shape of an image:", img_shape)
```

```
Shape of an image: torch.Size([1, 64, 64])
```

Let's make a dev set for ourselves:

[7]:
```
val_size = 1000
train_size = len(dataset) - val_size
train_ds, val_ds = random_split(dataset, [train_size, val_size])
len(train_ds), len(val_ds)
```

[7]:
```
(59000, 1000)
```

we suggest that you binarize the data in a first pass through this notebook, but as you will see, we can also model the continuous pixel intensities.

[8]:
```
bin_data = True
```

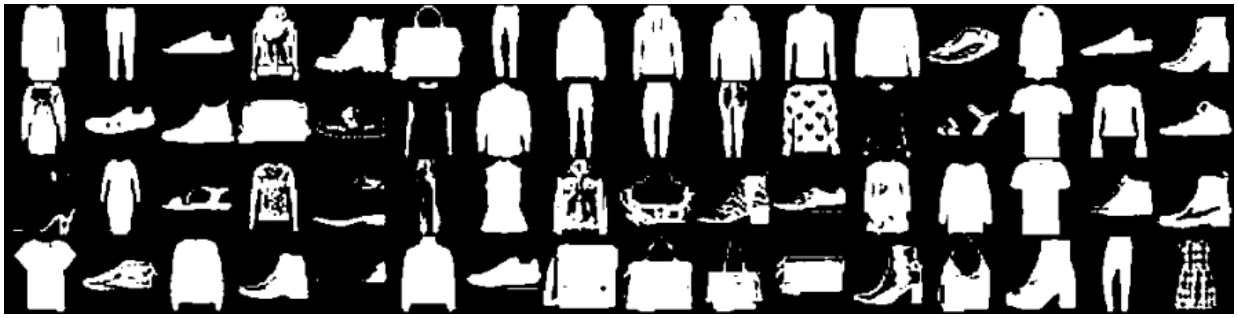
[9]:
```
if bin_data:
    train_ds = Binarizer(train_ds)
    val_ds = Binarizer(val_ds)
```

[10]:
```
batch_size = 64
train_loader = DataLoader(train_ds, batch_size, shuffle=True, num_workers=2, pin_
↪memory=True)
val_loader = DataLoader(val_ds, batch_size, num_workers=2, pin_memory=True)
```

Let's visualise a few samples

[11]:
```
for images, y in train_loader:
    print('images.shape:', images.shape)
    plt.figure(figsize=(16,8))
    plt.axis('off')
    plt.imshow(make_grid(images, nrow=16).permute((1, 2, 0)))
    plt.show()
    break
```

```
images.shape: torch.Size([64, 1, 64, 64])
```



4.44.3 2. Latent variable models

We will be using NNs to parameterise a latent variable model, that is, a joint distribution over a collection of random variables (rvs), some of which are observed, some of which are not.

We are interested in two random variables (rvs):

- a discrete latent code $Z \in \mathcal{Z}$
- and an image $X \in \mathcal{X} \subseteq \mathbb{R}^D$

In this tutorial, x is has a number C of channels, a certain width W and a certain height H, so $\mathcal{X} \subseteq \mathbb{R}^{C \times W \times H}$. Because we have fixed $D = C \times W \times H$, $\mathcal{X}$ is finite-dimensional, but this need not be the case in general (for example, in a different domain, $\mathcal{X}$ could be the unbounded space of all sentences of arbitrary lenght). We may treat the pixel intensities as discrete or continuous, as long as we choose an appropriate pmf/pdf for each case.

In this tutorial we will look into two types of latent code. A categorical code $z \in \{1, \dots, K\}$, and a combinatorial code $z \in \{0, 1\}^K$, in both cases $\mathcal{Z}$ is countably finite, but in general this need not be the case (for example, we could have $z \in \mathbb{N}$ or z be a latent sequence of arbitrary length).

In this tutorial, we specify a joint distribution over $\mathcal{Z} \times \mathcal{X}$ by specifying a joint probability density function (pdf):

$$p_{ZX}(z, x|\theta) = p_Z(z|\theta)p_{X|Z}(x|z, \theta) \tag{4.55}$$

Here θ denotes the parameters of the NNs that parameterise the pmf p_Z and the pdf $p_{X|Z=z}$ (for any given z).

In this tutorial, the prior is fixed, but in general it need not be. We do not have additional predictors to condition on, but in some application domains you may have (e.g., in imagine captioning, we may be interested in a joint for a caption y and a latent code z given an image x; in image generation, we may be interested in a joint distribution for an image x and a latent code z given a caption y).

2.1 Prior networks

We begin by specifying the component that parameterises the prior p_Z.

A prior network is an NN that parameterises a fixed prior distribution for the instances in a batch.

[12]:
```
class PriorNet(nn.Module):
    """
    An NN that parameterises a prior distribution.

    For this lab, our priors are fixed, so this NN's forward pass
     simply returns a fixed prior with a given batch_shape.
    """

    def __init__(self, outcome_shape: tuple):
        """
        outcome_shape: this is the shape of a single outcome
            if you use a single integer k, we will turn it into (k,)
        """
        super().__init__()
        if isinstance(outcome_shape, int):
            outcome_shape = (outcome_shape,)
        self.outcome_shape = outcome_shape

    def forward(self, batch_shape):
        """
        Returns a td object for the batch.
        """
        raise NotImplementedError("Implement me!")
```

Let's implement two priors.

A product of (uniform) Bernoulli distributions

Here the latent code is a K-dimensinoal bit vector, you can think of each coordinate of the code as an attribute of the data point. We use a uniform prior per coordinate:

$$p_Z(z) = \prod_{k=1}^{K} \text{Bernoulli}(z_k|0.5) \tag{4.56}$$

Uniform (one-hot) Categorical distribution

Here the latent code is the a class from a discrete set $\{1, \dots, K\}$, we use a uniform prior over classes:

$$p_Z(z) = \text{Categorical}(z|K^{-1}\mathbf{1}_K) \tag{4.57}$$

where $\mathbf{1}_K$ is the K-dimensional vector of ones.

In practice, we can use the "OneHotCategorical" distribution, which wraps Categorical samples around a call to `onehot(sample, K)`.

[13]:
```
class BernoulliPriorNet(PriorNet):
    """
    For z a D-dimensional bit vector:

        p(z) = prod_d Bernoulli(z[d]|0.5)
    """

    def __init__(self, outcome_shape):
        super().__init__(outcome_shape)
        # the product of Bernoulli priors will have Bernoulli(0.5) factors
        self.register_buffer("logits", torch.zeros(self.outcome_shape, requires_
↪grad=False).detach())

    def forward(self, batch_shape):
        shape = batch_shape + self.outcome_shape
        # we wrap around td.Independent to obtain a pmf over multivariate draws
        # without td.Independent, we would have multiple pmfs, rather than one
        # pmf over a multivariate outcome space
        # td.Independent will interpret the rightmost dimensions as part of
        # the shape of the outcome
        return td.Independent(td.Bernoulli(logits=self.logits.expand(shape)), len(self.
↪outcome_shape))


class CategoricalPriorNet(PriorNet):
    """
    For z the one-hot encoding of a category in a set of K categories:

        p(z) = OneHotCategorical(z|torch.ones(K) / K)
    """

    def __init__(self, outcome_shape):
        super().__init__(outcome_shape)
        self.register_buffer("logits", torch.zeros(self.outcome_shape, requires_
↪grad=False).detach())

    def forward(self, batch_shape):
        shape = batch_shape + self.outcome_shape
        # OneHotCategorical is a wrapper around Categorical,
        # after drawing a Categorical sample, td.OneHotCategorical
        # encodes it using onehot(sample, support_size)
        # Here we do not need td.Independent, because OneHotCategorical
        # is a distribution over a multivariate draw (the one-hot
        # encoding of a category), which is different from the product of
        # Bernoulli prior
        return td.OneHotCategorical(logits=self.logits.expand(shape))
```

[14]:
```
def test_priors(batch_size=3):
    prior_net = BernoulliPriorNet(7)
    print("\nBernoulli")
    print(f" outcome_shape={prior_net.outcome_shape}")
    p = prior_net(batch_shape=(batch_size,))
```

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```
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")

    prior_net = CategoricalPriorNet(7)
    print("\nCategorical")
    print(f" outcome_shape={prior_net.outcome_shape}")
    p = prior_net(batch_shape=(batch_size,))
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")


test_priors()
```

```
Bernoulli
 outcome_shape=(7,)
 distribution: Independent(Bernoulli(logits: torch.Size([3, 7])), 1)
 sample: tensor([[0., 0., 0., 1., 1., 1., 0.],
        [1., 0., 1., 0., 1., 0., 0.],
        [1., 0., 0., 1., 1., 1., 1.]])
 shapes: sample=torch.Size([3, 7]) log_prob=torch.Size([3])

Categorical
 outcome_shape=(7,)
 distribution: OneHotCategorical()
 sample: tensor([[0., 0., 1., 0., 0., 0., 0.],
        [1., 0., 0., 0., 0., 0., 0.],
        [0., 0., 0., 0., 1., 0., 0.]])
 shapes: sample=torch.Size([3, 7]) log_prob=torch.Size([3])
```

2.2 Conditional probability distributions

Next, we create code to parameterise conditional probability distributions (cpds), which we do by having an NN parameterise a choice of pmf/pdf. This will be useful in parameterising the $p_{X|Z=z}$ component of our latent variable models (and, later on, it will also be useful for variational inference, when we develop $q_{Z|X=x}$).

Our general strategy is to map from a number of inputs (which the user will choose) to the parameters of a pmf/pdf support by `torch.distributions`.

[15]:
```
class CPDNet(nn.Module):
    """
    Let L be a choice of distribution
        and x ~ L is an outcome with shape outcome_shape

    This is an NN whose forward method maps from a number of inputs to the
        parameters of L's pmf/pdf and returns a torch.distributions
        object representing L's pmf/pdf.
    """
```

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```
    def __init__(self, outcome_shape):
        """
        outcome_shape: this is the shape of a single outcome
            if you use a single integer k, we will turn it into (k,)
        """
        super().__init__()
        if isinstance(outcome_shape, int):
            outcome_shape = (outcome_shape,)
        self.outcome_shape = outcome_shape

    def forward(self, inputs):
        """
        Return a torch.distribution object predicted from `inputs`.

        inputs: a tensor with shape batch_shape + (num_inputs,)
        """
        raise NotImplementedError("Implemented me")
```

2.2.1 Observational model

The observational model prescribes the distribution of $X|Z=z$.

If we assume our pixel intensities are binary, we can use a product of $C \times W \times H$ Bernoulli distributions, which we parameterise jointly using an NN:

$$p_{X|Z}(x|z,\theta) = \prod_{c=1}^{C}\prod_{w=1}^{W}\prod_{h=1}^{H} \text{Bernoulli}(x_{c,w,h}|f_{c,w,h}(z;\theta)) \tag{4.58}$$

Here $\mathbf{f}(z;\theta) \in (0,1)^C \times (0,1)^W \times (0,1)^H$ is an NN architecture such as a feed-forward net or a stack of transposed convolution layers. In NN literature, such architectures are often called *decoders*.

If we assume our pixel intensities are real values in $[0,1]$ (0 and 1 included), we need to parameterise a pdf. A good choice of pdf is the ContinuousBernoulli distributions, which is a single-parameter distribution (much like the Bernoulli) whose support is the set $[0,1]$.

Let's start by designing $\mathbf{f}$.

A very basic design uses a FFNN:

[16]:
```
class ReshapeLast(nn.Module):
    """
    Helper layer to reshape the rightmost dimension of a tensor.

    This can be used as a component of nn.Sequential.
    """

    def __init__(self, shape: tuple):
        """
        shape: desired rightmost shape
        """
```

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```
        super().__init__()
        self._shape = shape

    def forward(self, input):
        # reshapes the last dimension into self.shape
        return input.reshape(input.shape[:-1] + self._shape)


def build_ffnn_decoder(latent_size, num_channels, width=64, height=64, hidden_size=512,␣
↪p_drop=0.):
    """
    Map the latent code to a tensor with shape [num_channels, width, height]
    using a FFNN with 2 hidden layers.

    latent_size: size of latent code
    num_channels: number of channels in the output
    width: image shape
    height: image shape
    hidden_size: we first map from latent_size to hidden_size and
        then use feed forward NNs to map it to [num_channels, width, height]
    p_drop: dropout rate before linear layers
    """
    decoder = nn.Sequential(
        nn.Dropout(p_drop),
        nn.Linear(latent_size, hidden_size),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(hidden_size, hidden_size),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(hidden_size, num_channels * width * height),
        ReshapeLast((num_channels, width, height)),
    )
    return decoder
```

[17]:
```
# mapping from 10-dimensional latent code
build_ffnn_decoder(latent_size=10, num_channels=1)(torch.zeros((5, 10))).shape
```

[17]:
```
torch.Size([5, 1, 64, 64])
```

[18]:
```
# we can also have a structured batch shape (e.g., [3, 5])
build_ffnn_decoder(latent_size=10, num_channels=1)(torch.zeros((3, 5, 10))).shape
```

[18]:
```
torch.Size([3, 5, 1, 64, 64])
```

The downside is that the output layer is rather large.

An architecture with inductive biases that are more appropriate for our data type is a CNN, in particular, a transposed CNN. Here we design one such decoder:

[19]:
```
class MySequential(nn.Sequential):
    """
    This is a version of nn.Sequential that works with structured batches
```

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```
     (i.e., batches that have multiple dimensions)
    even when some of the nn layers in it does not.

    The idea is to just wrap nn.Sequential around two calls to reshape
     which remove and restore the batch dimensions.
    """

    def __init__(self, *args, event_dims=1):
        super().__init__(*args)
        self._event_dims = event_dims

    def forward(self, input):
        # memorise batch shape
        batch_shape = input.shape[:-self._event_dims]
        # memorise latent shape
        event_shape = input.shape[-self._event_dims:]
        # flatten batch shape and obtain outputs
        output = super().forward(input.reshape( (-1,) + event_shape))
        # restore batch shape
        return output.reshape(batch_shape + output.shape[1:])


def build_cnn_decoder(latent_size, num_channels, width=64, height=64, hidden_size=1024,␣
↪p_drop=0.):
    """
    Map the latent code to a tensor with shape [num_channels, width, height].

    latent_size: size of latent code
    num_channels: number of channels in the output
    width: must be 64 (for now)
    height: must be 64 (for now)
    hidden_size: we first map from latent_size to hidden_size and
        then use transposed 2d convolutions to [num_channels, width, height]
    p_drop: dropout rate before linear layers
    """
    if width != 64:
        raise ValueError("The width is hardcoded")
    if height != 64:
        raise ValueError("The height is hardcoded")

    # TODO: change the architecture so width and height are not hardcoded
    decoder = MySequential(
        nn.Dropout(p_drop),
        nn.Linear(latent_size, hidden_size),
        ReshapeLast((hidden_size, 1, 1)),
        nn.ConvTranspose2d(hidden_size, 128, 5, 2),
        nn.ReLU(),
        nn.ConvTranspose2d(128, 64, 5, 2),
        nn.ReLU(),
        nn.ConvTranspose2d(64, 32, 6, 2),
        nn.ReLU(),
        nn.ConvTranspose2d(32, num_channels, 6, 2),
```

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```
        event_dims=1
    )
    return decoder
```

[20]:
```
# a batch of five 10-dimensional latent codes is transformed
# into a batch of 5 images, each with shape [1,64,64]
build_cnn_decoder(latent_size=10, num_channels=1)(torch.zeros((5, 10))).shape
```

[20]:
```
torch.Size([5, 1, 64, 64])
```

[21]:
```
# note that because we use MySequential,
# we can have a batch of [3, 5] assignments
# (this is useful, for example, when we have multiple draws of the latent
# variable for each of the data points in the batch)
build_cnn_decoder(latent_size=10, num_channels=1)(torch.zeros((3, 5, 10))).shape
```

[21]:
```
torch.Size([3, 5, 1, 64, 64])
```

Now we are in position to design a CPDNet for our image model, it simply combines a choice of decoder with a choice of distribution:

[22]:
```
class BinarizedImageModel(CPDNet):

    def __init__(self, num_channels, width, height, latent_size, decoder_type=build_ffnn_
↪decoder, p_drop=0.):
        super().__init__((num_channels, width, height))
        self.decoder =  decoder_type(
            latent_size=latent_size,
            num_channels=num_channels,
            width=width,
            height=height,
            p_drop=p_drop
        )

    def forward(self, z):
        """
        Return the cpd X|Z=z

        z: batch_shape + (latent_dim,)
        """
        # batch_shape + (num_channels, width, height)
        h = self.decoder(z)
        return td.Independent(td.Bernoulli(logits=h), len(self.outcome_shape))


class ContinuousImageModel(CPDNet):

    def __init__(self, num_channels, width, height, latent_size, decoder_type=build_ffnn_
↪decoder, p_drop=0.):
        super().__init__((num_channels, width, height))
        self.decoder =  decoder_type(
            latent_size=latent_size,
            num_channels=num_channels,
```

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```
            width=width,
            height=height,
            p_drop=p_drop
        )

    def forward(self, z):
        """
        Return the cpd X|Z=z

        z: batch_shape + (latent_dim,)
        """
        # batch_shape + (num_channels, width, height)
        h = self.decoder(z)
        return td.Independent(td.ContinuousBernoulli(logits=h), len(self.outcome_shape))
```

[23]:
```
obs_model = BinarizedImageModel(
    num_channels=img_shape[0],
    width=img_shape[1],
    height=img_shape[2],
    latent_size=10,
    p_drop=0.1,
)
print(obs_model)
# a batch of five zs is mapped to 5 distributions over [1,64,64]-dimensional
# binary tensors
print(obs_model(torch.zeros([5, 10])))
```

```
BinarizedImageModel(
  (decoder): Sequential(
    (0): Dropout(p=0.1, inplace=False)
    (1): Linear(in_features=10, out_features=512, bias=True)
    (2): ReLU()
    (3): Dropout(p=0.1, inplace=False)
    (4): Linear(in_features=512, out_features=512, bias=True)
    (5): ReLU()
    (6): Dropout(p=0.1, inplace=False)
    (7): Linear(in_features=512, out_features=4096, bias=True)
    (8): ReshapeLast()
  )
)
Independent(Bernoulli(logits: torch.Size([5, 1, 64, 64])), 3)
```

We can also use a different decoder

[24]:
```
obs_model = BinarizedImageModel(
    num_channels=img_shape[0],
    width=img_shape[1],
    height=img_shape[2],
    latent_size=10,
    p_drop=0.1,
    decoder_type=build_cnn_decoder
)
```

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```
print(obs_model)
# a batch of five zs is mapped to 5 distributions over [1,64,64]-dimensional
# binary tensors
print(obs_model(torch.zeros([5, 10])))
```

```
BinarizedImageModel(
  (decoder): MySequential(
    (0): Dropout(p=0.1, inplace=False)
    (1): Linear(in_features=10, out_features=1024, bias=True)
    (2): ReshapeLast()
    (3): ConvTranspose2d(1024, 128, kernel_size=(5, 5), stride=(2, 2))
    (4): ReLU()
    (5): ConvTranspose2d(128, 64, kernel_size=(5, 5), stride=(2, 2))
    (6): ReLU()
    (7): ConvTranspose2d(64, 32, kernel_size=(6, 6), stride=(2, 2))
    (8): ReLU()
    (9): ConvTranspose2d(32, 1, kernel_size=(6, 6), stride=(2, 2))
  )
)
Independent(Bernoulli(logits: torch.Size([5, 1, 64, 64])), 3)
```

2.3 Joint distribution

We can now combine a prior and an observational model into a joint distribution. A joint distribution supports a few important operations such as marginal and posterior pdf assessments, as well as sampling from the joint distribution. Marginal and posterior assessments require computations that may or may not be tractable, see below.

From a joint pdf, we can compute the marginal density of x via

$$p_X(x|\theta) = \sum_{z \in \mathcal{Z}} p_{ZX}(z, x|\theta) \tag{4.59}$$

$$= \sum_{z \in \mathcal{Z}} p_Z(z|\theta) p_{X|Z}(x|z, \theta) \tag{4.60}$$

Under the assumption that $\mathcal{Z}$ is countably finite, this can be done via enumeration in time proportional to $\mathcal{O}(|\mathcal{Z}|)$. This marginalisation is therefore intractable for countably infinite $\mathcal{Z}$ or for $\mathcal{Z}$ that is combinatorially large (e.g., the space of K-dimensinoal bit vectors).

Assuming enumeration is tractable, we can also assess the posterior mass of z given x via

$$p_{Z|X}(z|x, \theta) = \frac{p_Z(z|\theta) p_{X|Z}(x|z, \theta)}{p_X(x|\theta)} \tag{4.61}$$

When marginalisation is intractable, we can obtain a naive lowerbound by direct application of Jensen's inequality:

$$\log p_X(x|\theta) = \log \sum_{z \in \mathcal{Z}} p_Z(z|\theta) p_{X|Z}(x|z,\theta) \tag{4.62}$$

$$\overset{\text{JI}}{\geq} \sum_{z \in \mathcal{Z}} p_Z(z|\theta) \log p_{X|Z}(x|z,\theta) \tag{4.63}$$

$$\overset{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^{S} \log p_{X|Z}(x|z_s,\theta) \quad \text{where } z_s \sim p_Z \tag{4.64}$$

A better lowerbound could be obtained via importance sampling, but it would require training an approximating distribution (as we will do in variational inference).

Recall that, given a dataset $\mathcal{D}$, the log-likelihood function $\mathcal{L}(\theta|\mathcal{D}) = \sum_{x \in \mathcal{D}} \log p_X(x|\theta)$ requires performing marginal density assessments. Whenever exact marginalisation is intractable, we are unaible to assess $\mathcal{L}(\theta|\mathcal{D})$ and its gradient with respect to θ. If the prior is fixed, we can use the naive lowerbound to obtain a gradient estimate, but, again, our naive application of JI leads to a generally rather loose bound.

[25]:
```
class JointDistribution(nn.Module):
    """
    A wrapper to combine a prior net and a cpd net into a joint distribution.
    """

    def __init__(self, prior_net: PriorNet, cpd_net: CPDNet):
        """
        prior_net: object to parameterise p_Z
        cpd_net: object to parameterise p_{X|Z=z}
        """
        super().__init__()
        self.prior_net = prior_net
        self.cpd_net = cpd_net

    def prior(self, shape):
        return self.prior_net(shape)

    def obs_model(self, z):
        return self.cpd_net(z)

    def sample(self, shape):
        """
        Return z via prior_net(shape).sample()
            and x via cpd_net(z).sample()
        """
        pz = self.prior_net(shape)
        z = pz.sample()
        px_z = self.cpd_net(z)
        x = px_z.sample()
        return z, x

    def log_prob(self, z, x):
        """
        Assess the log density of the joint outcome.
        """
        batch_shape = z.shape[:-len(self.prior_net.outcome_shape)]
```

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```
        pz = self.prior_net(batch_shape)
        px_z = self.cpd_net(z)
        return pz.log_prob(z) + px_z.log_prob(x)

    def log_marginal(self, x, enumerate_fn):
        """
        Return log marginal density of x.

        enumerate_fn: function that enumerates the support of the prior
            (this is needed for marginalisation p(x) = \int p(z, x) dz)

            This only really makes sense if the support is a
            (small) countably finite set. In such cases, you can use
                enumerate=lambda p: p.enumerate_support()
            which is supported, for example, by Categorical and OneHotCategorical.

            If the support is discrete (eg, bit vectors) you can still dare to
            enumerate it explicitly, but you will need to write cutomised code,
            as torch.distributions will not offer that functionality for you.

            If the support is uncountable, countably infinite, or just large
            anyway, you need approximate tools (such as VI, importance sampling, etc)
        """
        batch_shape = x.shape[:-len(self.cpd_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        log_joint = []
        # (support_size,) + batch_shape
        z = enumerate_fn(pz)
        px_z = self.cpd_net(z)
        # (support_size,) + batch_shape
        log_joint = pz.log_prob(z) + px_z.log_prob(x.unsqueeze(0))
        # batch_shape
        return torch.logsumexp(log_joint, 0)

    def posterior(self, x, enumerate_fn):
        """
        Return the posterior distribution Z|X=x.

        As the code is discrete, we return a discrete distribution over
        the complete space of all possible latent codes. This is done via
        exhaustive enumeration provided by `enumerate_fn`.
        """
        batch_shape = x.shape[:-len(self.cpd_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        # (support_size,) + batch_shape
        z = enumerate_fn(pz)
        px_z = self.cpd_net(z)
        # (support_size,) + batch_shape
        log_joint = pz.log_prob(z) + px_z.log_prob(x.unsqueeze(0))
        # batch_shape + (support_size,)
        log_joint = torch.swapaxes(log_joint, 0, -1)
        return td.Categorical(logits=log_joint)
```

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```
    def naive_lowerbound(self, x, num_samples: int):
        """
        Return an MC lowerbound on log marginal density of x:
            log p(x) >= 1/S \sum_s log p(x|z[s])
                with z[s] ~ p_Z
        """
        batch_shape = x.shape[:-len(self.cpd_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        # (num_samples,) + batch_shape + prior_outcome_shape
        log_probs = []
        # I'm using a for loop, but note that with enough GPU memory
        # one could parallelise this step
        for z in pz.sample((num_samples,)):
            px_z = self.cpd_net(z)
            log_probs.append(px_z.log_prob(x))
        # (num_samples,) + batch_shape
        log_probs = torch.stack(log_probs)
        # batch_shape
        return torch.mean(log_probs, 0)
```

[26]:
```
def test_joint_dist(latent_size=10, data_shape=(1, 64, 64), batch_size=2, hidden_
↪size=32):
    p = JointDistribution(
        prior_net=CategoricalPriorNet(latent_size),
        cpd_net=BinarizedImageModel(
            num_channels=data_shape[0],
            width=data_shape[1],
            height=data_shape[2],
            latent_size=latent_size,
            decoder_type=build_cnn_decoder
        )
    )
    print("Model for binarized data")
    print(p)
    z, x = p.sample((batch_size,))
    print("sampled z")
    print(z)
    print("sampled x")
    print(x)
    enumerate_fn = lambda p: p.enumerate_support()
    print("marginal")
    print(p.log_marginal(x, enumerate_fn))
    print("MC lowerbound")
    print(" 1:", p.naive_lowerbound(x, 10))
    print(" 2:", p.naive_lowerbound(x, 10))
    print("posterior distribution")
    print(p.posterior(x, enumerate_fn).probs)

    print("\n\n")

    p = JointDistribution(
```

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```
        prior_net=CategoricalPriorNet(latent_size),
        cpd_net=ContinuousImageModel(
            num_channels=data_shape[0],
            width=data_shape[1],
            height=data_shape[2],
            latent_size=latent_size,
            decoder_type=build_cnn_decoder
        )
    )
    print("Model for continuous data")
    print(p)
    z, x = p.sample((batch_size,))
    print("sampled z")
    print(z)
    print("sampled x")
    print(x)
    enumerate_fn = lambda p: p.enumerate_support()
    print("marginal")
    print(p.log_marginal(x, enumerate_fn))
    print("MC lowerbound")
    print(" 1:", p.naive_lowerbound(x, 10))
    print(" 2:", p.naive_lowerbound(x, 10))
    print("posterior distribution")
    print(p.posterior(x, enumerate_fn).probs)

test_joint_dist(10)
```

```
Model for binarized data
JointDistribution(
  (prior_net): CategoricalPriorNet()
  (cpd_net): BinarizedImageModel(
    (decoder): MySequential(
      (0): Dropout(p=0.0, inplace=False)
      (1): Linear(in_features=10, out_features=1024, bias=True)
      (2): ReshapeLast()
      (3): ConvTranspose2d(1024, 128, kernel_size=(5, 5), stride=(2, 2))
      (4): ReLU()
      (5): ConvTranspose2d(128, 64, kernel_size=(5, 5), stride=(2, 2))
      (6): ReLU()
      (7): ConvTranspose2d(64, 32, kernel_size=(6, 6), stride=(2, 2))
      (8): ReLU()
      (9): ConvTranspose2d(32, 1, kernel_size=(6, 6), stride=(2, 2))
    )
  )
)
sampled z
tensor([[0., 0., 0., 0., 0., 1., 0., 0., 0., 0.],
        [0., 0., 0., 1., 0., 0., 0., 0., 0., 0.]])
sampled x
tensor([[[[0., 0., 1.,  ..., 0., 1., 1.],
          [1., 0., 1.,  ..., 1., 0., 0.],
          [0., 1., 1.,  ..., 0., 1., 0.],
```

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```
          ...,
          [1., 1., 0.,  ..., 1., 1., 0.],
          [0., 0., 1.,  ..., 0., 0., 1.],
          [1., 0., 1.,  ..., 1., 0., 0.]]],


        [[[0., 0., 0.,  ..., 1., 1., 1.],
          [1., 0., 1.,  ..., 0., 0., 1.],
          [0., 1., 1.,  ..., 1., 1., 0.],
          ...,
          [0., 0., 0.,  ..., 1., 1., 1.],
          [1., 0., 0.,  ..., 0., 0., 0.],
          [1., 0., 1.,  ..., 1., 0., 0.]]]])
marginal
tensor([-2833.0503, -2840.0588], grad_fn=<LogsumexpBackward0>)
MC lowerbound
 1: tensor([-2833.0542, -2840.0547], grad_fn=<MeanBackward1>)
 2: tensor([-2833.0972, -2840.0427], grad_fn=<MeanBackward1>)
posterior distribution
tensor([[0.0848, 0.1013, 0.1000, 0.1056, 0.0816, 0.0984, 0.1063, 0.1045, 0.1015,
         0.1161],
        [0.0965, 0.1006, 0.0892, 0.0886, 0.1072, 0.1042, 0.1156, 0.1104, 0.1010,
         0.0867]], grad_fn=<SoftmaxBackward0>)



Model for continuous data
JointDistribution(
  (prior_net): CategoricalPriorNet()
  (cpd_net): ContinuousImageModel(
    (decoder): MySequential(
      (0): Dropout(p=0.0, inplace=False)
      (1): Linear(in_features=10, out_features=1024, bias=True)
      (2): ReshapeLast()
      (3): ConvTranspose2d(1024, 128, kernel_size=(5, 5), stride=(2, 2))
      (4): ReLU()
      (5): ConvTranspose2d(128, 64, kernel_size=(5, 5), stride=(2, 2))
      (6): ReLU()
      (7): ConvTranspose2d(64, 32, kernel_size=(6, 6), stride=(2, 2))
      (8): ReLU()
      (9): ConvTranspose2d(32, 1, kernel_size=(6, 6), stride=(2, 2))
    )
  )
)
sampled z
tensor([[0., 0., 0., 0., 1., 0., 0., 0., 0., 0.],
        [0., 0., 0., 0., 1., 0., 0., 0., 0., 0.]])
sampled x
tensor([[[[0.0177, 0.4419, 0.8944,  ..., 0.1530, 0.0298, 0.2958],
          [0.3006, 0.2818, 0.9756,  ..., 0.3906, 0.3666, 0.5736],
          [0.5353, 0.1523, 0.1889,  ..., 0.1321, 0.3172, 0.1197],
          ...,
```

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```
          [0.5384, 0.4939, 0.3950,  ..., 0.1797, 0.4078, 0.8856],
          [0.8161, 0.1738, 0.2747,  ..., 0.3477, 0.0262, 0.0069],
          [0.5498, 0.7573, 0.8136,  ..., 0.1438, 0.7143, 0.1651]]],


        [[[0.3061, 0.7684, 0.9373,  ..., 0.3133, 0.9556, 0.9470],
          [0.6662, 0.7195, 0.2499,  ..., 0.1698, 0.7220, 0.4024],
          [0.9018, 0.6794, 0.7495,  ..., 0.5036, 0.7543, 0.2213],
          ...,
          [0.9679, 0.9352, 0.9314,  ..., 0.1054, 0.8021, 0.6079],
          [0.4803, 0.2586, 0.0312,  ..., 0.7962, 0.8062, 0.9996],
          [0.2138, 0.5723, 0.5005,  ..., 0.7090, 0.4256, 0.8469]]]])
marginal
tensor([2.4405, 1.3252], grad_fn=<LogsumexpBackward0>)
MC lowerbound
 1: tensor([2.4240, 1.3365], grad_fn=<MeanBackward1>)
 2: tensor([2.4259, 1.3594], grad_fn=<MeanBackward1>)
posterior distribution
tensor([[0.1080, 0.1020, 0.0954, 0.1017, 0.0990, 0.1036, 0.0978, 0.0957, 0.0963,
         0.1006],
        [0.0995, 0.1146, 0.0970, 0.1074, 0.1070, 0.0973, 0.0960, 0.0972, 0.0957,
         0.0882]], grad_fn=<SoftmaxBackward0>)
```

4.44.4 3. Learning

We estimate θ using stochastic gradient-based maximum likelihood estimation. For a tractable model, we can assess the log-likelihood function

$$\mathcal{L}(\theta|\mathcal{D}) = \sum_{x \in \mathcal{D}} \log p_X(x|\theta) \tag{4.65}$$

and estimate $\nabla_\theta \mathcal{L}(\theta|\mathcal{D})$ using random mini-batches:

$$\nabla_\theta \mathcal{L}(\theta|\mathcal{D}) \overset{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^{S} \nabla_\theta \log p_X(x^{(s)}|\theta) \tag{4.66}$$

$$\text{where } x^{(s)} \sim \mathcal{D} \tag{4.67}$$

3.1 Tractable LVMs

A mixture model with K components is in principle a tractable LVM:

$$p_X(x|\theta) = \sum_{z=1}^{K} \frac{1}{K} p_{X|Z}(x|z,\theta) \tag{4.68}$$

For $p_{X|Z=z}$ we use the image model above, which conditions on the one-hot encoding of z.

[27]:
```
print(JointDistribution(
    prior_net=CategoricalPriorNet(10),
    cpd_net=BinarizedImageModel(
        num_channels=img_shape[0],
        width=img_shape[1],
        height=img_shape[2],
        latent_size=10,
        decoder_type=build_ffnn_decoder
    )
))
```

```
JointDistribution(
  (prior_net): CategoricalPriorNet()
  (cpd_net): BinarizedImageModel(
    (decoder): Sequential(
      (0): Dropout(p=0.0, inplace=False)
      (1): Linear(in_features=10, out_features=512, bias=True)
      (2): ReLU()
      (3): Dropout(p=0.0, inplace=False)
      (4): Linear(in_features=512, out_features=512, bias=True)
      (5): ReLU()
      (6): Dropout(p=0.0, inplace=False)
      (7): Linear(in_features=512, out_features=4096, bias=True)
      (8): ReshapeLast()
    )
  )
)
```

3.2 Training algorithm

Here we have some helper code to assess and train an LVM using its exact log-likelihood function.

[28]:
```
def assess_exact(model: JointDistribution, enumerate_fn, dl, device):
    """
    Wrapper for estimating the model's log-likelihood.
    As data samples, we use all data points in a data loader.

    model: a joint distribution for which Z can be exactly marginalised
    enumerate_fn: algorithm to enumerate the support of Z for a batch
        this will be used to assess `model.log_prob(batch, enumerate_fn)`
    dl: torch data loader
    device: torch device
    """
    L = 0
    data_size = 0
    with torch.no_grad():
        for batch_x, batch_y in dl:
            L = L + model.log_marginal(batch_x.to(device), enumerate_fn).sum(0)
            data_size += batch_x.shape[0]
    L = L / data_size
    return L
```

[29]:
```
def train_exact(model: JointDistribution, enumerate_fn, optimiser,
    training_data, dev_data,
    batch_size=64, num_epochs=10, check_every=10,
    grad_clip=5.,
    report_metrics=['L'],
    num_workers=2,
    device=torch.device('cuda:0')
    ):
    """
    model: a joint distribution where Z can be exactly marginalised
    enumerate_fn: function to enumerate the support of Z
        (used in combintation with model.log_prob)
    optimiser: pytorch optimiser
    training_corpus: a torchvision corpus for training
    dev_corpus: a torchvision corpus for validation
    batch_size: use more if you have more memory
    num_epochs: use more for improved convergence
    check_every: use less to check performance on dev set more often
    device: where we run the experiment

    Return a log of quantities computed during training (for plotting)
    """
    batcher = DataLoader(training_data, batch_size, shuffle=True, num_workers=num_
↪workers, pin_memory=True)
    dev_batcher = DataLoader(dev_data, batch_size, num_workers=num_workers, pin_
↪memory=True)

    total_steps = num_epochs * len(batcher)
    log = defaultdict(list)

    step = 0
    model.eval()

    log['dev.L'].append((step, assess_exact(model, enumerate_fn, dev_batcher,␣
↪device=device).item()))


    with tqdm(range(total_steps)) as bar:
        for epoch in range(num_epochs):
            for batch_x, batch_y in batcher:
                model.train()
                optimiser.zero_grad()

                loss = - model.log_marginal(
                    batch_x.to(device),
                    enumerate_fn
                ).mean(0)
                log['loss'].append((step, loss.item()))

                loss.backward()

                nn.utils.clip_grad_norm_(
                    model.parameters(),
```

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```
                    grad_clip
                )
                optimiser.step()


                bar_dict = OrderedDict()
                bar_dict['loss'] = f"{loss.item():.2f}"
                bar_dict[f"dev.L"] =  "{:.2f}".format(log[f"dev.L"][-1][1])
                bar.set_postfix(bar_dict)
                bar.update()

                if step % check_every == 0:
                    model.eval()
                    log['dev.L'].append((step, assess_exact(model, enumerate_fn, dev_
↪batcher, device=device).item()))

                step += 1

    model.eval()
    log['dev.L'].append((step, assess_exact(model, enumerate_fn, dev_batcher,␣
↪device=device).item()))

    return log
```

Here's some helper code to inspect samples from a mixture model

[30]:
```
def inspect_mixture_model(model: JointDistribution, support_size):
    # Display some samples from the prior
    _, x_ = model.sample((support_size, 5))
    x_ = x_.cpu().reshape(-1, 1, 64, 64)
    plt.figure(figsize=(12,6))
    plt.axis('off')
    plt.imshow(make_grid(x_, nrow=support_size).permute((1, 2, 0)))
    plt.title("Prior samples")
    plt.show()

    # Display samples from each of the 10 components
    # [support_size, latent_dim]
    support = model.prior(tuple()).enumerate_support()
    # [support_size, 1, 64, 64]
    x_ = model.obs_model(support).sample((5,)).cpu().reshape(-1, 1, 64, 64)
    plt.figure(figsize=(12,6))
    plt.axis('off')
    plt.imshow(make_grid(x_, nrow=support_size).permute((1, 2, 0)))
    plt.title("Component samples")
    plt.show()
```

3.2.1 Experiment

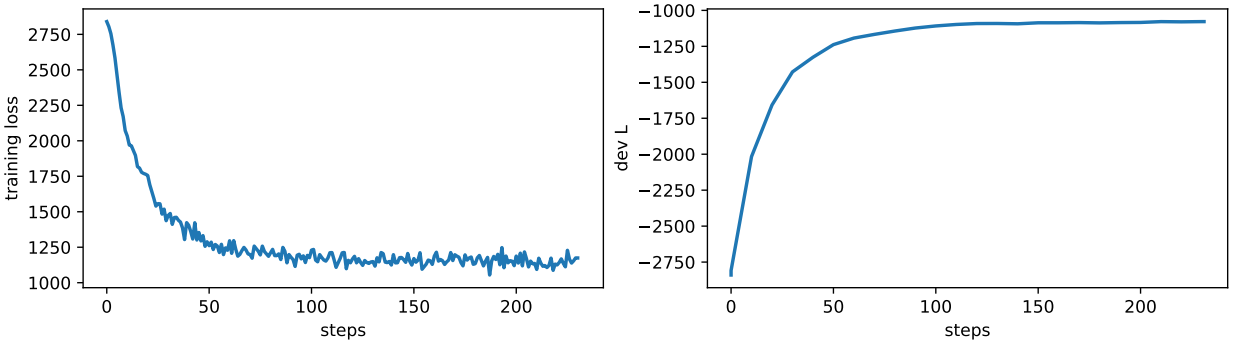
[31]:
```
seed_all()

mixture_model = JointDistribution(
    prior_net=CategoricalPriorNet(10),
    cpd_net=BinarizedImageModel(  # could also be continuous (but then change the␣
↪preprocessing in the beginning)
        num_channels=img_shape[0],
        width=img_shape[1],
        height=img_shape[2],
        latent_size=10,
        decoder_type=build_ffnn_decoder, # could also be CNN (but consider less latent␣
↪classes, as the transposed CNN decoder is a bit too slow for exact enumeration)
        p_drop=0.1,
    )
).to(my_device)

print(mixture_model)

mm_optim = opt.Adam(mixture_model.parameters(), lr=1e-3, weight_decay=1e-6)
```

```
JointDistribution(
  (prior_net): CategoricalPriorNet()
  (cpd_net): BinarizedImageModel(
    (decoder): Sequential(
      (0): Dropout(p=0.1, inplace=False)
      (1): Linear(in_features=10, out_features=512, bias=True)
      (2): ReLU()
      (3): Dropout(p=0.1, inplace=False)
      (4): Linear(in_features=512, out_features=512, bias=True)
      (5): ReLU()
      (6): Dropout(p=0.1, inplace=False)
      (7): Linear(in_features=512, out_features=4096, bias=True)
      (8): ReshapeLast()
    )
  )
)
```

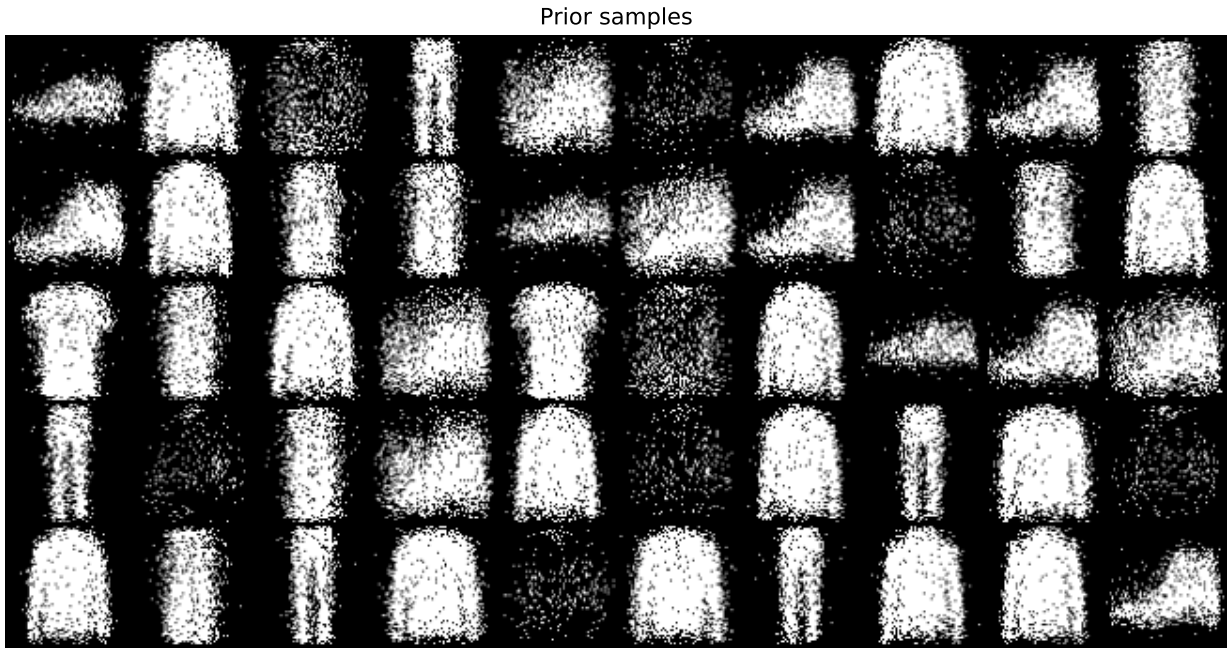
[32]:
```
log = train_exact(
    model=mixture_model,
    optimiser=mm_optim,
    enumerate_fn=lambda p: p.enumerate_support(),
    training_data=train_ds,
    dev_data=val_ds,
    batch_size=256,
    num_epochs=1,  # use more for a better model
    check_every=10,
    grad_clip=5.,
    device=my_device
)
```

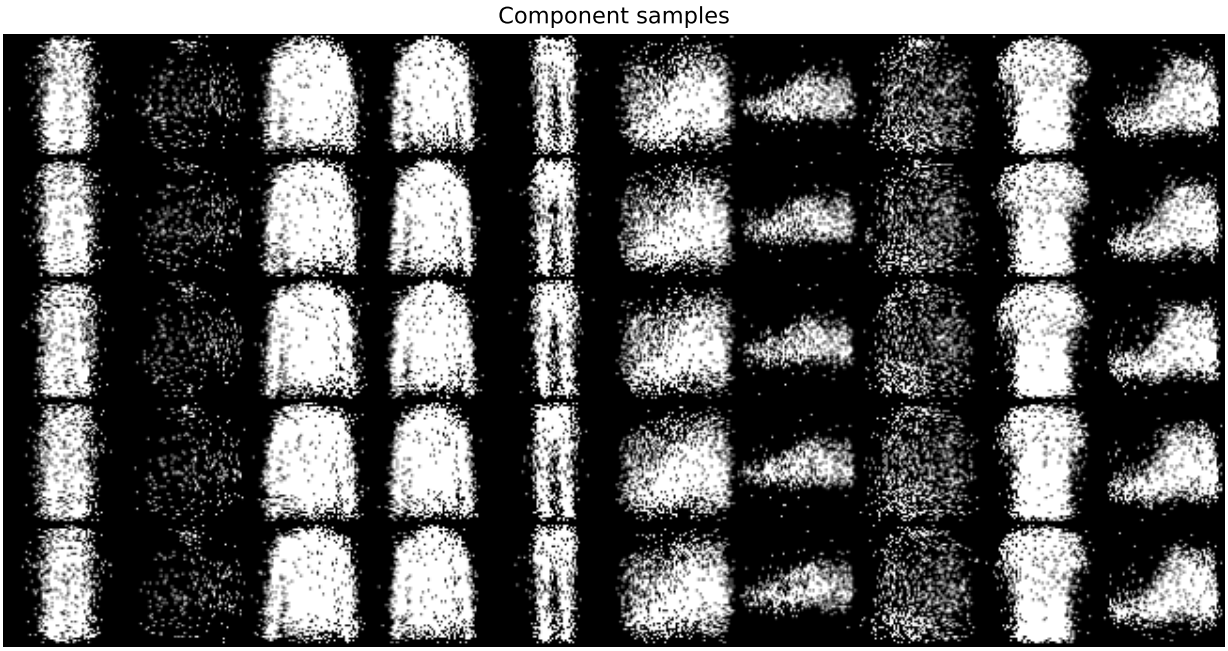
```
  0%|          | 0/231 [00:00<?, ?it/s]
```

[33]:
```
fig, axs = plt.subplots(1, 2, sharex=True, sharey=False, figsize=(12, 3))

_ = axs[0].plot(np.array(log['loss'])[:,0], np.array(log['loss'])[:,1])
_ = axs[0].set_ylabel("training loss")
_ = axs[0].set_xlabel("steps")

_ = axs[1].plot(np.array(log['dev.L'])[:,0], np.array(log['dev.L'])[:,1])
_ = axs[1].set_ylabel("dev L")
_ = axs[1].set_xlabel("steps")
```



[34]:
```
inspect_mixture_model(mixture_model, 10)
```





A mixture model offers very limited capacity to the observational model, it can at best partition the data space into K groups.

A factor model instead offers up 2^K codes to the observational model, next we will design a factor model.

3.3 Intractable LVMs

When marginalisation is intractable (e.g., $\mathcal{Z} = \{0,1\}^K$ for moderate K) or just plain incovenient (e.g., $\mathcal{Z} = \{1,\dots,K\}$ for large K, e.g., $K > 10$), we resort to variational inference introducing a parametric approximation $q_{Z|X=x}$ to the model's true posterior distribution $p_{Z|X=x}$ and estimate both the approximation and the joint distribution by maximising the evidence lowerbound (ELBO), show below for a single observation x:

$$\mathcal{E}(\lambda,\theta|\mathcal{D}) = \mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}\left[\log \frac{p_{ZX}(z,x|\theta)}{q_{Z|X}(z|x,\lambda)}\right]\right] \tag{4.69}$$

$$= \underbrace{\mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}[\log p_{ZX}(x|z,\theta)]\right]}_{-D} - \underbrace{\mathbb{E}_{x\sim\mathcal{D}}\left[\mathrm{KL}(q_{Z|X=x}||p_Z)\right]}_{R} \tag{4.70}$$

where the inner expectation is taken with respect to $q_{Z|X}(z|x,\lambda)$.

When computed in expectation under the data distribution, the two components of the ELBO, namely, the expected log-likelihood $\mathbb{E}[\log p_{ZX}(x|z,\theta)]$ and the "KL term" $\mathrm{KL}(q_{Z|X=x}||p_Z)$, are related to two information-theoretic quantities known as *distortion* and *rate*.

We choose our approximation to be such that: its support is embeded in the support of the prior, it is simple enough to sample from, and it is simple enough to assess the mass of a sample. If possible, we choose it such that other quantities are also tractable (e.g., entropy, relative entropy).

For a multivariate z, we normally choose a factorised family, for example, if z is a D-dimensional bit vector:

$$q_{Z|X}(z|x,\lambda) = \prod_{k=1}^{K} \text{Bernoulli}(z_k|g_k(x;\lambda)) \tag{4.71}$$

with $\mathbf{g}(x;\lambda) \in (0,1)^K$. This is called a *mean field assumption*.

For a Categorical z, the marginalisation is tractable in principle (it takes time linear in the number K of possible assignments), but for certain decoders, even K forward passes might be too much, so we use an independently parameterised Categorical distribution:

$$q_{Z|X}(z|x,\lambda) = \text{Categorical}(z|\mathbf{g}(x;\lambda)) \tag{4.72}$$

with $\mathbf{g}(x;\lambda) \in \Delta_{K-1}$.

3.4 Inference model

The inference model is a conditional model of the latent variable, for which we design CPD nets.

Before we go on, it is useful to design an "encoder" a function that maps an image $x \in \mathcal{X}$ to a fixed-size vector that we can use as a compact representation of x. Next, we design one such encoder employing FFNNs and another employing CNNs.

[35]:
```
class FlattenImage(nn.Module):
    def forward(self, input):
        return input.reshape(input.shape[:-3] + (-1,))

def build_ffnn_encoder(num_channels, width=64, height=64, output_size=1024, p_drop=0.):
    encoder = nn.Sequential(
        FlattenImage(),
        nn.Dropout(p_drop),
        nn.Linear(num_channels * width * height, output_size//2),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(output_size//2, output_size//2),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(output_size//2, output_size),
    )
    return encoder

def build_cnn_encoder(num_channels, width=64, height=64, output_size=1024, p_drop=0.):
    if width != 64:
        raise ValueError("The width is hardcoded")
    if height != 64:
        raise ValueError("The height is hardcoded")
    if output_size != 1024:
        raise ValueError("The output_size is hardcoded")
    # TODO: change the architecture so width, height and output_size are not hardcoded
    encoder = MySequential(
        nn.Conv2d(num_channels, 32, 4, 2),
        nn.LeakyReLU(0.2),
```

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```
        nn.Conv2d(32, 64, 4, 2),
        nn.LeakyReLU(0.2),
        nn.Conv2d(64, 128, 4, 2),
        nn.LeakyReLU(0.2),
        nn.Conv2d(128, 256, 4, 2),
        nn.LeakyReLU(0.2),
        FlattenImage(),
        event_dims=3
    )
    return encoder
```

[36]:
```
# a batch of five [1, 64, 64]-dimensional images is encoded into
# five 1024-dimensional vectors
build_ffnn_encoder(num_channels=1)(torch.zeros((5, 1, 64, 64))).shape
```

[36]:
```
torch.Size([5, 1024])
```

[37]:
```
# and, again, we can have structured batches
# (here trying with (3,5))
build_ffnn_encoder(num_channels=1)(torch.zeros((3, 5, 1, 64, 64))).shape
```

[37]:
```
torch.Size([3, 5, 1024])
```

[38]:
```
# a batch of five [1, 64, 64]-dimensional images is encoded into
# five 1024-dimensional vectors
build_cnn_encoder(num_channels=1)(torch.zeros((5, 1, 64, 64))).shape
```

[38]:
```
torch.Size([5, 1024])
```

[39]:
```
# and, again, since we use MySequential we can have structured batches
# (here trying with (3,5))
build_cnn_encoder(num_channels=1)(torch.zeros((3, 5, 1, 64, 64))).shape
```

[39]:
```
torch.Size([3, 5, 1024])
```

We can now design some CPD nets, assuming they map from an encoding of an image to a pmf over $\mathcal{Z}$.

Product of Bernoullis

This can be used to parameterise a cpd over binary vectors of fixed dimensionality.

OneHotCategorical

This can be used to parameterise a cpd over the one-hot encoding of categories from a finite set.

[40]:
```
class BernoulliCPDNet(CPDNet):
    """
    Output distribution is a product of Bernoulli distributions
    """

    def __init__(self, outcome_shape, num_inputs: int, hidden_size: int=None, p_drop:␣
↪float=0.):
        """
        outcome_shape: shape of the outcome (int or tuple)
            if int, we turn it into a singleton tuple
```

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```
        num_inputs: rightmost dimensionality of the inputs to forward
        hidden_size: size of hidden layers for the CPDNet (use None to skip)
        p_drop: configure dropout before every Linear layer
        """
        super().__init__(outcome_shape)
        num_outputs = np.prod(self.outcome_shape)

        if hidden_size:
            self.encoder = nn.Sequential(
                nn.Dropout(p_drop),
                nn.Linear(num_inputs, hidden_size),
                nn.ReLU()
            )
        else:
            self.encoder = nn.Identity()
            hidden_size = num_inputs

        self.logits = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_outputs),
            ReshapeLast(self.outcome_shape)
        )

    def forward(self, inputs):
        h = self.encoder(inputs)
        return td.Independent(td.Bernoulli(logits=self.logits(h)), len(self.outcome_
↪shape))


class CategoricalCPDNet(CPDNet):
    """
    Output distribution is a product of Bernoulli distributions
    """

    def __init__(self, outcome_shape, num_inputs: int, hidden_size: int=None, p_drop:␣
↪float=0.):
        """
        outcome_shape: shape of the outcome (int or tuple)
            if int, we turn it into a singleton tuple
        num_inputs: rightmost dimensionality of the inputs to forward
        hidden_size: size of hidden layers for the CPDNet (use None to skip)
        p_drop: configure dropout before every Linear layer
        """
        super().__init__(outcome_shape)
        num_outputs = np.prod(self.outcome_shape)

        if hidden_size:
            self.encoder = nn.Sequential(
                nn.Dropout(p_drop),
                nn.Linear(num_inputs, hidden_size),
                nn.ReLU()
            )
```

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```
        else:
            self.encoder = nn.Identity()
            hidden_size = num_inputs

        self.logits = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_outputs),
            ReshapeLast(self.outcome_shape)
        )

    def forward(self, inputs):
        h = self.encoder(inputs)
        return td.OneHotCategorical(logits=self.logits(h))
```

[41]:
```
def test_cpds(outcome_shape, batch_size=3, input_dim=5, hidden_size=2):

    cpd_net = BernoulliCPDNet(outcome_shape, num_inputs=input_dim, hidden_size=hidden_
↪size)
    print("\nBernoulli")
    print(cpd_net)
    print(f" outcome_shape={cpd_net.outcome_shape}")
    inputs = torch.from_numpy(np.random.uniform(size=(batch_size, input_dim))).float()
    print(f" shape of inputs: {inputs.shape}")
    p = cpd_net(inputs)
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")


# Try a few
test_cpds(12)
test_cpds(12, hidden_size=None)
test_cpds((4, 5))
```

```
Bernoulli
BernoulliCPDNet(
  (encoder): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=5, out_features=2, bias=True)
    (2): ReLU()
  )
  (logits): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=12, bias=True)
    (2): ReshapeLast()
  )
)
 outcome_shape=(12,)
 shape of inputs: torch.Size([3, 5])
 distribution: Independent(Bernoulli(logits: torch.Size([3, 12])), 1)
```

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```
 sample: tensor([[1., 0., 1., 1., 1., 0., 1., 1., 1., 0., 1., 1.],
        [0., 1., 1., 0., 0., 1., 1., 1., 0., 0., 1., 0.],
        [1., 0., 0., 0., 1., 1., 1., 0., 0., 0., 0., 0.]])
 shapes: sample=torch.Size([3, 12]) log_prob=torch.Size([3])

Bernoulli
BernoulliCPDNet(
  (encoder): Identity()
  (logits): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=5, out_features=12, bias=True)
    (2): ReshapeLast()
  )
)
 outcome_shape=(12,)
 shape of inputs: torch.Size([3, 5])
 distribution: Independent(Bernoulli(logits: torch.Size([3, 12])), 1)
 sample: tensor([[0., 0., 0., 0., 0., 0., 1., 1., 0., 0., 0., 1.],
        [0., 0., 0., 1., 1., 1., 0., 0., 1., 1., 0., 1.],
        [1., 0., 0., 0., 0., 1., 0., 0., 1., 0., 1., 0.]])
 shapes: sample=torch.Size([3, 12]) log_prob=torch.Size([3])

Bernoulli
BernoulliCPDNet(
  (encoder): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=5, out_features=2, bias=True)
    (2): ReLU()
  )
  (logits): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=20, bias=True)
    (2): ReshapeLast()
  )
)
 outcome_shape=(4, 5)
 shape of inputs: torch.Size([3, 5])
 distribution: Independent(Bernoulli(logits: torch.Size([3, 4, 5])), 2)
 sample: tensor([[[1., 1., 0., 0., 1.],
         [0., 1., 1., 0., 0.],
         [0., 0., 0., 1., 1.],
         [1., 1., 1., 1., 1.]],

        [[1., 1., 0., 0., 0.],
         [0., 1., 1., 0., 1.],
         [0., 0., 1., 0., 1.],
         [1., 0., 0., 0., 1.]],

        [[1., 1., 1., 0., 1.],
         [0., 0., 0., 1., 0.],
         [1., 0., 1., 1., 1.],
         [1., 0., 0., 1., 0.]]])
```

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```
shapes: sample=torch.Size([3, 4, 5]) log_prob=torch.Size([3])
```

Last, but certainly not least, we can combine our encoder and a choice of CPD net.

[42]:
```
class InferenceModel(CPDNet):

    def __init__(
        self, cpd_net_type,
        latent_size, num_channels=1, width=64, height=64,
        hidden_size=1024, p_drop=0.,
        encoder_type=build_ffnn_encoder):

        super().__init__(latent_size)

        self.latent_size = latent_size
        # encodes an image to a hidden_size-dimensional vector
        self.encoder = encoder_type(
            num_channels=num_channels,
            width=width,
            height=height,
            output_size=hidden_size,
            p_drop=p_drop
        )
        # maps from a hidden_size-dimensional encoding
        # to a cpd for Z|X=x
        self.cpd_net = cpd_net_type(
             latent_size,
             num_inputs=hidden_size,
             hidden_size=2*latent_size,
             p_drop=p_drop
        )

    def forward(self, x):
        h = self.encoder(x)
        return self.cpd_net(h)
```

[43]:
```
InferenceModel(BernoulliCPDNet, latent_size=10)(torch.zeros(5, 1, 64, 64))
```

[43]:
```
Independent(Bernoulli(logits: torch.Size([5, 10])), 1)
```

We now have everything in place to use variational inference.

3.5 Neural Variational Inference

We will train our generative model via variational inference, for which we need to train an inference model along with it. We will se the ELBO objective, and gradient estimator based on score function estimation.

It's common to refer to any one such model as a variational auto-encoder (VAE), even though the original VAE was a very different generative model and employed a different gradient estimator.

Given a data point x, we estimate the gradient of the ELBO with respect to λ by MC estimating the following expression:

$$\nabla_\lambda \mathcal{E}(\lambda, \theta|x) = \mathbb{E}\left[r(z, x; \theta, \lambda)\nabla_\lambda \log \frac{p_{ZX}(z, x|\theta)}{q_{Z|X}(z|x, \lambda)}\right] \tag{4.73}$$

where the "reward" function is

$$r(z, x; \theta, \lambda) = \log p_{X|Z}(x|z, \theta) \tag{4.74}$$

And, because this gradient estimator is rather noisy, it's commong to transform the reward function by further employing control variates. The simplest control variates are functions of x and possibly of θ and λ, but not a function of the action z with respect to which we evaluate the reward function. We will implement those as wrappers around the reward function. So, let's start by agreeing on the API of our control variates.

[44]:
```
class VarianceReduction(nn.Module):
    """
    We will be using simple forms of control variates for variance reduction.
    These are transformations of the reward that are independent of the sampled
    latent variable, but they can, in principle, depend on x, and on the
    parameters of the generative and inference model.

    Some of these are trainable components, thus they also contribute to the loss.
    """

    def __init__(self):
        super().__init__()

    def forward(self, r, x, q, r_fn):
        """
        Return the transformed reward and a contribution to the loss.

        r: a batch of rewards
        x: a batch of observations
        q: policy
        r_fn: reward function
        """
        return r, torch.zeros_like(r)
```

Now we can work on our general NVIL model. The following class implements the NVIL objective as well as a lot of helper code to manipulate the model components in interesting ways (e.g., sampling, sampling conditionally, estimating marginal density, etc.)

[45]:
```
class NVIL(nn.Module):
    """
    A generative model p(z)p(x|z) and an approximation q(z|x) to that
     model's true posterior.

    The approximation is estimated to maximise the ELBO, and so is the joint
     distribution.
    """

    def __init__(self, gen_model: JointDistribution, inf_model: InferenceModel, cv_model:
↪ VarianceReduction):
```

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```
        """
        gen_model: p(z)p(x|z)
        inf_model: q(z|x) which approximates p(z|x)
        cv_model: optional transformations of the reward
        """
        super().__init__()
        self.gen_model = gen_model
        self.inf_model = inf_model
        self.cv_model = cv_model

    def gen_params(self):
        return self.gen_model.parameters()

    def inf_params(self):
        return self.inf_model.parameters()

    def cv_params(self):
        return self.cv_model.parameters()

    def sample(self, batch_size, sample_size=None, oversample=False):
        """
        A sample from the joint distribution:
            z ~ prior
            x|z ~ obs model
        batch_size: number of samples in a batch
        sample_size: if None, the output tensor has shape [batch_size] + data_shape
            if 1 or more, the output tensor has shape [sample_size, batch_size] + data_
↪shape
            while batch_size controls a parallel computation,
            sample_size controls a sequential computation (a for loop)
        oversample: if True, samples z (batch_size times), hold it fixed,
            and sample x (sample_size times)
        """
        pz = self.gen_model.prior((batch_size,))
        samples = [None] * (sample_size or 1)
        px_z = self.gen_model.obs_model(pz.sample()) if oversample else None
        for k in range(sample_size or 1):
            if not oversample:
                px_z = self.gen_model.obs_model(pz.sample())
            samples[k] = px_z.sample()
        x = torch.stack(samples)
        return x if sample_size else x.squeeze(0)

    def cond_sample(self, x, sample_size=None, oversample=False):
        """
        Condition on x and draw a sample:
            z|x ~ inf model
            x'|z ~ obs model

        x: a batch of seed data samples
        sample_size: if None, the output tensor has shape [batch_size] + data_shape
            if 1 or more, the output tensor has shape [sample_size, batch_size] + data_
↪shape
```

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```
            sample_size controls a sequential computation (a for loop)
        oversample: if True, samples z (batch_size times), hold it fixed,
            and sample x' (sample_size times)
        """
        qz = self.inf_model(x)
        samples = [None] * (sample_size or 1)
        px_z = self.gen_model.obs_model(qz.sample()) if oversample else None
        for k in range(sample_size or 1):
            if not oversample:
                px_z = self.gen_model.obs_model(qz.sample())
            samples[k] = px_z.sample()
        x = torch.stack(samples)
        return x if sample_size else x.squeeze(0)

    def log_prob(self, z, x):
        """
        The log density of the joint outcome under the generative model
        z: [batch_size, latent_dim]
        x: [batch_size] + data_shape
        """
        return self.gen_model.log_prob(z=z, x=x)

    def DRL(self, x, sample_size=None):
        """
        MC estimates of a model's
            * distortion D
            * rate R
            * and log-likelihood L
        The estimates are based on single data points
         but multiple latent samples.

        x: batch_shape + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        """
        sample_size = sample_size or 1
        obs_dims = len(self.gen_model.cpd_net.outcome_shape)
        batch_shape = x.shape[:-obs_dims]
        with torch.no_grad():
            qz = self.inf_model(x)
            pz = self.gen_model.prior(batch_shape)
            R = td.kl_divergence(qz, pz)
            D = 0
            ratios = [None] * sample_size
            for k in range(sample_size):
                z = qz.sample()
                px_z = self.gen_model.obs_model(z)
                ratios[k] = pz.log_prob(z) + px_z.log_prob(x) - qz.log_prob(z)
                D = D - px_z.log_prob(x)
            ratios = torch.stack(ratios, dim=-1)
            L = torch.logsumexp(ratios, dim=-1) - np.log(sample_size)
            D = D / sample_size
```

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```
            return D, R, L

    def elbo(self, x, sample_size=None):
        """
        An MC estimate of ELBO = -D -R

        x: [batch_size] + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        """
        D, R, _ = self.DRL(x, sample_size=sample_size)
        return -D -R

    def log_prob_estimate(self, x, sample_size=None):
        """
        An importance sampling estimate of log p(x)

        x: [batch_size] + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        """
        _, _, L = self.DRL(x, sample_size=sample_size)
        return L

    def forward(self, x, sample_size=None, rate_weight=1.):
        """
        A surrogate for an MC estimate of - grad ELBO

        x: [batch_size] + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        cv: optional module for variance reduction
        """
        sample_size = sample_size or 1
        obs_dims = len(self.gen_model.cpd_net.outcome_shape)
        batch_shape = x.shape[:-obs_dims]

        qz = self.inf_model(x)
        pz = self.gen_model.prior(batch_shape)
        D = 0
        sfe = 0
        reward = 0
        cv_reward = 0
        raw_r = 0
        cv_loss = 0
        for _ in range(sample_size):
            z = qz.sample()
            px_z = self.gen_model.obs_model(z)
            raw_r = px_z.log_prob(x) + pz.log_prob(z) - qz.log_prob(z)
            r, l = self.cv_model(raw_r.detach(), x=x, q=qz, r_fn=lambda a: self.gen_
↪model(a).log_prob(x))
            cv_loss = cv_loss + l
```

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```
            sfe = sfe + r.detach() * qz.log_prob(z)
            D = D - px_z.log_prob(x)
        D = (D / sample_size)
        sfe = (sfe / sample_size)
        R = td.kl_divergence(qz, pz)
        cv_loss = cv_loss / sample_size

        elbo_grad_surrogate = (-D + sfe)
        loss = -elbo_grad_surrogate + cv_loss

        return {'loss': loss.mean(0), 'ELBO': (-D -R).mean(0).item(), 'D': D.mean(0).
↪item(), 'R': R.mean(0).item(), 'cv_loss': cv_loss.mean(0).item()}
```

Here's an example

[46]:
```
nvil = NVIL(
    JointDistribution(
        BernoulliPriorNet(10),
        BinarizedImageModel(
            num_channels=img_shape[0],
            width=img_shape[1],
            height=img_shape[2],
            latent_size=10,
            p_drop=0.1,
            decoder_type=build_ffnn_decoder
        )
    ),
    InferenceModel(
        cpd_net_type=BernoulliCPDNet,
        latent_size=10,
        num_channels=img_shape[0],
        width=img_shape[1],
        height=img_shape[2],
        encoder_type=build_ffnn_encoder
    ),
    VarianceReduction()
)
nvil
```

[46]:
```
NVIL(
  (gen_model): JointDistribution(
    (prior_net): BernoulliPriorNet()
    (cpd_net): BinarizedImageModel(
      (decoder): Sequential(
        (0): Dropout(p=0.1, inplace=False)
        (1): Linear(in_features=10, out_features=512, bias=True)
        (2): ReLU()
        (3): Dropout(p=0.1, inplace=False)
        (4): Linear(in_features=512, out_features=512, bias=True)
        (5): ReLU()
        (6): Dropout(p=0.1, inplace=False)
        (7): Linear(in_features=512, out_features=4096, bias=True)
        (8): ReshapeLast()
```

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```
      )
    )
  )
  (inf_model): InferenceModel(
    (encoder): Sequential(
      (0): FlattenImage()
      (1): Dropout(p=0.0, inplace=False)
      (2): Linear(in_features=4096, out_features=512, bias=True)
      (3): ReLU()
      (4): Dropout(p=0.0, inplace=False)
      (5): Linear(in_features=512, out_features=512, bias=True)
      (6): ReLU()
      (7): Dropout(p=0.0, inplace=False)
      (8): Linear(in_features=512, out_features=1024, bias=True)
    )
    (cpd_net): BernoulliCPDNet(
      (encoder): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=1024, out_features=20, bias=True)
        (2): ReLU()
      )
      (logits): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=20, out_features=10, bias=True)
        (2): ReshapeLast()
      )
    )
  )
  (cv_model): VarianceReduction()
)
```

[47]:
```
for x, y in train_loader:
    print('x.shape:', x.shape)
    print(nvil(x))
    break
```

```
x.shape: torch.Size([64, 1, 64, 64])
{'loss': tensor(-16754.9395, grad_fn=<MeanBackward1>), 'ELBO': -2844.470947265625, 'D':␣
↪2844.458740234375, 'R': 0.012489881366491318, 'cv_loss': 0.0}
```

3.5.1 Training algorithm

We have up to three components (recall that some control variates can have their own parameters), so we will be manipulating up to three optimisers:

[48]:
```
class OptCollection:

    def __init__(self, gen, inf, cv=None):
        self.gen = gen
        self.inf = inf
        self.cv = cv
```

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```
    def zero_grad(self):
        self.gen.zero_grad()
        self.inf.zero_grad()
        if self.cv:
            self.cv.zero_grad()

    def step(self):
        self.gen.step()
        self.inf.step()
        if self.cv:
            self.cv.step()
```

Here's some helper code to assess and train the model

[49]:
```
from collections import defaultdict, OrderedDict
from tqdm.auto import tqdm


def assess(model, sample_size, dl, device):
    """
    Wrapper for estimating a model's ELBO, distortion, rate, and log-likelihood
     using all data points in a data loader.
    """
    D = 0
    R = 0
    L = 0
    data_size = 0
    with torch.no_grad():
        for batch_x, batch_y in dl:
            Dx, Rx, Lx = model.DRL(batch_x.to(device), sample_size=sample_size)
            D = D + Dx.sum(0)
            R = R + Rx.sum(0)
            L = L + Lx.sum(0)
            data_size += batch_x.shape[0]
    D = D / data_size
    R = R / data_size
    L = L / data_size
    return {'ELBO': (-D -R).item(), 'D': D.item(), 'R': R.item(), 'L': L.item()}


def train_vae(model: NVIL, opts: OptCollection,
    training_data, dev_data,
    batch_size=64, num_epochs=10, check_every=10,
    sample_size_training=1,
    sample_size_eval=10,
    grad_clip=5.,
    num_workers=2,
    device=torch.device('cuda:0')
    ):
    """
    model: pytorch model
```

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```
    optimiser: pytorch optimiser
    training_corpus: a TaggedCorpus for trianing
    dev_corpus: a TaggedCorpus for dev
    batch_size: use more if you have more memory
    num_epochs: use more for improved convergence
    check_every: use less to check performance on dev set more often
    device: where we run the experiment

    Return a log of quantities computed during training (for plotting)
    """
    batcher = DataLoader(training_data, batch_size, shuffle=True, num_workers=num_
↪workers, pin_memory=True)
    dev_batcher = DataLoader(dev_data, batch_size, num_workers=num_workers, pin_
↪memory=True)

    total_steps = num_epochs * len(batcher)
    log = defaultdict(list)

    step = 0
    model.eval()
    for k, v in assess(model, sample_size_eval, dev_batcher, device=device).items():
        log[f"dev.{k}"].append((step, v))

    with tqdm(range(total_steps)) as bar:
        for epoch in range(num_epochs):
            for batch_x, batch_y in batcher:
                model.train()
                opts.zero_grad()

                loss_dict = model(
                    batch_x.to(device),
                    sample_size=sample_size_training,
                )
                for metric, value in loss_dict.items():
                    log[f'training.{metric}'].append((step, value))

                loss_dict['loss'].backward()

                nn.utils.clip_grad_norm_(
                    model.parameters(),
                    grad_clip
                )
                opts.step()

                bar_dict = OrderedDict()
                for metric, value in loss_dict.items():
                    bar_dict[f'training.{metric}'] = f"{loss_dict[metric]:.2f}"
                for metric in ['ELBO', 'D', 'R', 'L']:
                    bar_dict[f"dev.{metric}"] =  "{:.2f}".format(log[f"dev.{metric}"][-
↪1][1])
                bar.set_postfix(bar_dict)
                bar.update()
```

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```
                if step % check_every == 0:
                    model.eval()
                    for k, v in assess(model, sample_size_eval, dev_batcher,␣
↪device=device).items():
                        log[f"dev.{k}"].append((step, v))

                step += 1


    model.eval()
    for k, v in assess(model, sample_size_eval, dev_batcher, device=device).items():
        log[f"dev.{k}"].append((step, v))

    return log
```

And, finally, some code to help inspect samples

[50]:
```
def inspect_discrete_lvm(model, dl, device):
    for x, y in dl:

        x_ = model.sample(16, 4, oversample=True).cpu().reshape(-1, 1, 64, 64)
        plt.figure(figsize=(12,6))
        plt.axis('off')
        plt.imshow(make_grid(x_, nrow=16).permute((1, 2, 0)))
        plt.title("Prior samples")
        plt.show()

        plt.figure(figsize=(12,6))
        plt.axis('off')
        plt.imshow(make_grid(x, nrow=16).permute((1, 2, 0)))
        plt.title("Observations")
        plt.show()

        x_ = model.cond_sample(x.to(device)).cpu().reshape(-1, 1, 64, 64)
        plt.figure(figsize=(12,6))
        plt.axis('off')
        plt.imshow(make_grid(x_, nrow=16).permute((1, 2, 0)))
        plt.title("Conditional samples")
        plt.show()

        break
```

3.5.2 Variance reduction

Here are some concrete strategies for variance reduction. You can skip those in a first pass.

[51]:
```
class CentredReward(VarianceReduction):
    """
    This control variate does not have trainable parameters,
     it maintains a running estimate of the average reward and updates
     a batch of rewards by computing reward - avg.
    """

    def __init__(self, alpha=0.9):
        super().__init__()
        self._alpha = alpha
        self._r_mean = 0.

    def forward(self, r, x=None, q=None, r_fn=None):
        """
        Centre the reward and update running estimates of mean.
        """
        with torch.no_grad():
            # sufficient statistics for next updates
            r_mean = torch.mean(r, dim=0)
            # centre the signal
            r = r - self._r_mean
            # update running estimate of mean
            self._r_mean = (1-self._alpha) * self._r_mean + self._alpha * r_mean.item()
            return r, torch.zeros_like(r)


class ScaledReward(VarianceReduction):
    """
    This control variate does not have trainable parameters,
     it maintains a running estimate of the reward's standard deviation and
     updates a batch of rewards by computing reward / maximum(stddev, 1).
    """

    def __init__(self, alpha=0.9):
        super().__init__()
        self._alpha = alpha
        self._r_std = 1.0

    def forward(self, r, x=None, q=None, r_fn=None):
        """
        Scale the reward by a running estimate of std, and also update the estimate.
        """
        with torch.no_grad():
            # sufficient statistics for next updates
            r_std = torch.std(r, dim=0)
            # standardise the signal
            r = r / self._r_std
            # update running estimate of std
            self._r_std = (1-self._alpha) * self._r_std + self._alpha * r_std.item()
```

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```
            # it's not safe to standardise with scales less than 1
            self._r_std = np.maximum(self._r_std, 1.)
            return r, torch.zeros_like(r)


class SelfCritic(VarianceReduction):
    """
    This control variate does not have trainable parameters,
     it updates a batch of rewards by computing reward - reward', where
     reward' is (log p(X=x|Z=z')).detach() assessed for a novel sample
     z' ~ Z|X=x.
    """

    def __init__(self):
        super().__init__()

    def forward(self, r, x, q, r_fn):
        """
        Standardise the reward and update running estimates of mean/std.
        """
        with torch.no_grad():
            z = q.sample()
            r = r - r_fn(z, x)
            return r, torch.zeros_like(r)


class Baseline(VarianceReduction):
    """
    An input-dependent baseline implemented as an MLP.
    The trainable parameters are adjusted via MSE.
    """

    def __init__(self, num_inputs, hidden_size, p_drop=0.):
        super().__init__()
        self.baseline = nn.Sequential(
            FlattenImage(),
            nn.Dropout(p_drop),
            nn.Linear(num_inputs, hidden_size),
            nn.ReLU(),
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, 1)
        )

    def forward(self, r, x, q=None, r_fn=None):
        """
        Return r - baseline(x) and Baseline's loss.
        """
        # batch_shape + (1,)
        r_hat = self.baseline(x)
        # batch_shape
        r_hat = r_hat.squeeze(-1)
        loss = (r - r_hat)**2
```

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```
        return r - r_hat.detach(), loss


class CVChain(VarianceReduction):

    def __init__(self, *args):
        super().__init__()
        if len(args) == 1 and isinstance(args[0], OrderedDict):
            for key, module in args[0].items():
                self.add_module(key, module)
        else:
            for idx, module in enumerate(args):
                self.add_module(str(idx), module)

    def forward(self, r, x, q, r_fn):
        loss = 0
        for cv in self._modules.values():
            r, l = cv(r, x=x, q=q, r_fn=r_fn)
            loss = loss + l
        return r, loss
```

3.5.3 Experiment

[52]:
```
seed_all()

model = NVIL(
    JointDistribution(
        BernoulliPriorNet(10),
        BinarizedImageModel(
            num_channels=img_shape[0],
            width=img_shape[1],
            height=img_shape[2],
            latent_size=10,
            p_drop=0.1
        )
    ),
    InferenceModel(
        latent_size=10,
        num_channels=img_shape[0],
        width=img_shape[1],
        height=img_shape[2],
        cpd_net_type=BernoulliCPDNet
    ),
    VarianceReduction(), # no variance reduction
    # In the NVIL paper, this is what they use:
    # CVChain(
    #     CentredReward(),
    #     #Baseline(np.prod(img_shape), 512), # this is how you would use a trained␣
↪baselined
    #     #ScaledReward()
```

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```
    # )
).to(my_device)

opts = OptCollection(
    opt.RMSprop(model.gen_params(), lr=5e-4, weight_decay=1e-6),
    opt.RMSprop(model.inf_params(), lr=1e-4),
    #opt.RMSprop(model.cv_params(), lr=1e-4, weight_decay=1e-6) # you need this if your baseline has trainable parameters
)

model
```

[52]:
```
NVIL(
  (gen_model): JointDistribution(
    (prior_net): BernoulliPriorNet()
    (cpd_net): BinarizedImageModel(
      (decoder): Sequential(
        (0): Dropout(p=0.1, inplace=False)
        (1): Linear(in_features=10, out_features=512, bias=True)
        (2): ReLU()
        (3): Dropout(p=0.1, inplace=False)
        (4): Linear(in_features=512, out_features=512, bias=True)
        (5): ReLU()
        (6): Dropout(p=0.1, inplace=False)
        (7): Linear(in_features=512, out_features=4096, bias=True)
        (8): ReshapeLast()
      )
    )
  )
  (inf_model): InferenceModel(
    (encoder): Sequential(
      (0): FlattenImage()
      (1): Dropout(p=0.0, inplace=False)
      (2): Linear(in_features=4096, out_features=512, bias=True)
      (3): ReLU()
      (4): Dropout(p=0.0, inplace=False)
      (5): Linear(in_features=512, out_features=512, bias=True)
      (6): ReLU()
      (7): Dropout(p=0.0, inplace=False)
      (8): Linear(in_features=512, out_features=1024, bias=True)
    )
    (cpd_net): BernoulliCPDNet(
      (encoder): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=1024, out_features=20, bias=True)
        (2): ReLU()
      )
      (logits): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=20, out_features=10, bias=True)
        (2): ReshapeLast()
      )
```

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```
    )
  )
  (cv_model): VarianceReduction()
)
```

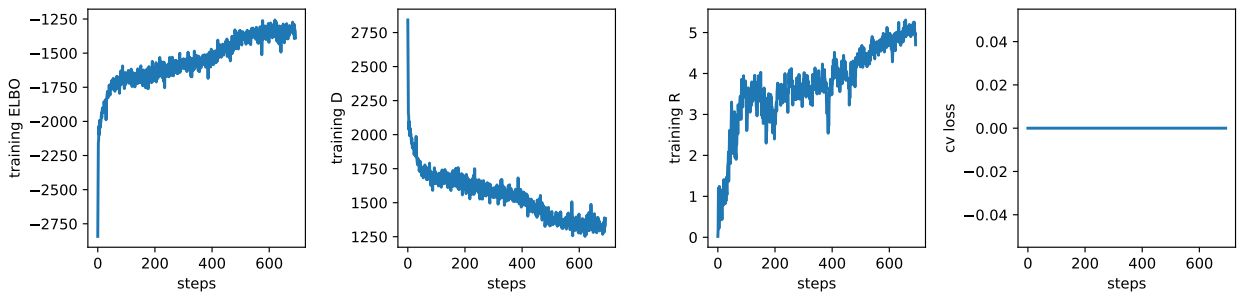
[53]:
```
log = train_vae(
    model=model,
    opts=opts,
    training_data=train_ds,
    dev_data=val_ds,
    batch_size=256,
    num_epochs=3,  # use more for better models
    check_every=100,
    sample_size_training=1,
    sample_size_eval=1,
    grad_clip=5.,
    device=my_device
)
```

```
  0%|          | 0/693 [00:00<?, ?it/s]
```

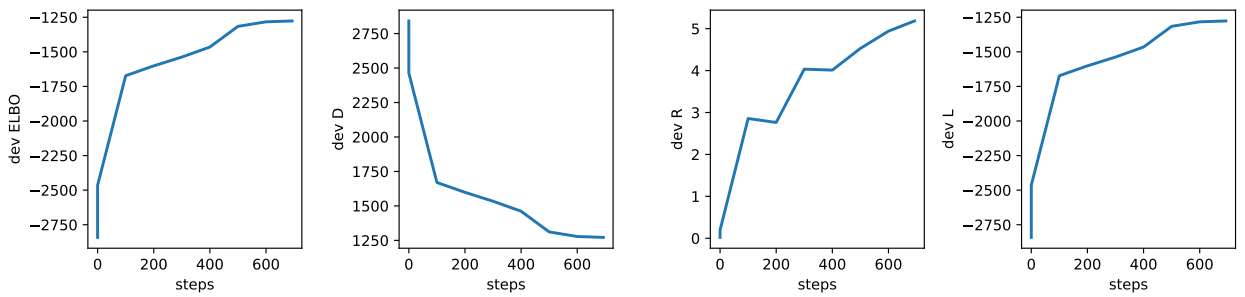
[54]:
```
log.keys()
```

[54]:
```
dict_keys(['dev.ELBO', 'dev.D', 'dev.R', 'dev.L', 'training.loss', 'training.ELBO',
↪'training.D', 'training.R', 'training.cv_loss'])
```

[55]:
```
fig, axs = plt.subplots(1, 3 + int('training.cv_loss' in log), sharex=True, sharey=False,
↪ figsize=(12, 3))

_ = axs[0].plot(np.array(log['training.ELBO'])[:,0], np.array(log['training.ELBO'])[:,1])
_ = axs[0].set_ylabel("training ELBO")
_ = axs[0].set_xlabel("steps")

_ = axs[1].plot(np.array(log['training.D'])[:,0], np.array(log['training.D'])[:,1])
_ = axs[1].set_ylabel("training D")
_ = axs[1].set_xlabel("steps")

_ = axs[2].plot(np.array(log['training.R'])[:,0], np.array(log['training.R'])[:,1])
_ = axs[2].set_ylabel("training R")
_ = axs[2].set_xlabel("steps")

if 'training.cv_loss' in log:
    _ = axs[3].plot(np.array(log['training.cv_loss'])[:,0], np.array(log['training.cv_
↪loss'])[:,1])
    _ = axs[3].set_ylabel("cv loss")
    _ = axs[3].set_xlabel("steps")

fig.tight_layout(h_pad=1.2, w_pad=1.2)
```

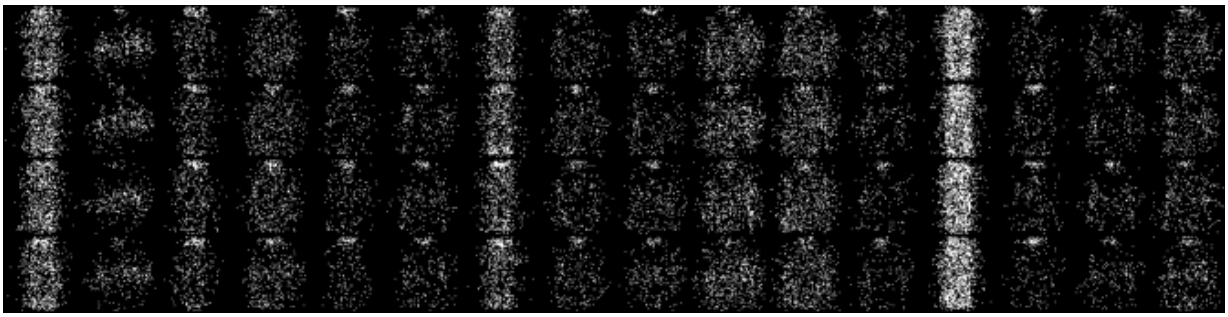


[56]:
```
fig, axs = plt.subplots(1, 4, sharex=True, sharey=False, figsize=(12, 3))

_ = axs[0].plot(np.array(log['dev.ELBO'])[:,0], np.array(log['dev.ELBO'])[:,1])
_ = axs[0].set_ylabel("dev ELBO")
_ = axs[0].set_xlabel("steps")

_ = axs[1].plot(np.array(log['dev.D'])[:,0], np.array(log['dev.D'])[:,1])
_ = axs[1].set_ylabel("dev D")
_ = axs[1].set_xlabel("steps")

_ = axs[2].plot(np.array(log['dev.R'])[:,0], np.array(log['dev.R'])[:,1])
_ = axs[2].set_ylabel("dev R")
_ = axs[2].set_xlabel("steps")

_ = axs[3].plot(np.array(log['dev.L'])[:,0], np.array(log['dev.L'])[:,1])
_ = axs[3].set_ylabel("dev L")
_ = axs[3].set_xlabel("steps")

fig.tight_layout(h_pad=1.2, w_pad=1.2)
```



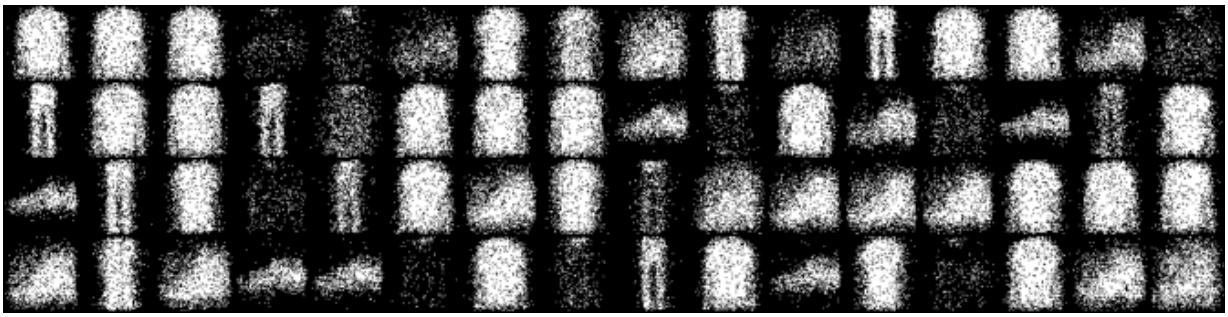
[57]:
```
inspect_discrete_lvm(model, DataLoader(val_ds, 64, num_workers=2, pin_memory=True), my_
↪device)
```

Prior samples



Observations

Conditional samples



4.44.5 4. Beyond

There are various things you can try.

- You can play with continuous output distributions and CNN encoder/decoders.
- Try switching baselines on and off.
- With VI, you should be able to use mixture models with larger K, even with the CNN decoder.
- You can change the dataset (e.g., use SVHN, whose images are coloured, thus you will be using 3 channels).
- You can attempt to (semi-)supervise the latent code (since these datasets offer some amount of supervision). For that you can use a log-likelihood side loss based on a model component that predicts a pmf $p_{Y|Z}(y|z, \phi)$ for the image's class given the latent code.

4.45 DPM 2 - Variational Inference for Deep Continuous LVMs

Filled notebook:
Authors: Wilker Aziz

4.45.1 0. Intended Learning Outcomes

After this tutorial the student should be able to

- parameterise a latent variable model with continuous latent variables
- estimate parameters using neural variational inference

Remark This tutorial builds upon the previous one and there is a lot of shared/unchanged code. The only changes are:

- additional prior nets (for continuous variables)
- additional CPD nets (for continuous variables)
- we changed DRL and forward in the NVIL class such that it can support LVMs trained via SFE or via reparameterisation

[1]:
```
import torch
import numpy as np
import random
import matplotlib.pyplot as plt
import torch.nn as nn
import torch.nn.functional as F
import torch.distributions as td

from functools import partial
from itertools import chain
from collections import defaultdict, OrderedDict
from tqdm.auto import tqdm
```

[2]:
```
def seed_all(seed=42):
    np.random.seed(seed)
    random.seed(seed)
    torch.manual_seed(seed)

seed_all()
```

4.45.2 1. Data

We are going to use toy image datsets for this notebook. These are fixed-dimensional observations for which encoder and decoders are relatively easy to design. This way we can focus on the aspects that are probabilistic in nature.

[3]:
```
from torchvision.datasets import FashionMNIST
from torchvision import transforms
from torchvision.transforms import ToTensor
from torch.utils.data import random_split, Dataset
from torch.utils.data.dataloader import DataLoader
from torchvision.utils import make_grid
```

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```
import torch.optim as opt

%matplotlib inline
```

A helper to binarize datasets:

[4]:
```
class Binarizer(Dataset):

    def __init__(self, ds, threshold=0.5):
        self._ds = ds
        self._threshold = threshold

    def __len__(self):
        """Size of the corpus in number of sequence pairs"""
        return len(self._ds)

    def __getitem__(self, idx):
        """
        Return corpus_x[idx] and corpus_y[idx] converted to codes
        the latter has the EOS code in the end
        """
        x, y = self._ds[idx]
        return (x >= self._threshold).float(), y
```

FashionMNIST

[5]:
```
dataset = FashionMNIST(root='data/', train=True, download=True,
                       transform=transforms.Compose([transforms.Resize(64), transforms.
↪ToTensor()]))
```

[6]:
```
img_shape = dataset[0][0].shape
print("Shape of an image:", img_shape)
```

```
Shape of an image: torch.Size([1, 64, 64])
```

Let's make a dev set for ourselves:

[7]:
```
val_size = 1000
train_size = len(dataset) - val_size
train_ds, val_ds = random_split(dataset, [train_size, val_size])
len(train_ds), len(val_ds)
```

[7]:
```
(59000, 1000)
```

we suggest that you binarize the data in a first pass through this notebook, but as you will see, we can also model the continuous pixel intensities.

[8]:
```
bin_data = True
```

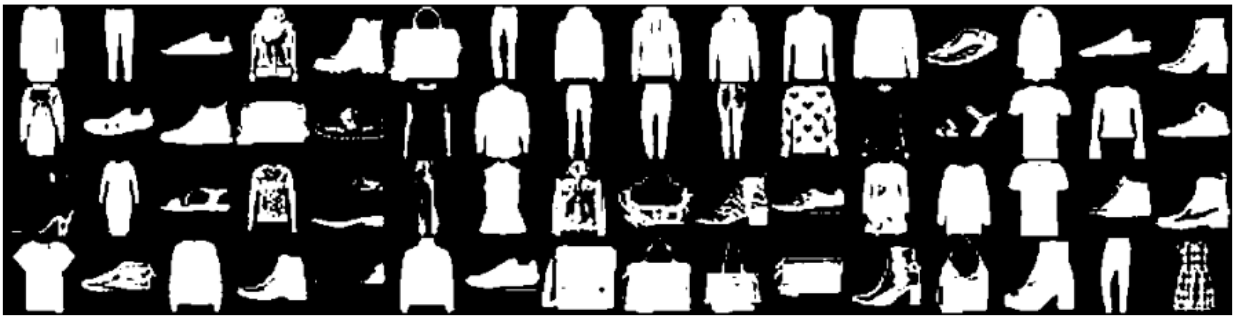
[9]:
```
if bin_data:
    train_ds = Binarizer(train_ds)
    val_ds = Binarizer(val_ds)
```

[10]:
```
batch_size = 64
train_loader = DataLoader(train_ds, batch_size, shuffle=True, num_workers=2, pin_
↪memory=True)
val_loader = DataLoader(val_ds, batch_size, num_workers=2, pin_memory=True)
```

Let's visualise a few samples

[11]:
```
for images, y in train_loader:
    print('images.shape:', images.shape)
    plt.figure(figsize=(16,8))
    plt.axis('off')
    plt.imshow(make_grid(images, nrow=16).permute((1, 2, 0)))
    plt.show()
    break
```

```
images.shape: torch.Size([64, 1, 64, 64])
```



4.45.3 2. Latent variable models

We will be using NNs to parameterise a latent variable model, that is, a joint distribution over a collection of random variables (rvs), some of which are observed, some of which are not.

We are interested in two random variables (rvs):

- a discrete latent code $Z \in \mathcal{Z}$
- and an image $X \in \mathcal{X} \subseteq \mathbb{R}^D$

In this tutorial, x is has a number C of channels, a certain width W and a certain height H, so $\mathcal{X} \subseteq \mathbb{R}^{C \times W \times H}$. Because we have fixed $D = C \times W \times H$, $\mathcal{X}$ is finite-dimensional, but this need not be the case in general (for example, in a different domain, $\mathcal{X}$ could be the unbounded space of all sentences of arbitrary lenght). We may treat the pixel intensities as discrete or continuous, as long as we choose an appropriate pmf/pdf for each case.

In this tutorial we will look into continuous latent codes. That is, $z \in \mathcal{Z} \subseteq \mathbb{R}^K$.

We specify a joint distribution over $\mathcal{Z} \times \mathcal{X}$ by specifying a joint probability density function (pdf):

$$p_{ZX}(z, x|\theta) = p_Z(z|\theta)p_{X|Z}(x|z, \theta) \tag{4.75}$$

Here θ denotes the parameters of the NNs that parameterise the pdf p_Z and the pdf $p_{X|Z=z}$ (for any given z).

In this tutorial, the prior is fixed, but in general it need not be. We do not have additional predictors to condition on, but in some application domains you may have (e.g., in imagine captioning, we may be interested in a joint for a caption y and a latent code z given an image x; in image generation, we may be interested in a joint distribution for an image x and a latent code z given a caption y).

2.1 Prior networks

We begin by specifying the component that parameterises the prior p_Z.

A prior network is an NN that parameterises a fixed prior distribution for the instances in a batch.

[12]:
```
class PriorNet(nn.Module):
    """
    An NN that parameterises a prior distribution.

    For this lab, our priors are fixed, so this NN's forward pass
     simply returns a fixed prior with a given batch_shape.
    """

    def __init__(self, outcome_shape: tuple):
        """
        outcome_shape: this is the shape of a single outcome
            if you use a single integer k, we will turn it into (k,)
        """
        super().__init__()
        if isinstance(outcome_shape, int):
            outcome_shape = (outcome_shape,)
        self.outcome_shape = outcome_shape

    def forward(self, batch_shape):
        """
        Returns a td object for the batch.
        """
        raise NotImplementedError("Implement me!")
```

Let's implement two priors.

A standard Gaussian prior

Here the latent code is a point in the K-dimensional real coordinate space. We use a standard Gaussian per coordinate:

$$p_Z(z) = \prod_{k=1}^{K} \mathcal{N}(z_k|0,1) \tag{4.76}$$

A mixture of Gaussians prior

Here we learn a mixture of C Gaussians, each a product of K independent Gaussians:

$$p_Z(z|\theta) = \sum_{c=1}^{C} \omega_c \prod_{k=1}^{K} \mathcal{N}(z_k|\mu_c, \sigma_c^2) \tag{4.77}$$

where the prior parameters are the mixing coefficients $\omega_{1:C} \in \Delta_{C-1}$, the locations $\mu_{1:C} \in \mathbb{R}^C$ and the scales $\sigma_{1:C} \in \mathbb{R}^C_{>0}$.

[13]:
```
class GaussianPriorNet(PriorNet):
    """
    For z a K-dimensional code:
```

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```
        p(z) = prod_k Normal(z[k]|0, 1)
    """

    def __init__(self, outcome_shape):
        super().__init__(outcome_shape)
        # the product of Bernoulli priors will have Bernoulli(0.5) factors
        self.register_buffer("locs", torch.zeros(self.outcome_shape, requires_
↪grad=False).detach())
        self.register_buffer("scales", torch.ones(self.outcome_shape, requires_
↪grad=False).detach())

    def forward(self, batch_shape):
        shape = batch_shape + self.outcome_shape
        # we wrap around td.Independent to obtain a pdf over multivariate draws
        return td.Independent(td.Normal(loc=self.locs.expand(shape), scale=self.scales.
↪expand(shape)), len(self.outcome_shape))


class MoGPriorNet(PriorNet):
    """
    For z a K-dimensional code:

        p(z|w_1...w_C, u_1...u_C, s_1...s_C)
         = \sum_c w_c prod_k Normal(z[k]|u[c], s[c]^2)
    """

    def __init__(self, outcome_shape, num_components, lbound=-10, rbound=10):
        super().__init__(outcome_shape)
        # [C]
        self.logits = nn.Parameter(torch.rand(num_components, requires_grad=True),␣
↪requires_grad=True)
        # (C,) + outcome_shape
        shape = (num_components,) + self.outcome_shape
        self.locs = nn.Parameter(torch.rand(shape, requires_grad=True), requires_
↪grad=True)
        self.scales = nn.Parameter(1 + torch.rand(shape, requires_grad=True), requires_
↪grad=True)
        self.num_components = num_components

    def forward(self, batch_shape):
        # e.g., with batch_shape (B,) and outcome_shape (K,) this is
        # [B, C, K]
        shape = batch_shape + (self.num_components,) + self.outcome_shape
        # we wrap around td.Independent to obtain a pdf over multivariate draws
        # (note that C is not part of the event_shape, thus td.Independent will
        #  should not treat that dimension as part of the outcome)
        # in our example, a draw from independent would return [B, C] draws of K-
↪dimensional outcomes
        comps = td.Independent(td.Normal(loc=self.locs.expand(shape), scale=self.scales.
↪expand(shape)), len(self.outcome_shape))
        # a batch of component selectors
```

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```
        pc = td.Categorical(logits=self.logits.expand(batch_shape + (self.num_components,
↪)))
        # and finally, a mixture
        return td.MixtureSameFamily(pc, comps)
```

[14]:
```
def test_priors(batch_size=2, latent_dim=3, num_comps=5):

    prior_net = GaussianPriorNet(latent_dim)
    print("\nGaussian")
    print(" trainable parameters")
    print(list(prior_net.parameters()))
    print(f" outcome_shape={prior_net.outcome_shape}")
    p = prior_net(batch_shape=(batch_size,))
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")

    prior_net = MoGPriorNet(latent_dim, num_comps)
    print("\nMixture of Gaussian")
    print(" trainable parameters")
    print(list(prior_net.parameters()))
    print(f" outcome_shape={prior_net.outcome_shape}")
    p = prior_net(batch_shape=(batch_size,))
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")


test_priors()
```

```
Gaussian
 trainable parameters
[]
 outcome_shape=(3,)
 distribution: Independent(Normal(loc: torch.Size([2, 3]), scale: torch.Size([2, 3])), 1)
 sample: tensor([[-0.3545, -0.5105, -0.7530],
        [ 0.6498, -0.0851, -1.2621]])
 shapes: sample=torch.Size([2, 3]) log_prob=torch.Size([2])

Mixture of Gaussian
 trainable parameters
[Parameter containing:
tensor([0.8617, 0.8520, 0.3585, 0.6196, 0.5566], requires_grad=True), Parameter␣
↪containing:
tensor([[0.4819, 0.0711, 0.2805],
        [0.4312, 0.1763, 0.3839],
        [0.0172, 0.8007, 0.8341],
        [0.6358, 0.9348, 0.1698],
        [0.6220, 0.4291, 0.3030]], requires_grad=True), Parameter containing:
```

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```
tensor([[1.5164, 1.3117, 1.3240],
        [1.5596, 1.3319, 1.5549],
        [1.1613, 1.6315, 1.0815],
        [1.9174, 1.9954, 1.5884],
        [1.8620, 1.4976, 1.3426]], requires_grad=True)]
 outcome_shape=(3,)
 distribution: MixtureSameFamily(
  Categorical(logits: torch.Size([2, 5])),
  Independent(Normal(loc: torch.Size([2, 5, 3]), scale: torch.Size([2, 5, 3])), 1))
 sample: tensor([[-1.5431, -0.7577,  0.3158],
        [ 3.9455, -0.1169,  0.7572]])
 shapes: sample=torch.Size([2, 3]) log_prob=torch.Size([2])
```

2.2 Conditional probability distributions

Next, we create code to parameterise conditional probability distributions (cpds), which we do by having an NN parameterise a choice of pmf/pdf. This will be useful in parameterising the $p_{X|Z=z}$ component of our latent variable models (and, later on, it will also be useful for variational inference, when we develop $q_{Z|X=x}$).

Our general strategy is to map from a number of inputs (which the user will choose) to the parameters of a pmf/pdf support by `torch.distributions`.

[15]:
```
class CPDNet(nn.Module):
    """
    Let L be a choice of distribution
        and x ~ L is an outcome with shape outcome_shape

    This is an NN whose forward method maps from a number of inputs to the
        parameters of L's pmf/pdf and returns a torch.distributions
        object representing L's pmf/pdf.
    """

    def __init__(self, outcome_shape):
        """
        outcome_shape: this is the shape of a single outcome
            if you use a single integer k, we will turn it into (k,)
        """
        super().__init__()
        if isinstance(outcome_shape, int):
            outcome_shape = (outcome_shape,)
        self.outcome_shape = outcome_shape

    def forward(self, inputs):
        """
        Return a torch.distribution object predicted from `inputs`.

        inputs: a tensor with shape batch_shape + (num_inputs,)
        """
        raise NotImplementedError("Implemented me")
```

2.2.1 Observational model

The observational model prescribes the distribution of $X|Z = z$.

If we assume our pixel intensities are binary, we can use a product of $C \times W \times H$ Bernoulli distributions, which we parameterise jointly using an NN:

$$p_{X|Z}(x|z,\theta) = \prod_{c=1}^{C}\prod_{w=1}^{W}\prod_{h=1}^{H} \text{Bernoulli}(x_{c,w,h}|f_{c,w,h}(z;\theta)) \tag{4.78}$$

Here $\mathbf{f}(z;\theta) \in (0,1)^C \times (0,1)^W \times (0,1)^H$ is an NN architecture such as a feed-forward net or a stack of transposed convolution layers. In NN literature, such architectures are often called *decoders*.

If we assume our pixel intensities are real values in $[0,1]$ (0 and 1 included), we need to parameterise a pdf. A good choice of pdf is the ContinuousBernoulli distributions, which is a single-parameter distribution (much like the Bernoulli) whose support is the set $[0,1]$.

Let's start by designing $\mathbf{f}$.

A very basic design uses a FFNN:

[16]:
```
class ReshapeLast(nn.Module):
    """
    Helper layer to reshape the rightmost dimension of a tensor.

    This can be used as a component of nn.Sequential.
    """

    def __init__(self, shape: tuple):
        """
        shape: desired rightmost shape
        """
        super().__init__()
        self._shape = shape

    def forward(self, input):
        # reshapes the last dimension into self.shape
        return input.reshape(input.shape[:-1] + self._shape)


def build_ffnn_decoder(latent_size, num_channels, width=64, height=64, hidden_size=512,␣
↪p_drop=0.):
    """
    Map the latent code to a tensor with shape [num_channels, width, height]
    using a FFNN with 2 hidden layers.

    latent_size: size of latent code
    num_channels: number of channels in the output
    width: image shape
    height: image shape
    hidden_size: we first map from latent_size to hidden_size and
        then use feed forward NNs to map it to [num_channels, width, height]
    p_drop: dropout rate before linear layers
```

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```
    """
    decoder = nn.Sequential(
        nn.Dropout(p_drop),
        nn.Linear(latent_size, hidden_size),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(hidden_size, hidden_size),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(hidden_size, num_channels * width * height),
        ReshapeLast((num_channels, width, height)),
    )
    return decoder
```

[17]:
```
# mapping from 10-dimensional latent code
build_ffnn_decoder(latent_size=10, num_channels=1)(torch.zeros((5, 10))).shape
```

[17]:
```
torch.Size([5, 1, 64, 64])
```

[18]:
```
# we can also have a structured batch shape (e.g., [3, 5])
build_ffnn_decoder(latent_size=10, num_channels=1)(torch.zeros((3, 5, 10))).shape
```

[18]:
```
torch.Size([3, 5, 1, 64, 64])
```

The downside is that the output layer is rather large.

An architecture with inductive biases that are more appropriate for our data type is a CNN, in particular, a transposed CNN. Here we design one such decoder:

[19]:
```
class MySequential(nn.Sequential):
    """
    This is a version of nn.Sequential that works with structured batches
     (i.e., batches that have multiple dimensions)
    even when some of the nn layers in it does not.

    The idea is to just wrap nn.Sequential around two calls to reshape
     which remove and restore the batch dimensions.
    """

    def __init__(self, *args, event_dims=1):
        super().__init__(*args)
        self._event_dims = event_dims

    def forward(self, input):
        # memorise batch shape
        batch_shape = input.shape[:-self._event_dims]
        # memorise latent shape
        event_shape = input.shape[-self._event_dims:]
        # flatten batch shape and obtain outputs
        output = super().forward(input.reshape( (-1,) + event_shape))
        # restore batch shape
        return output.reshape(batch_shape + output.shape[1:])
```

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```
def build_cnn_decoder(latent_size, num_channels, width=64, height=64, hidden_size=1024,␣
↪p_drop=0.):
    """
    Map the latent code to a tensor with shape [num_channels, width, height].

    latent_size: size of latent code
    num_channels: number of channels in the output
    width: must be 64 (for now)
    height: must be 64 (for now)
    hidden_size: we first map from latent_size to hidden_size and
        then use transposed 2d convolutions to [num_channels, width, height]
    p_drop: dropout rate before linear layers
    """
    if width != 64:
        raise ValueError("The width is hardcoded")
    if height != 64:
        raise ValueError("The height is hardcoded")

    # TODO: change the architecture so width and height are not hardcoded
    decoder = MySequential(
        nn.Dropout(p_drop),
        nn.Linear(latent_size, hidden_size),
        ReshapeLast((hidden_size, 1, 1)),
        nn.ConvTranspose2d(hidden_size, 128, 5, 2),
        nn.ReLU(),
        nn.ConvTranspose2d(128, 64, 5, 2),
        nn.ReLU(),
        nn.ConvTranspose2d(64, 32, 6, 2),
        nn.ReLU(),
        nn.ConvTranspose2d(32, num_channels, 6, 2),
        event_dims=1
    )
    return decoder
```

[20]:
```
# a batch of five 10-dimensional latent codes is transformed
# into a batch of 5 images, each with shape [1,64,64]
build_cnn_decoder(latent_size=10, num_channels=1)(torch.zeros((5, 10))).shape
```

[20]:
```
torch.Size([5, 1, 64, 64])
```

[21]:
```
# note that because we use MySequential,
# we can have a batch of [3, 5] assignments
# (this is useful, for example, when we have multiple draws of the latent
# variable for each of the data points in the batch)
build_cnn_decoder(latent_size=10, num_channels=1)(torch.zeros((3, 5, 10))).shape
```

[21]:
```
torch.Size([3, 5, 1, 64, 64])
```

Now we are in position to design a CPDNet for our image model, it simply combines a choice of decoder with a choice of distribution:

[22]:
```
class BinarizedImageModel(CPDNet):

    def __init__(self, num_channels, width, height, latent_size, decoder_type=build_ffnn_
↪decoder, p_drop=0.):
        super().__init__((num_channels, width, height))
        self.decoder =  decoder_type(
            latent_size=latent_size,
            num_channels=num_channels,
            width=width,
            height=height,
            p_drop=p_drop
        )

    def forward(self, z):
        """
        Return the cpd X|Z=z

        z: batch_shape + (latent_dim,)
        """
        # batch_shape + (num_channels, width, height)
        h = self.decoder(z)
        return td.Independent(td.Bernoulli(logits=h), len(self.outcome_shape))


class ContinuousImageModel(CPDNet):
    # TODO: this could be an exercise

    def __init__(self, num_channels, width, height, latent_size, decoder_type=build_ffnn_
↪decoder, p_drop=0.):
        super().__init__((num_channels, width, height))
        self.decoder =  decoder_type(
            latent_size=latent_size,
            num_channels=num_channels,
            width=width,
            height=height,
            p_drop=p_drop
        )

    def forward(self, z):
        """
        Return the cpd X|Z=z

        z: batch_shape + (latent_dim,)
        """
        # batch_shape + (num_channels, width, height)
        h = self.decoder(z)
        return td.Independent(td.ContinuousBernoulli(logits=h), len(self.outcome_shape))
```

[23]:
```
obs_model = BinarizedImageModel(
    num_channels=img_shape[0],
    width=img_shape[1],
    height=img_shape[2],
```

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```
    latent_size=10,
    p_drop=0.1,
)
print(obs_model)
# a batch of five zs is mapped to 5 distributions over [1,64,64]-dimensional
# binary tensors
print(obs_model(torch.zeros([5, 10])))
```

```
BinarizedImageModel(
  (decoder): Sequential(
    (0): Dropout(p=0.1, inplace=False)
    (1): Linear(in_features=10, out_features=512, bias=True)
    (2): ReLU()
    (3): Dropout(p=0.1, inplace=False)
    (4): Linear(in_features=512, out_features=512, bias=True)
    (5): ReLU()
    (6): Dropout(p=0.1, inplace=False)
    (7): Linear(in_features=512, out_features=4096, bias=True)
    (8): ReshapeLast()
  )
)
Independent(Bernoulli(logits: torch.Size([5, 1, 64, 64])), 3)
```

We can also use a different decoder

[24]:
```
obs_model = BinarizedImageModel(
    num_channels=img_shape[0],
    width=img_shape[1],
    height=img_shape[2],
    latent_size=10,
    p_drop=0.1,
    decoder_type=build_cnn_decoder
)
print(obs_model)
# a batch of five zs is mapped to 5 distributions over [1,64,64]-dimensional
# binary tensors
print(obs_model(torch.zeros([5, 10])))
```

```
BinarizedImageModel(
  (decoder): MySequential(
    (0): Dropout(p=0.1, inplace=False)
    (1): Linear(in_features=10, out_features=1024, bias=True)
    (2): ReshapeLast()
    (3): ConvTranspose2d(1024, 128, kernel_size=(5, 5), stride=(2, 2))
    (4): ReLU()
    (5): ConvTranspose2d(128, 64, kernel_size=(5, 5), stride=(2, 2))
    (6): ReLU()
    (7): ConvTranspose2d(64, 32, kernel_size=(6, 6), stride=(2, 2))
    (8): ReLU()
    (9): ConvTranspose2d(32, 1, kernel_size=(6, 6), stride=(2, 2))
  )
)
Independent(Bernoulli(logits: torch.Size([5, 1, 64, 64])), 3)
```

2.3 Joint distribution

We can now combine a prior and an observational model into a joint distribution. A joint distribution supports a few important operations such as marginal and posterior pdf assessments, as well as sampling from the joint distribution. Marginal and posterior assessments require computations that may or may not be tractable, see below.

From a joint pdf, we can compute the marginal density of x via

$$p_X(x|\theta) = \int_{\mathcal{Z}} p_{ZX}(z, x|\theta)\mathrm{d}z \tag{4.79}$$

$$= \int_{\mathcal{Z}} p_Z(z|\theta)p_{X|Z}(x|z, \theta)\mathrm{d}z \tag{4.80}$$

For uncountable $\mathcal{Z}$ and a general enough parameterisation of $p_{X|Z=z}$, this is intractable (a special case where this is tractable is that where $p_{X|Z=z}$ is itself a Gaussian whose mean depend linearly on z, such a conditional is unreasonably simple for interesting datasets).

The posterior density of z given x depends on the intractable marginal:

$$p_{Z|X}(z|x, \theta) = \frac{p_Z(z|\theta)p_{X|Z}(x|z, \theta)}{p_X(x|\theta)} \tag{4.81}$$

As marginalisation is intractable, we can obtain a naive lowerbound by direct application of Jensen's inequality:

$$\log p_X(x|\theta) = \log \int_{\mathcal{Z}} p_Z(z|\theta)p_{X|Z}(x|z, \theta)\mathrm{d}z \tag{4.82}$$

$$\overset{\text{JI}}{\geq} \int_{\mathcal{Z}} p_Z(z|\theta) \log p_{X|Z}(x|z, \theta)\mathrm{d}z \tag{4.83}$$

$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} \log p_{X|Z}(x|z_s, \theta) \quad \text{where } z_s \sim p_Z \tag{4.84}$$

A better lowerbound could be obtained via importance sampling, but it would require training an approximating distribution (as we will do in variational inference).

Recall that, given a dataset $\mathcal{D}$, the log-likelihood function $\mathcal{L}(\theta|\mathcal{D}) = \sum_{x\in\mathcal{D}} \log p_X(x|\theta)$ requires performing marginal density assessments. Whenever exact marginalisation is intractable, we are unaible to assess $\mathcal{L}(\theta|\mathcal{D})$ and its gradient with respect to θ. If the prior is fixed, we can use the naive lowerbound to obtain a gradient estimate, but, again, our naive application of JI leads to a generally rather loose bound.

[25]:
```
class JointDistribution(nn.Module):
    """
    A wrapper to combine a prior net and a cpd net into a joint distribution.
    """

    def __init__(self, prior_net: PriorNet, cpd_net: CPDNet):
        """
        prior_net: object to parameterise p_Z
        cpd_net: object to parameterise p_{X|Z=z}
        """
        super().__init__()
        self.prior_net = prior_net
```

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```
        self.cpd_net = cpd_net

    def prior(self, shape):
        return self.prior_net(shape)

    def obs_model(self, z):
        return self.cpd_net(z)

    def sample(self, shape):
        """
        Return z via prior_net(shape).sample()
            and x via cpd_net(z).sample()
        """
        pz = self.prior_net(shape)
        z = pz.sample()
        px_z = self.cpd_net(z)
        x = px_z.sample()
        return z, x

    def log_prob(self, z, x):
        """
        Assess the log density of the joint outcome.
        """
        batch_shape = z.shape[:-len(self.prior_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        px_z = self.cpd_net(z)
        return pz.log_prob(z) + px_z.log_prob(x)

    def log_marginal(self, x, enumerate_fn):
        """
        Return log marginal density of x.

        enumerate_fn: function that enumerates the support of the prior
            (this is needed for marginalisation p(x) = \int p(z, x) dz)

            This only really makes sense if the support is a
            (small) countably finite set. In such cases, you can use
                enumerate=lambda p: p.enumerate_support()
            which is supported, for example, by Categorical and OneHotCategorical.

            If the support is discrete (eg, bit vectors) you can still dare to
            enumerate it explicitly, but you will need to write cutomised code,
            as torch.distributions will not offer that functionality for you.

            If the support is uncountable, countably infinite, or just large
            anyway, you need approximate tools (such as VI, importance sampling, etc)
        """
        batch_shape = x.shape[:-len(self.cpd_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        log_joint = []
        # (support_size,) + batch_shape
        z = enumerate_fn(pz)
```

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```
        px_z = self.cpd_net(z)
        # (support_size,) + batch_shape
        log_joint = pz.log_prob(z) + px_z.log_prob(x.unsqueeze(0))
        # batch_shape
        return torch.logsumexp(log_joint, 0)

    def posterior(self, x, enumerate_fn):
        """
        Return the posterior distribution Z|X=x.

        As the code is discrete, we return a discrete distribution over
        the complete space of all possible latent codes. This is done via
        exhaustive enumeration provided by `enumerate_fn`.
        """
        batch_shape = x.shape[:-len(self.cpd_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        # (support_size,) + batch_shape
        z = enumerate_fn(pz)
        px_z = self.cpd_net(z)
        # (support_size,) + batch_shape
        log_joint = pz.log_prob(z) + px_z.log_prob(x.unsqueeze(0))
        # batch_shape + (support_size,)
        log_joint = torch.swapaxes(log_joint, 0, -1)
        return td.Categorical(logits=log_joint)

    def naive_lowerbound(self, x, num_samples: int):
        """
        Return an MC lowerbound on log marginal density of x:
            log p(x) >= 1/S \sum_s log p(x|z[s])
                with z[s] ~ p_Z
        """
        batch_shape = x.shape[:-len(self.cpd_net.outcome_shape)]
        pz = self.prior_net(batch_shape)
        # (num_samples,) + batch_shape + prior_outcome_shape
        log_probs = []
        # I'm using a for loop, but note that with enough GPU memory
        # one could parallelise this step
        for z in pz.sample((num_samples,)):
            px_z = self.cpd_net(z)
            log_probs.append(px_z.log_prob(x))
        # (num_samples,) + batch_shape
        log_probs = torch.stack(log_probs)
        # batch_shape
        return torch.mean(log_probs, 0)
```

[26]:
```
def test_joint_dist(latent_size=10, num_comps=3, data_shape=(1, 64, 64), batch_size=2,␣
↪hidden_size=32):
    p = JointDistribution(
        prior_net=GaussianPriorNet(latent_size),
        cpd_net=BinarizedImageModel(
            num_channels=data_shape[0],
            width=data_shape[1],
```

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```
            height=data_shape[2],
            latent_size=latent_size,
            decoder_type=build_cnn_decoder
        )
    )
    print("Model for binarized data")
    print(p)
    z, x = p.sample((batch_size,))
    print("sampled z")
    print(z)
    print("sampled x")
    print(x)
    print("MC lowerbound")
    print(" 1:", p.naive_lowerbound(x, 10))
    print(" 2:", p.naive_lowerbound(x, 10))

    print("\n\n")

    p = JointDistribution(
        prior_net=MoGPriorNet(latent_size, num_comps),
        cpd_net=ContinuousImageModel(
            num_channels=data_shape[0],
            width=data_shape[1],
            height=data_shape[2],
            latent_size=latent_size,
            decoder_type=build_cnn_decoder
        )
    )
    print("Model for continuous data")
    print(p)
    z, x = p.sample((batch_size,))
    print("sampled z")
    print(z)
    print("sampled x")
    print(x)
    print("MC lowerbound")
    print(" 1:", p.naive_lowerbound(x, 10))
    print(" 2:", p.naive_lowerbound(x, 10))

test_joint_dist(10)
```

```
Model for binarized data
JointDistribution(
  (prior_net): GaussianPriorNet()
  (cpd_net): BinarizedImageModel(
    (decoder): MySequential(
      (0): Dropout(p=0.0, inplace=False)
      (1): Linear(in_features=10, out_features=1024, bias=True)
      (2): ReshapeLast()
      (3): ConvTranspose2d(1024, 128, kernel_size=(5, 5), stride=(2, 2))
      (4): ReLU()
      (5): ConvTranspose2d(128, 64, kernel_size=(5, 5), stride=(2, 2))
```

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```
      (6): ReLU()
      (7): ConvTranspose2d(64, 32, kernel_size=(6, 6), stride=(2, 2))
      (8): ReLU()
      (9): ConvTranspose2d(32, 1, kernel_size=(6, 6), stride=(2, 2))
    )
  )
)
sampled z
tensor([[-0.8407,  0.2065, -1.2518, -0.9531,  0.1592, -0.1754, -1.6121,  0.1075,
         -0.7088, -0.3303],
        [-0.1712,  0.1613, -0.3089,  0.2564,  0.0636,  0.7447,  0.7566, -0.4789,
          1.1534, -0.8448]])
sampled x
tensor([[[[0., 1., 1.,  ..., 1., 1., 1.],
          [1., 1., 0.,  ..., 1., 0., 1.],
          [1., 0., 1.,  ..., 0., 0., 1.],
          ...,
          [0., 0., 1.,  ..., 0., 1., 0.],
          [1., 1., 0.,  ..., 1., 1., 1.],
          [1., 0., 0.,  ..., 0., 0., 1.]]],


        [[[0., 1., 0.,  ..., 1., 1., 1.],
          [1., 1., 0.,  ..., 1., 0., 0.],
          [0., 0., 0.,  ..., 1., 0., 1.],
          ...,
          [0., 1., 0.,  ..., 1., 1., 1.],
          [1., 1., 0.,  ..., 1., 0., 0.],
          [0., 0., 1.,  ..., 0., 1., 1.]]]])
MC lowerbound
 1: tensor([-2837.7363, -2837.9871], grad_fn=<MeanBackward1>)
 2: tensor([-2837.9243, -2838.0288], grad_fn=<MeanBackward1>)



Model for continuous data
JointDistribution(
  (prior_net): MoGPriorNet()
  (cpd_net): ContinuousImageModel(
    (decoder): MySequential(
      (0): Dropout(p=0.0, inplace=False)
      (1): Linear(in_features=10, out_features=1024, bias=True)
      (2): ReshapeLast()
      (3): ConvTranspose2d(1024, 128, kernel_size=(5, 5), stride=(2, 2))
      (4): ReLU()
      (5): ConvTranspose2d(128, 64, kernel_size=(5, 5), stride=(2, 2))
      (6): ReLU()
      (7): ConvTranspose2d(64, 32, kernel_size=(6, 6), stride=(2, 2))
      (8): ReLU()
      (9): ConvTranspose2d(32, 1, kernel_size=(6, 6), stride=(2, 2))
    )
  )
```

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```
)
sampled z
tensor([[ 0.5024,  0.1232,  1.0614,  1.5447,  1.1263,  1.0789,  2.7709,  1.9042,
         -1.0329,  3.2964],
        [ 1.0950, -1.1369,  1.0845,  1.6282, -0.8367,  1.1774, -0.4392, -0.3845,
          1.5312, -1.0509]])
sampled x
tensor([[[[0.2456, 0.6908, 0.2022,  ..., 0.9125, 0.4140, 0.0154],
          [0.9211, 0.8082, 0.1273,  ..., 0.0145, 0.6978, 0.2584],
          [0.9423, 0.6667, 0.8885,  ..., 0.8678, 0.2550, 0.1817],
          ...,
          [0.9706, 0.4656, 0.9801,  ..., 0.3806, 0.5779, 0.3176],
          [0.8841, 0.9396, 0.1979,  ..., 0.4812, 0.1924, 0.1274],
          [0.9042, 0.7917, 0.8952,  ..., 0.4248, 0.3569, 0.6764]]],


        [[[0.2313, 0.6762, 0.1603,  ..., 0.8595, 0.0705, 0.6296],
          [0.6333, 0.8830, 0.3072,  ..., 0.0994, 0.7293, 0.3187],
          [0.2723, 0.6290, 0.7742,  ..., 0.1179, 0.6817, 0.0761],
          ...,
          [0.2667, 0.3814, 0.9479,  ..., 0.4457, 0.3651, 0.0825],
          [0.7468, 0.6061, 0.9087,  ..., 0.1951, 0.1604, 0.0321],
          [0.6896, 0.4760, 0.0178,  ..., 0.3982, 0.9280, 0.0480]]]])
MC lowerbound
 1: tensor([0.0437, 0.5014], grad_fn=<MeanBackward1>)
 2: tensor([0.1282, 0.4484], grad_fn=<MeanBackward1>)
```

4.45.4 3. Learning

We estimate θ using stochastic gradient-based maximum likelihood estimation. For a tractable model, we can assess the log-likelihood function

$$\mathcal{L}(\theta|\mathcal{D}) = \sum_{x \in \mathcal{D}} \log p_X(x|\theta) \tag{4.85}$$

and estimate $\nabla_\theta \mathcal{L}(\theta|\mathcal{D})$ using random mini-batches:

$$\nabla_\theta \mathcal{L}(\theta|\mathcal{D}) \overset{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^{S} \nabla_\theta \log p_X(x^{(s)}|\theta) \tag{4.86}$$

$$\text{where } x^{(s)} \sim \mathcal{D} \tag{4.87}$$

An intractable model, such as the continuous LVM above requires approximate inference.

3.1 Intractable LVMs

When marginalisation is intractable, we resort to variational inference introducing a parametric approximation $q_{Z|X=x}$ to the model's true posterior distribution $p_{Z|X=x}$ and estimate both the approximation and the joint distribution by maximising the evidence lowerbound (ELBO), shown below for a single observation x:

$$\mathcal{E}(\lambda, \theta|\mathcal{D}) = \mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}\left[\log \frac{p_{ZX}(z, x|\theta)}{q_{Z|X}(z|x, \lambda)}\right]\right] \tag{4.88}$$

$$= \underbrace{\mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}[\log p_{Z|X}(x|z, \theta)]\right]}_{-D} - \underbrace{\mathbb{E}_{x\sim\mathcal{D}}\left[\mathrm{KL}(q_{Z|X=x}||p_Z)\right]}_{R} \tag{4.89}$$

where the inner expectation is taken with respect to $q_{Z|X}(z|x, \lambda)$.

When computed in expectation under the data distribution, the two components of the ELBO, namely, the expected log-likelihood $\mathbb{E}[\log p_{Z|X}(x|z, \theta)]$ and the "KL term" $\mathrm{KL}(q_{Z|X=x}||p_Z)$, are related to two information-theoretic quantities known as *distortion* and *rate*.

We choose our approximation to be such that: its support is embeded in the support of the prior, it is simple enough to sample from, and it is simple enough to assess the mass of a sample. If possible, we choose it such that other quantities are also tractable (e.g., entropy, relative entropy).

For a multivariate z, we normally choose a factorised family, for example, if z is a point in $\mathbb{R}^K$:

$$q_{Z|X}(z|x, \lambda) = \prod_{k=1}^{K} \mathcal{N}(z_k|\mu_k(x; \lambda), \sigma_k^2(x; \lambda)) \tag{4.90}$$

with $\boldsymbol{\mu}(x; \lambda) \in \mathbb{R}^K$ and $\boldsymbol{\sigma}(x; \lambda) \in \mathbb{R}^K_{>0}$. This is called a *mean field assumption*.

We can obtain a more complex approximation by, for example, using a mixture of mean field families:

$$q_{Z|X}(z|x, \lambda) = \sum_{c=1}^{C} \omega_c(x; \lambda) \prod_{k=1}^{K} \mathcal{N}(z_k|\mu_k(x; \lambda), \sigma_k^2(x; \lambda)) \tag{4.91}$$

with $\boldsymbol{\mu}(x; \lambda) \in \mathbb{R}^K$, $\boldsymbol{\sigma}(x; \lambda) \in \mathbb{R}^K_{>0}$, and $\boldsymbol{\omega}(x; \lambda) \in \Delta_{C-1}$.

There are other ways to inject structure in the variational approximation, a common example is to use a normalising flow. When designing a structured approximation a few things must be kept in mind:

- sampling should remain tractable
- assessing the density of a sample should remain tractable
- it's okay if we cannot compute entropy or KL in closed-form, we can always estimate the gradient of such terms (e.g., via score function estimation)

As we shall see the two approximations above differ in a crucial way, the simple Gaussian mean field is amenable to a continuously differentiable reparameterisation which leads to a lower variance estimator (compared to, for example, the score function estimator).

[ ]:

3.1.1 Reparameterised gradient

For some distributions, it is possible to obtain a sample via a continuously differentiable transformation of a fixed random source. This enables a class for gradient estimators known as *reparameterised gradient* (or the "reparameterisation trick"). In these cases $Z = \mathcal{T}(\epsilon, \lambda)$ with ϵ drawn from a distribution whose parameters are independent of λ. Moreover, $\mathcal{T}$ is differentiable and invertible.

3.2 Inference model

The inference model is a conditional model of the latent variable, for which we design CPD nets.

Before we go on, it is useful to design an "encoder" a function that maps an image $x \in \mathcal{X}$ to a fixed-size vector that we can use as a compact representation of x. Next, we design one such encoder employing FFNNs and another employing CNNs.

[27]:
```
class FlattenImage(nn.Module):
    def forward(self, input):
        return input.reshape(input.shape[:-3] + (-1,))

def build_ffnn_encoder(num_channels, width=64, height=64, output_size=1024, p_drop=0.):
    encoder = nn.Sequential(
        FlattenImage(),
        nn.Dropout(p_drop),
        nn.Linear(num_channels * width * height, output_size//2),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(output_size//2, output_size//2),
        nn.ReLU(),
        nn.Dropout(p_drop),
        nn.Linear(output_size//2, output_size),
    )
    return encoder

def build_cnn_encoder(num_channels, width=64, height=64, output_size=1024, p_drop=0.):
    if width != 64:
        raise ValueError("The width is hardcoded")
    if height != 64:
        raise ValueError("The height is hardcoded")
    if output_size != 1024:
        raise ValueError("The output_size is hardcoded")
    # TODO: change the architecture so width, height and output_size are not hardcoded
    encoder = MySequential(
        nn.Conv2d(num_channels, 32, 4, 2),
        nn.LeakyReLU(0.2),
        nn.Conv2d(32, 64, 4, 2),
        nn.LeakyReLU(0.2),
        nn.Conv2d(64, 128, 4, 2),
        nn.LeakyReLU(0.2),
        nn.Conv2d(128, 256, 4, 2),
        nn.LeakyReLU(0.2),
        FlattenImage(),
        event_dims=3
```

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```
    )
    return encoder
```

[28]:
```
# a batch of five [1, 64, 64]-dimensional images is encoded into
# five 1024-dimensional vectors
build_ffnn_encoder(num_channels=1)(torch.zeros((5, 1, 64, 64))).shape
```

[28]:
```
torch.Size([5, 1024])
```

[29]:
```
# and, again, we can have structured batches
# (here trying with (3,5))
build_ffnn_encoder(num_channels=1)(torch.zeros((3, 5, 1, 64, 64))).shape
```

[29]:
```
torch.Size([3, 5, 1024])
```

[30]:
```
# a batch of five [1, 64, 64]-dimensional images is encoded into
# five 1024-dimensional vectors
build_cnn_encoder(num_channels=1)(torch.zeros((5, 1, 64, 64))).shape
```

[30]:
```
torch.Size([5, 1024])
```

[31]:
```
# and, again, since we use MySequential we can have structured batches
# (here trying with (3,5))
build_cnn_encoder(num_channels=1)(torch.zeros((3, 5, 1, 64, 64))).shape
```

[31]:
```
torch.Size([3, 5, 1024])
```

We can now design some CPD nets, assuming they map from an encoding of an image to a pmf over $\mathcal{Z}$.

Gaussian mean field

This can be used to parameterise a cpd over real vectors of fixed dimensionality.

Mixture of Gaussian mean fields

This can also be used to parameterise a cpd over real vectors of fixed dimensionality, but it achieves a more complex density (e.g., multimodal).

[32]:
```
class GaussianCPDNet(CPDNet):
    """
    Output distribution is a product of Gaussian distributions
    """

    def __init__(self, outcome_shape, num_inputs: int, hidden_size: int=None, p_drop:␣
↪float=0.):
        """
        outcome_shape: shape of the outcome (int or tuple)
            if int, we turn it into a singleton tuple
        num_inputs: rightmost dimensionality of the inputs to forward
        hidden_size: size of hidden layers for the CPDNet (use None to skip)
        p_drop: configure dropout before every Linear layer
        """
        super().__init__(outcome_shape)
        num_outputs = np.prod(self.outcome_shape)
```

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```
        if hidden_size:
            self.encoder = nn.Sequential(
                nn.Dropout(p_drop),
                nn.Linear(num_inputs, hidden_size),
                nn.ReLU()
            )
        else:
            self.encoder = nn.Identity()
            hidden_size = num_inputs

        self.locs = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_outputs),
            ReshapeLast(self.outcome_shape)
        )
        self.scales = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_outputs),
            nn.Softplus(), # we use the softplus activations for the scales
            ReshapeLast(self.outcome_shape)
        )

    def forward(self, inputs):
        h = self.encoder(inputs)
        return td.Independent(td.Normal(loc=self.locs(h), scale=self.scales(h)),␣
↪len(self.outcome_shape))

class MoGCPDNet(CPDNet):
    """
    Output distribution is a mixture of products of Gaussian distributions
    """

    def __init__(self, outcome_shape, num_inputs: int, hidden_size: int=None, p_drop:␣
↪float=0., num_components=2):
        """
        outcome_shape: shape of the outcome (int or tuple)
            if int, we turn it into a singleton tuple
        num_inputs: rightmost dimensionality of the inputs to forward
        hidden_size: size of hidden layers for the CPDNet (use None to skip)
        p_drop: configure dropout before every Linear layer
        num_components: number of Gaussians to be mixed
        """
        super().__init__(outcome_shape)
        self.num_components = num_components

        num_outputs = num_components * np.prod(self.outcome_shape)

        if hidden_size:
            self.encoder = nn.Sequential(
                nn.Dropout(p_drop),
                nn.Linear(num_inputs, hidden_size),
                nn.ReLU()
```

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```
            )
        else:
            self.encoder = nn.Identity()
            hidden_size = num_inputs

        self.locs = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_outputs),
            ReshapeLast((num_components,) + self.outcome_shape)
        )
        self.scales = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_outputs),
            nn.Softplus(), # we use the softplus activations for the scales
            ReshapeLast((num_components,) + self.outcome_shape)
        )
        self.logits = nn.Sequential(
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, num_components),
            ReshapeLast((num_components,))
        )

    def forward(self, inputs):
        h = self.encoder(inputs)
        comps = td.Independent(td.Normal(loc=self.locs(h), scale=self.scales(h)),␣
↪len(self.outcome_shape))
        pc = td.Categorical(logits=self.logits(h))
        return td.MixtureSameFamily(pc, comps)
```

[33]:
```
def test_cpds(outcome_shape, num_comps=2, batch_size=3, input_dim=5, hidden_size=2):

    cpd_net = GaussianCPDNet(outcome_shape, num_inputs=input_dim, hidden_size=hidden_
↪size)
    print("\nGaussian")
    print(cpd_net)
    print(f" outcome_shape={cpd_net.outcome_shape}")
    inputs = torch.from_numpy(np.random.uniform(size=(batch_size, input_dim))).float()
    print(f" shape of inputs: {inputs.shape}")
    p = cpd_net(inputs)
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")

    cpd_net = MoGCPDNet(outcome_shape, num_inputs=input_dim, hidden_size=hidden_size,␣
↪num_components=num_comps)
    print("\nMixture of Gaussians")
    print(cpd_net)
    print(f" outcome_shape={cpd_net.outcome_shape}")
    inputs = torch.from_numpy(np.random.uniform(size=(batch_size, input_dim))).float()
    print(f" shape of inputs: {inputs.shape}")
    p = cpd_net(inputs)
```

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```
    print(f" distribution: {p}")
    z = p.sample()
    print(f" sample: {z}")
    print(f" shapes: sample={z.shape} log_prob={p.log_prob(z).shape}")


# Try a few
test_cpds(12)
#test_cpds(12, hidden_size=None)
# your latent code could be a metrix (we talk about it as a "vector" for convenience)
#test_cpds((4, 5))
```

```
Gaussian
GaussianCPDNet(
  (encoder): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=5, out_features=2, bias=True)
    (2): ReLU()
  )
  (locs): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=12, bias=True)
    (2): ReshapeLast()
  )
  (scales): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=12, bias=True)
    (2): Softplus(beta=1, threshold=20)
    (3): ReshapeLast()
  )
)
 outcome_shape=(12,)
 shape of inputs: torch.Size([3, 5])
 distribution: Independent(Normal(loc: torch.Size([3, 12]), scale: torch.Size([3, 12])),␣
↪1)
 sample: tensor([[-0.2740,  1.4641, -0.1492,  0.8619,  0.8987, -0.6384,  0.1898, -0.0084,
          0.0154, -0.0720,  0.5614, -0.7824],
        [ 1.4560, -0.2668, -0.2343, -0.8925,  0.0078, -0.1212,  0.3651, -0.8519,
          1.0650, -1.2128, -0.4736, -0.1115],
        [ 0.1504, -0.5747,  0.1681,  0.4921,  1.2217, -0.4474, -0.9136, -1.1818,
          0.9822, -0.6862, -0.0885, -0.3536]])
 shapes: sample=torch.Size([3, 12]) log_prob=torch.Size([3])

Mixture of Gaussians
MoGCPDNet(
  (encoder): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=5, out_features=2, bias=True)
    (2): ReLU()
  )
  (locs): Sequential(
```

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```
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=24, bias=True)
    (2): ReshapeLast()
  )
  (scales): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=24, bias=True)
    (2): Softplus(beta=1, threshold=20)
    (3): ReshapeLast()
  )
  (logits): Sequential(
    (0): Dropout(p=0.0, inplace=False)
    (1): Linear(in_features=2, out_features=2, bias=True)
    (2): ReshapeLast()
  )
)
 outcome_shape=(12,)
 shape of inputs: torch.Size([3, 5])
 distribution: MixtureSameFamily(
  Categorical(logits: torch.Size([3, 2])),
  Independent(Normal(loc: torch.Size([3, 2, 12]), scale: torch.Size([3, 2, 12])), 1))
 sample: tensor([[ 2.2989,  0.6416, -0.7611, -0.2090, -0.4584,  0.5179, -0.1198,  0.0880,
          0.7712, -0.4315, -0.3756,  0.2588],
         [-0.1332, -0.0895, -0.0302,  1.7607, -0.6219,  0.5210,  1.3052,  0.4076,
          0.2439, -0.4406,  0.0756,  0.6263],
         [-0.1179,  1.3194, -0.2864,  1.0093,  1.1053,  0.9005,  0.6088,  0.2438,
          0.7631, -0.8659,  0.4035,  0.1295]])
 shapes: sample=torch.Size([3, 12]) log_prob=torch.Size([3])
```

Last, but certainly not least, we can combine our encoder and a choice of CPD net.

[34]:
```
class InferenceModel(CPDNet):

    def __init__(
        self, cpd_net_type,
        latent_size, num_channels=1, width=64, height=64,
        hidden_size=1024, p_drop=0.,
        encoder_type=build_ffnn_encoder):

        super().__init__(latent_size)

        self.latent_size = latent_size
        # encodes an image to a hidden_size-dimensional vector
        self.encoder = encoder_type(
            num_channels=num_channels,
            width=width,
            height=height,
            output_size=hidden_size,
            p_drop=p_drop
        )
        # maps from a hidden_size-dimensional encoding
        # to a cpd for Z|X=x
```

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```
        self.cpd_net = cpd_net_type(
            latent_size,
            num_inputs=hidden_size,
            hidden_size=2*latent_size,
            p_drop=p_drop
        )

    def forward(self, x):
        h = self.encoder(x)
        return self.cpd_net(h)
```

[35]:
```
InferenceModel(GaussianCPDNet, latent_size=10)(torch.zeros(5, 1, 64, 64))
```

[35]:
```
Independent(Normal(loc: torch.Size([5, 10]), scale: torch.Size([5, 10])), 1)
```

[36]:
```
InferenceModel(partial(MoGCPDNet, num_components=3), latent_size=10)(torch.zeros(5, 1,␣
↪64, 64))
```

[36]:
```
MixtureSameFamily(
  Categorical(logits: torch.Size([5, 3])),
  Independent(Normal(loc: torch.Size([5, 3, 10]), scale: torch.Size([5, 3, 10])), 1))
```

We now have everything in place to use variational inference.

3.3 Neural Variational Inference

We will train our generative model via variational inference, for which we need to train an inference model along with it. We will use the ELBO objective, and gradient estimators based on score function estimation and differentiable reparameterisation.

It's common to refer to any one such model as a variational auto-encoder (VAE), especially so when using reparameterised gradients.

Let's start with score function estimation.

Given a data point x, we estimate the gradient of the ELBO with respect to λ by MC estimating the following expressions:

$$\nabla_\lambda \mathcal{E}(\lambda, \theta | x) = \mathbb{E}\left[r(z, x; \theta, \lambda) \nabla_\lambda \log \frac{p_{ZX}(z, x|\theta)}{q_{Z|X}(z|x, \lambda)} \right] \tag{4.92}$$

$$\nabla_\theta \mathcal{E}(\lambda, \theta | x) = \mathbb{E}\left[\nabla_\theta \log p_{ZX}(z, x|\theta) \right] \tag{4.93}$$

where the "reward" function in the gradient estimator for λ is

$$r(z, x; \theta, \lambda) = \log p_{X|Z}(x|z, \theta) \tag{4.94}$$

And, because this gradient estimator is rather noisy, it's commong to transform the reward function by further employing control variates. The simplest control variates are functions of x and possibly of θ and λ, but not a function of the action z with respect to which we evaluate the reward function. We will implement those as wrappers around the reward function. So, let's start by agreeing on the API of our control variates.

[37]:
```
class VarianceReduction(nn.Module):
    """
    We will be using simple forms of control variates for variance reduction.
    These are transformations of the reward that are independent of the sampled
    latent variable, but they can, in principle, depend on x, and on the
    parameters of the generative and inference model.

    Some of these are trainable components, thus they also contribute to the loss.
    """

    def __init__(self):
        super().__init__()

    def forward(self, r, x, q, r_fn):
        """
        Return the transformed reward and a contribution to the loss.

        r: a batch of rewards
        x: a batch of observations
        q: policy
        r_fn: reward function
        """
        return r, torch.zeros_like(r)
```

In case a reparameterisation trick is available for the approximate posterior, we can MC estimate the following expressions:

$$\nabla_\lambda \mathcal{E}(\lambda, \theta | x) = \mathbb{E}_{\epsilon \sim s(\cdot)} \left[\nabla_\lambda \log \frac{p_{XZ}(x, Z = \mathcal{T}(\epsilon, \lambda) | \theta)}{q_{Z|X}(Z = \mathcal{T}(\epsilon, \lambda) | x, \lambda)} \right] \tag{4.95}$$

and

$$\nabla_\theta \mathcal{E}(\lambda, \theta | x) = \mathbb{E}_{\epsilon \sim s(\cdot)} \left[\nabla_\theta \log \frac{p_{XZ}(x, Z = \mathcal{T}(\epsilon, \lambda) | \theta)}{q_{Z|X}(Z = \mathcal{T}(\epsilon, \lambda) | x, \lambda)} \right] \tag{4.96}$$

Gradients of these kind are commonly referred to as *path derivatives*. We don't need to implement the path derivatives ourselves, nor the transformations, rather we use a distribution object which supports an `rsample` method (for "reparameterised sample"), this distribution will be able to assess the density of the sample should we need it and if we obtained the sample via `rsample` the path derivative will be automatically available to backprop.

If KL divergence from the prior to the approximate posterior is computable, we use a different gradient estimator for λ and θ, namely:

$$\nabla_\lambda \mathcal{E}(\lambda, \theta | x) = \mathbb{E}_{\epsilon \sim s(\cdot)} \left[\nabla_\lambda \log p_{X|Z}(x | Z = \mathcal{T}(\epsilon, \lambda), \theta) \right] - \nabla_\lambda \mathrm{KL}(q_{Z|X} || p_Z) \tag{4.97}$$

and

$$\nabla_\theta \mathcal{E}(\lambda, \theta | x) = \mathbb{E}_{\epsilon \sim s(\cdot)} \left[\nabla_\theta \log p_{X|Z}(x | Z = \mathcal{T}(\epsilon, \lambda), \theta) \right] - \nabla_\theta \mathrm{KL}(q_{Z|X} || p_Z) \tag{4.98}$$

Recall that, in practice, we will need to design a surrogate loss: a node in the computation graph whose backward corresponds to the gradient estimator we want. Check carefully the changes we made to the forward method of the NVIL class.

Now we can work on our general NVIL model. The following class implements the NVIL objective as well as a lot of helper code to manipulate the model components in interesting ways (e.g., sampling, sampling conditionally, estimating marginal density, etc.)

[38]:
```
class NVIL(nn.Module):
    """
    A generative model p(z)p(x|z) and an approximation q(z|x) to that
     model's true posterior.

    The approximation is estimated to maximise the ELBO, and so is the joint
     distribution.
    """

    def __init__(self, gen_model: JointDistribution, inf_model: InferenceModel, cv_model:
↪ VarianceReduction):
        """
        gen_model: p(z)p(x|z)
        inf_model: q(z|x) which approximates p(z|x)
        cv_model: optional transformations of the reward
        """
        super().__init__()
        self.gen_model = gen_model
        self.inf_model = inf_model
        self.cv_model = cv_model

    def gen_params(self):
        return self.gen_model.parameters()

    def inf_params(self):
        return self.inf_model.parameters()

    def cv_params(self):
        return self.cv_model.parameters()

    def sample(self, batch_size, sample_size=None, oversample=False):
        """
        A sample from the joint distribution:
            z ~ prior
            x|z ~ obs model
        batch_size: number of samples in a batch
        sample_size: if None, the output tensor has shape [batch_size] + data_shape
            if 1 or more, the output tensor has shape [sample_size, batch_size] + data_
↪shape
            while batch_size controls a parallel computation,
            sample_size controls a sequential computation (a for loop)
        oversample: if True, samples z (batch_size times), hold it fixed,
            and sample x (sample_size times)
        """
        pz = self.gen_model.prior((batch_size,))
        samples = [None] * (sample_size or 1)
        px_z = self.gen_model.obs_model(pz.sample()) if oversample else None
        for k in range(sample_size or 1):
            if not oversample:
```

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```
                px_z = self.gen_model.obs_model(pz.sample())
            samples[k] = px_z.sample()
        x = torch.stack(samples)
        return x if sample_size else x.squeeze(0)

    def cond_sample(self, x, sample_size=None, oversample=False):
        """
        Condition on x and draw a sample:
            z|x ~ inf model
            x'|z ~ obs model

        x: a batch of seed data samples
        sample_size: if None, the output tensor has shape [batch_size] + data_shape
            if 1 or more, the output tensor has shape [sample_size, batch_size] + data_
↪shape
            sample_size controls a sequential computation (a for loop)
        oversample: if True, samples z (batch_size times), hold it fixed,
            and sample x' (sample_size times)
        """
        qz = self.inf_model(x)
        samples = [None] * (sample_size or 1)
        px_z = self.gen_model.obs_model(qz.sample()) if oversample else None
        for k in range(sample_size or 1):
            if not oversample:
                px_z = self.gen_model.obs_model(qz.sample())
            samples[k] = px_z.sample()
        x = torch.stack(samples)
        return x if sample_size else x.squeeze(0)

    def log_prob(self, z, x):
        """
        The log density of the joint outcome under the generative model
        z: [batch_size, latent_dim]
        x: [batch_size] + data_shape
        """
        return self.gen_model.log_prob(z=z, x=x)

    def DRL(self, x, sample_size=None):
        """
        MC estimates of a model's
            * distortion D
            * rate R
            * and log-likelihood L
        The estimates are based on single data points
         but multiple latent samples.

        x: batch_shape + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        """
        sample_size = sample_size or 1
        obs_dims = len(self.gen_model.cpd_net.outcome_shape)
```

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```
        batch_shape = x.shape[:-obs_dims]
        with torch.no_grad():
            qz = self.inf_model(x)
            pz = self.gen_model.prior(batch_shape)
            try:  # not every design admits tractable KL
                R = td.kl_divergence(qz, pz)
            except NotImplementedError:
                # MC estimation of KL(q(z|x)||p(z))
                z = qz.sample((sample_size,))
                R = (qz.log_prob(z) - pz.log_prob(z)).mean(0)
            D = 0
            ratios = [None] * sample_size
            for k in range(sample_size):
                z = qz.sample()
                px_z = self.gen_model.obs_model(z)
                ratios[k] = pz.log_prob(z) + px_z.log_prob(x) - qz.log_prob(z)
                D = D - px_z.log_prob(x)
            ratios = torch.stack(ratios, dim=-1)
            L = torch.logsumexp(ratios, dim=-1) - np.log(sample_size)
            D = D / sample_size
            return D, R, L

    def elbo(self, x, sample_size=None):
        """
        An MC estimate of ELBO = -D -R

        x: [batch_size] + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        """
        D, R, _ = self.DRL(x, sample_size=sample_size)
        return -D -R

    def log_prob_estimate(self, x, sample_size=None):
        """
        An importance sampling estimate of log p(x)

        x: [batch_size] + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        """
        _, _, L = self.DRL(x, sample_size=sample_size)
        return L

    def forward(self, x, sample_size=None, rate_weight=1.):
        """
        A surrogate for an MC estimate of - grad ELBO

        x: [batch_size] + data_shape
        sample_size: if 1 or more, we use multiple samples
            sample_size controls a sequential computation (a for loop)
        cv: optional module for variance reduction
```

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```
        """
        sample_size = sample_size or 1
        obs_dims = len(self.gen_model.cpd_net.outcome_shape)
        batch_shape = x.shape[:-obs_dims]

        qz = self.inf_model(x)
        pz = self.gen_model.prior(batch_shape)

        # we can *always* make use of the score function estimator (SFE)
        use_sfe = True

        # these 3 log densities will contribute to the different parts of the objective
        log_p_x_z = 0.
        log_p_z = 0.
        log_q_z_x = 0.

        # these quantities will help us compute the SFE part of the objective
        # (if needed)
        sfe = 0
        reward = 0
        cv_reward = 0
        raw_r = 0
        cv_loss = 0

        for _ in range(sample_size):

            # Obtain a sample
            if qz.has_rsample:  # this is how td objects tell us whether they are␣
↪continuously reparameterisable
                z = qz.rsample()
                use_sfe = False  # with path derivatives, we do not need SFE
            else:
                z = qz.sample()

            # Parameterise the observational model
            px_z = self.gen_model.obs_model(z)

            # Compute all three relevant densities:
            # p(x|z,theta)
            log_p_x_z = log_p_x_z + px_z.log_prob(x)
            # q(z|x,lambda)
            log_q_z_x = log_q_z_x + qz.log_prob(z)
            # p(z|theta)
            log_p_z = log_p_z + pz.log_prob(z)

            # Compute the "reward" for SFE
            raw_r = log_p_x_z + log_p_z - log_q_z_x

            # Apply variance reduction techniques
            r, l = self.cv_model(raw_r.detach(), x=x, q=qz, r_fn=lambda a: self.gen_
↪model(a).log_prob(x))
            cv_loss = cv_loss + l
```

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```
            # SFE part for updating lambda
            sfe = sfe + r.detach() * qz.log_prob(z)

        # Compute the sample mean for the different terms
        sfe = (sfe / sample_size)
        cv_loss = cv_loss / sample_size
        log_p_x_z = log_p_x_z / sample_size
        log_p_z = log_p_z / sample_size
        log_q_z_x = log_q_z_x / sample_size

        D = - log_p_x_z
        try:  # not every design admits tractable KL
            R = td.kl_divergence(qz, pz)
        except NotImplementedError:
            R = log_q_z_x - log_p_z

        if use_sfe:
            # the first two terms update theta
            # the last term updates lambda
            elbo_grad_surrogate = log_p_x_z + log_p_z + sfe
            # note that the term (log_p_x_z + log_p_z) is also part of sfe
            # but there it is detached, meaning that it won't contribute to
            # grad theta
        else:
            # without SFE, we can use the classic form of the ELBO
            elbo_grad_surrogate = -D - R

        loss = -elbo_grad_surrogate + cv_loss

        return {'loss': loss.mean(0), 'ELBO': (-D -R).mean(0).item(), 'D': D.mean(0).
↪item(), 'R': R.mean(0).item(), 'cv_loss': cv_loss.mean(0).item()}
```

Here's an example

[39]:
```
vae = NVIL(
    JointDistribution(
        GaussianPriorNet(10),
        BinarizedImageModel(
            num_channels=img_shape[0],
            width=img_shape[1],
            height=img_shape[2],
            latent_size=10,
            p_drop=0.1,
            decoder_type=build_ffnn_decoder
        )
    ),
    InferenceModel(
        cpd_net_type=GaussianCPDNet,
        latent_size=10,
        num_channels=img_shape[0],
        width=img_shape[1],
```

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```
        height=img_shape[2],
        encoder_type=build_ffnn_encoder
    ),
    VarianceReduction()
)
vae
```

[39]:
```
NVIL(
  (gen_model): JointDistribution(
    (prior_net): GaussianPriorNet()
    (cpd_net): BinarizedImageModel(
      (decoder): Sequential(
        (0): Dropout(p=0.1, inplace=False)
        (1): Linear(in_features=10, out_features=512, bias=True)
        (2): ReLU()
        (3): Dropout(p=0.1, inplace=False)
        (4): Linear(in_features=512, out_features=512, bias=True)
        (5): ReLU()
        (6): Dropout(p=0.1, inplace=False)
        (7): Linear(in_features=512, out_features=4096, bias=True)
        (8): ReshapeLast()
      )
    )
  )
  (inf_model): InferenceModel(
    (encoder): Sequential(
      (0): FlattenImage()
      (1): Dropout(p=0.0, inplace=False)
      (2): Linear(in_features=4096, out_features=512, bias=True)
      (3): ReLU()
      (4): Dropout(p=0.0, inplace=False)
      (5): Linear(in_features=512, out_features=512, bias=True)
      (6): ReLU()
      (7): Dropout(p=0.0, inplace=False)
      (8): Linear(in_features=512, out_features=1024, bias=True)
    )
    (cpd_net): GaussianCPDNet(
      (encoder): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=1024, out_features=20, bias=True)
        (2): ReLU()
      )
      (locs): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=20, out_features=10, bias=True)
        (2): ReshapeLast()
      )
      (scales): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=20, out_features=10, bias=True)
        (2): Softplus(beta=1, threshold=20)
        (3): ReshapeLast()
```

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```
      )
    )
  )
  (cv_model): VarianceReduction()
)
```

[40]:
```
for x, y in train_loader:
    print('x.shape:', x.shape)
    print(vae(x))
    break
```

```
x.shape: torch.Size([64, 1, 64, 64])
{'loss': tensor(2845.1970, grad_fn=<MeanBackward1>), 'ELBO': -2845.197021484375, 'D':␣
↪2843.9189453125, 'R': 1.27774977684021, 'cv_loss': 0.0}
```

3.3.1 Training algorithm

We have up to three components (recall that some control variates can have their own parameters), so we will be manipulating up to three optimisers:

[41]:
```
class OptCollection:

    def __init__(self, gen, inf, cv=None):
        self.gen = gen
        self.inf = inf
        self.cv = cv

    def zero_grad(self):
        self.gen.zero_grad()
        self.inf.zero_grad()
        if self.cv:
            self.cv.zero_grad()

    def step(self):
        self.gen.step()
        self.inf.step()
        if self.cv:
            self.cv.step()
```

Here's some helper code to assess and train the model

[42]:
```
from collections import defaultdict, OrderedDict
from tqdm.auto import tqdm


def assess(model, sample_size, dl, device):
    """
    Wrapper for estimating a model's ELBO, distortion, rate, and log-likelihood
     using all data points in a data loader.
    """
    D = 0
```

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```
    R = 0
    L = 0
    data_size = 0
    with torch.no_grad():
        for batch_x, batch_y in dl:
            Dx, Rx, Lx = model.DRL(batch_x.to(device), sample_size=sample_size)
            D = D + Dx.sum(0)
            R = R + Rx.sum(0)
            L = L + Lx.sum(0)
            data_size += batch_x.shape[0]
    D = D / data_size
    R = R / data_size
    L = L / data_size
    return {'ELBO': (-D -R).item(), 'D': D.item(), 'R': R.item(), 'L': L.item()}


def train_vae(model: NVIL, opts: OptCollection,
    training_data, dev_data,
    batch_size=64, num_epochs=10, check_every=10,
    sample_size_training=1,
    sample_size_eval=10,
    grad_clip=5.,
    num_workers=2,
    device=torch.device('cuda:0')
    ):
    """
    model: pytorch model
    optimiser: pytorch optimiser
    training_corpus: a TaggedCorpus for trianing
    dev_corpus: a TaggedCorpus for dev
    batch_size: use more if you have more memory
    num_epochs: use more for improved convergence
    check_every: use less to check performance on dev set more often
    device: where we run the experiment

    Return a log of quantities computed during training (for plotting)
    """
    batcher = DataLoader(training_data, batch_size, shuffle=True, num_workers=num_
↪workers, pin_memory=True)
    dev_batcher = DataLoader(dev_data, batch_size, num_workers=num_workers, pin_
↪memory=True)

    total_steps = num_epochs * len(batcher)
    log = defaultdict(list)

    step = 0
    model.eval()
    for k, v in assess(model, sample_size_eval, dev_batcher, device=device).items():
        log[f"dev.{k}"].append((step, v))

    with tqdm(range(total_steps)) as bar:
        for epoch in range(num_epochs):
```

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```
            for batch_x, batch_y in batcher:
                model.train()
                opts.zero_grad()

                loss_dict = model(
                    batch_x.to(device),
                    sample_size=sample_size_training,
                )
                for metric, value in loss_dict.items():
                    log[f'training.{metric}'].append((step, value))

                loss_dict['loss'].backward()

                nn.utils.clip_grad_norm_(
                    model.parameters(),
                    grad_clip
                )
                opts.step()

                bar_dict = OrderedDict()
                for metric, value in loss_dict.items():
                    bar_dict[f'training.{metric}'] = f"{loss_dict[metric]:.2f}"
                for metric in ['ELBO', 'D', 'R', 'L']:
                    bar_dict[f"dev.{metric}"] =  "{:.2f}".format(log[f"dev.{metric}"][-
↪1][1])
                bar.set_postfix(bar_dict)
                bar.update()

                if step % check_every == 0:
                    model.eval()
                    for k, v in assess(model, sample_size_eval, dev_batcher,␣
↪device=device).items():
                        log[f"dev.{k}"].append((step, v))

                step += 1


    model.eval()
    for k, v in assess(model, sample_size_eval, dev_batcher, device=device).items():
        log[f"dev.{k}"].append((step, v))

    return log
```

And, finally, some code to help inspect samples

[43]:
```
def inspect_lvm(model, dl, device):
    for x, y in dl:

        x_ = model.sample(16, 4, oversample=True).cpu().reshape(-1, 1, 64, 64)
        plt.figure(figsize=(16,8))
        plt.axis('off')
        plt.imshow(make_grid(x_, nrow=16).permute((1, 2, 0)))
```

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```
        plt.title("Prior samples")
        plt.show()

        plt.figure(figsize=(16,8))
        plt.axis('off')
        plt.imshow(make_grid(x, nrow=16).permute((1, 2, 0)))
        plt.title("Observations")
        plt.show()

        x_ = model.cond_sample(x.to(device)).cpu().reshape(-1, 1, 64, 64)
        plt.figure(figsize=(16,8))
        plt.axis('off')
        plt.imshow(make_grid(x_, nrow=16).permute((1, 2, 0)))
        plt.title("Conditional samples")
        plt.show()

        break
```

3.3.2 Variance reduction

Here are some concrete strategies for variance reduction. You can skip those in a first pass.

[44]:
```
class CentredReward(VarianceReduction):
    """
    This control variate does not have trainable parameters,
     it maintains a running estimate of the average reward and updates
     a batch of rewards by computing reward - avg.
    """

    def __init__(self, alpha=0.9):
        super().__init__()
        self._alpha = alpha
        self._r_mean = 0.

    def forward(self, r, x=None, q=None, r_fn=None):
        """
        Centre the reward and update running estimates of mean.
        """
        with torch.no_grad():
            # sufficient statistics for next updates
            r_mean = torch.mean(r, dim=0)
            # centre the signal
            r = r - self._r_mean
            # update running estimate of mean
            self._r_mean = (1-self._alpha) * self._r_mean + self._alpha * r_mean.item()
            return r, torch.zeros_like(r)


class ScaledReward(VarianceReduction):
    """
    This control variate does not have trainable parameters,
```

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```
     it maintains a running estimate of the reward's standard deviation and
     updates a batch of rewards by computing reward / maximum(stddev, 1).
    """

    def __init__(self, alpha=0.9):
        super().__init__()
        self._alpha = alpha
        self._r_std = 1.0

    def forward(self, r, x=None, q=None, r_fn=None):
        """
        Scale the reward by a running estimate of std, and also update the estimate.
        """
        with torch.no_grad():
            # sufficient statistics for next updates
            r_std = torch.std(r, dim=0)
            # standardise the signal
            r = r / self._r_std
            # update running estimate of std
            self._r_std = (1-self._alpha) * self._r_std + self._alpha * r_std.item()
            # it's not safe to standardise with scales less than 1
            self._r_std = np.maximum(self._r_std, 1.)
            return r, torch.zeros_like(r)


class SelfCritic(VarianceReduction):
    """
    This control variate does not have trainable parameters,
     it updates a batch of rewards by computing reward - reward', where
     reward' is (log p(X=x|Z=z')).detach() assessed for a novel sample
     z' ~ Z|X=x.
    """

    def __init__(self):
        super().__init__()

    def forward(self, r, x, q, r_fn):
        """
        Standardise the reward and update running estimates of mean/std.
        """
        with torch.no_grad():
            z = q.sample()
            r = r - r_fn(z, x)
            return r, torch.zeros_like(r)


class Baseline(VarianceReduction):
    """
    An input-dependent baseline implemented as an MLP.
    The trainable parameters are adjusted via MSE.
    """
```

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```
    def __init__(self, num_inputs, hidden_size, p_drop=0.):
        super().__init__()
        self.baseline = nn.Sequential(
            FlattenImage(),
            nn.Dropout(p_drop),
            nn.Linear(num_inputs, hidden_size),
            nn.ReLU(),
            nn.Dropout(p_drop),
            nn.Linear(hidden_size, 1)
        )

    def forward(self, r, x, q=None, r_fn=None):
        """
        Return r - baseline(x) and Baseline's loss.
        """
        # batch_shape + (1,)
        r_hat = self.baseline(x)
        # batch_shape
        r_hat = r_hat.squeeze(-1)
        loss = (r - r_hat)**2
        return r - r_hat.detach(), loss


class CVChain(VarianceReduction):

    def __init__(self, *args):
        super().__init__()
        if len(args) == 1 and isinstance(args[0], OrderedDict):
            for key, module in args[0].items():
                self.add_module(key, module)
        else:
            for idx, module in enumerate(args):
                self.add_module(str(idx), module)

    def forward(self, r, x, q, r_fn):
        loss = 0
        for cv in self._modules.values():
            r, l = cv(r, x=x, q=q, r_fn=r_fn)
            loss = loss + l
        return r, loss
```

3.3.3 Experiment

[45]:
```
seed_all()
my_device = torch.device('cuda:0')

model = NVIL(
    JointDistribution(
        GaussianPriorNet(10),
        BinarizedImageModel(
```

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```
            num_channels=img_shape[0],
            width=img_shape[1],
            height=img_shape[2],
            latent_size=10,
            p_drop=0.1
        )
    ),
    InferenceModel(
        latent_size=10,
        num_channels=img_shape[0],
        width=img_shape[1],
        height=img_shape[2],
        cpd_net_type=GaussianCPDNet # Gaussian prior and Gaussian posterior: this is a␣
↪classic VAE
    ),
    VarianceReduction(), # no variance reduction is needed for a VAE
    #CVChain(  # variance reduction helps SFE
    #    CentredReward(),
    #    #Baseline(np.prod(img_shape), 512), # this is how you would use a trained␣
↪baselined
    #    #ScaledReward()
    #)
).to(my_device)

opts = OptCollection(
    # Tips based on empirical practice:

    # Adam is the go-to choice for (reparameterised) VAEs
    opt.Adam(model.gen_params(), lr=5e-4, weight_decay=1e-6),
    opt.Adam(model.inf_params(), lr=1e-4),


    # Adam is not often a good choice for SFE-based optimisation
    #  a possible reason: SFE is too noisy and the design choices behind Adam
    #  were made having reparameterised gradients in mind
    #opt.RMSprop(model.gen_params(), lr=5e-4, weight_decay=1e-6),
    #opt.RMSprop(model.inf_params(), lr=1e-4),
    #opt.RMSprop(model.cv_params(), lr=1e-4, weight_decay=1e-6) # you need this if your␣
↪baseline has trainable parameters
)

model
```

[45]:
```
NVIL(
  (gen_model): JointDistribution(
    (prior_net): GaussianPriorNet()
    (cpd_net): BinarizedImageModel(
      (decoder): Sequential(
        (0): Dropout(p=0.1, inplace=False)
        (1): Linear(in_features=10, out_features=512, bias=True)
        (2): ReLU()
        (3): Dropout(p=0.1, inplace=False)
```

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```
        (4): Linear(in_features=512, out_features=512, bias=True)
        (5): ReLU()
        (6): Dropout(p=0.1, inplace=False)
        (7): Linear(in_features=512, out_features=4096, bias=True)
        (8): ReshapeLast()
      )
    )
  )
  (inf_model): InferenceModel(
    (encoder): Sequential(
      (0): FlattenImage()
      (1): Dropout(p=0.0, inplace=False)
      (2): Linear(in_features=4096, out_features=512, bias=True)
      (3): ReLU()
      (4): Dropout(p=0.0, inplace=False)
      (5): Linear(in_features=512, out_features=512, bias=True)
      (6): ReLU()
      (7): Dropout(p=0.0, inplace=False)
      (8): Linear(in_features=512, out_features=1024, bias=True)
    )
    (cpd_net): GaussianCPDNet(
      (encoder): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=1024, out_features=20, bias=True)
        (2): ReLU()
      )
      (locs): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=20, out_features=10, bias=True)
        (2): ReshapeLast()
      )
      (scales): Sequential(
        (0): Dropout(p=0.0, inplace=False)
        (1): Linear(in_features=20, out_features=10, bias=True)
        (2): Softplus(beta=1, threshold=20)
        (3): ReshapeLast()
      )
    )
  )
  (cv_model): VarianceReduction()
)
```

[46]:
```
log = train_vae(
    model=model,
    opts=opts,
    training_data=train_ds,
    dev_data=val_ds,
    batch_size=256,
    num_epochs=5,  # use more for better models
    check_every=100,
    sample_size_training=1,
    sample_size_eval=1,
```

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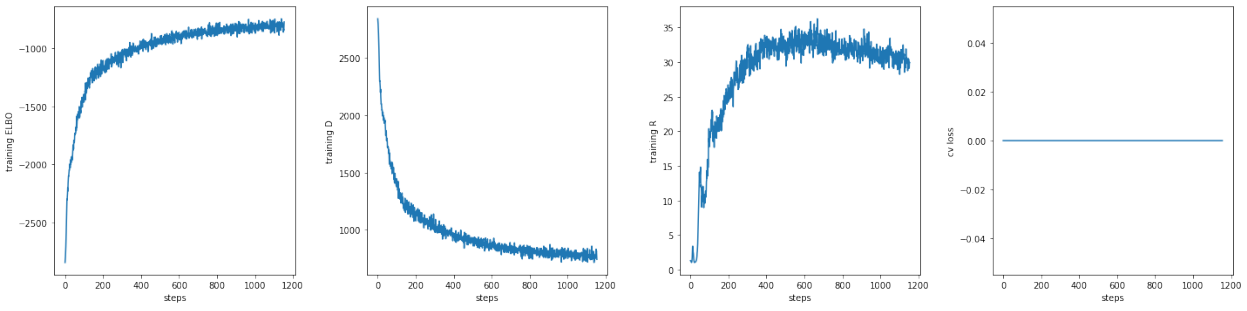
```
    grad_clip=5.,
    device=my_device
)
```

```
  0%|          | 0/1155 [00:00<?, ?it/s]
```

[47]:
```
log.keys()
```

[47]:
```
dict_keys(['dev.ELBO', 'dev.D', 'dev.R', 'dev.L', 'training.loss', 'training.ELBO',
↪'training.D', 'training.R', 'training.cv_loss'])
```

[48]:
```
fig, axs = plt.subplots(1, 3 + int('training.cv_loss' in log), sharex=True, sharey=False,
↪ figsize=(20, 5))

_ = axs[0].plot(np.array(log['training.ELBO'])[:,0], np.array(log['training.ELBO'])[:,1])
_ = axs[0].set_ylabel("training ELBO")
_ = axs[0].set_xlabel("steps")

_ = axs[1].plot(np.array(log['training.D'])[:,0], np.array(log['training.D'])[:,1])
_ = axs[1].set_ylabel("training D")
_ = axs[1].set_xlabel("steps")

_ = axs[2].plot(np.array(log['training.R'])[:,0], np.array(log['training.R'])[:,1])
_ = axs[2].set_ylabel("training R")
_ = axs[2].set_xlabel("steps")

if 'training.cv_loss' in log:
    _ = axs[3].plot(np.array(log['training.cv_loss'])[:,0], np.array(log['training.cv_
↪loss'])[:,1])
    _ = axs[3].set_ylabel("cv loss")
    _ = axs[3].set_xlabel("steps")

fig.tight_layout(h_pad=2, w_pad=2)
```



[49]:
```
fig, axs = plt.subplots(1, 4, sharex=True, sharey=False, figsize=(20, 5))

_ = axs[0].plot(np.array(log['dev.ELBO'])[:,0], np.array(log['dev.ELBO'])[:,1])
_ = axs[0].set_ylabel("dev ELBO")
_ = axs[0].set_xlabel("steps")

_ = axs[1].plot(np.array(log['dev.D'])[:,0], np.array(log['dev.D'])[:,1])
_ = axs[1].set_ylabel("dev D")
```

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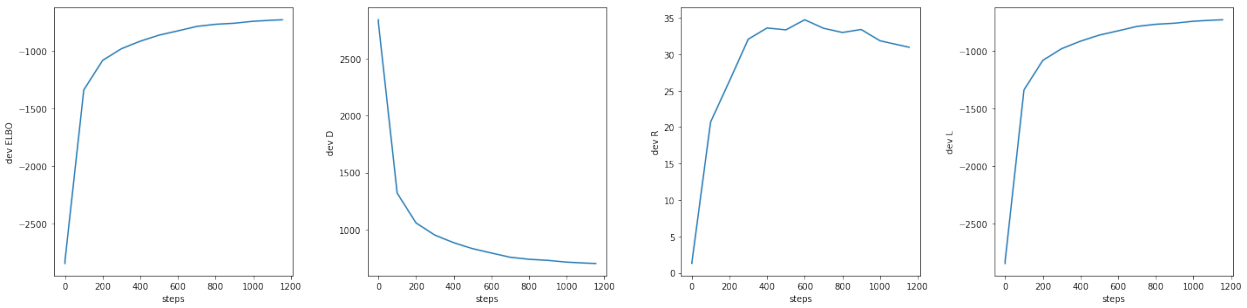
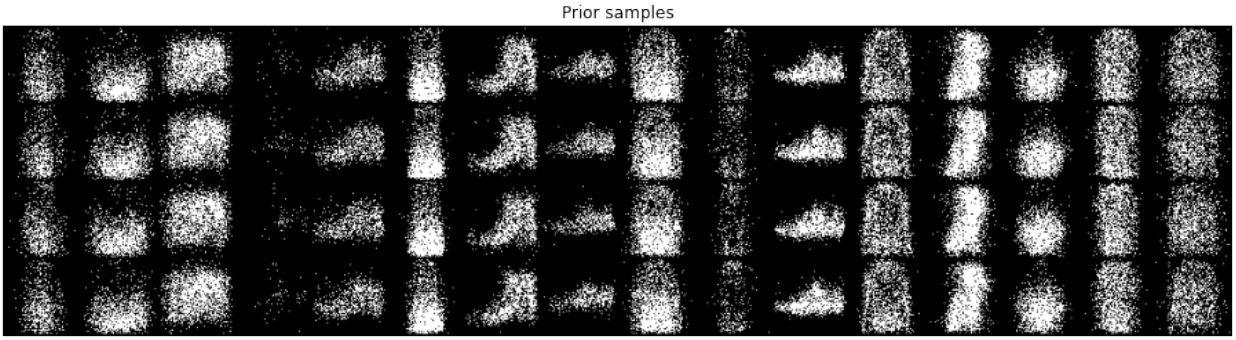
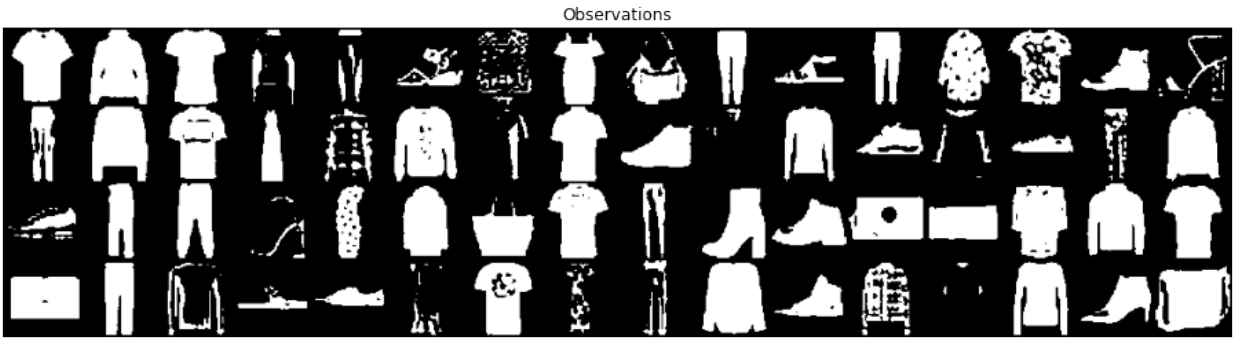
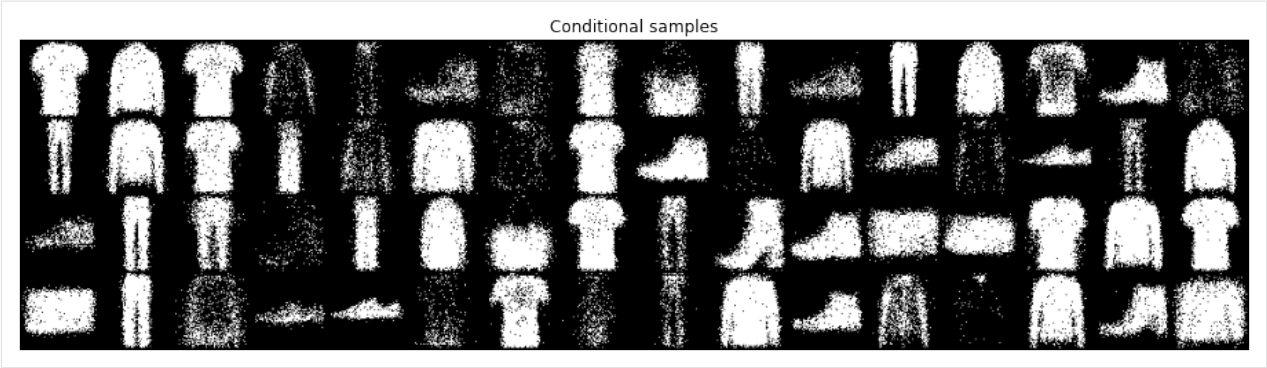
```
_ = axs[1].set_xlabel("steps")

_ = axs[2].plot(np.array(log['dev.R'])[:,0], np.array(log['dev.R'])[:,1])
_ = axs[2].set_ylabel("dev R")
_ = axs[2].set_xlabel("steps")

_ = axs[3].plot(np.array(log['dev.L'])[:,0], np.array(log['dev.L'])[:,1])
_ = axs[3].set_ylabel("dev L")
_ = axs[3].set_xlabel("steps")

fig.tight_layout(h_pad=2, w_pad=2)
```



[50]:
```
inspect_lvm(model, DataLoader(val_ds, 64, num_workers=2, pin_memory=True), my_device)
```







4.45.5 4. Beyond

There are various things you can try.

You can try to use a **trainable prior**. If you do, you will probably note that it is not trivial how to get the prior to be used in an interesting way. In fact, trained priors are completely data-driven, and there's no reason to believe that an NN will find a "data-driven" explanation of the data that is anything like what you would like it to. If you want the different components of your prior to specialise to certain types of output, you will need to design stronger pressures. For example, you may use some degree of annotation to inform what each component should typically be responsible for. Ideas that dispense with the need for annotation will have to focus on the architecture of the decoder or on other penalties in the loss. For example, a decoder that is built with some geometric properties.

If you use a trainable prior, it is a good idea to try and visualise what the final prior looks like. You can try sampling from it and plotting histograms of the different coordinates of the samples. You can flatten the samples and inspect the coordinates marginally, you can also use other plotting tools (see some examples from seaborn) to spot dependency, for example. And, of course, you can always use tools for dimensionality reduction (eg, t-SNE).

You can try to use a **stronger posterior approximation** that is reparameterisable. A good idea is to build a bijective transformation (ie., a normalising flow).

You can try to **improve the gradient estimator** of the mixture of mean field families. Within a mixture of C components that are each reparameterisable, only the component assigmment is a discrete operation, so with access to the sampling procedure internal to mixture, one can design a customised gradient estimator that updates $\omega(x;\lambda)$ through SFE, but updates $\mu(x;\lambda)$ and $\sigma(x;\lambda)$ through reparameterisation.

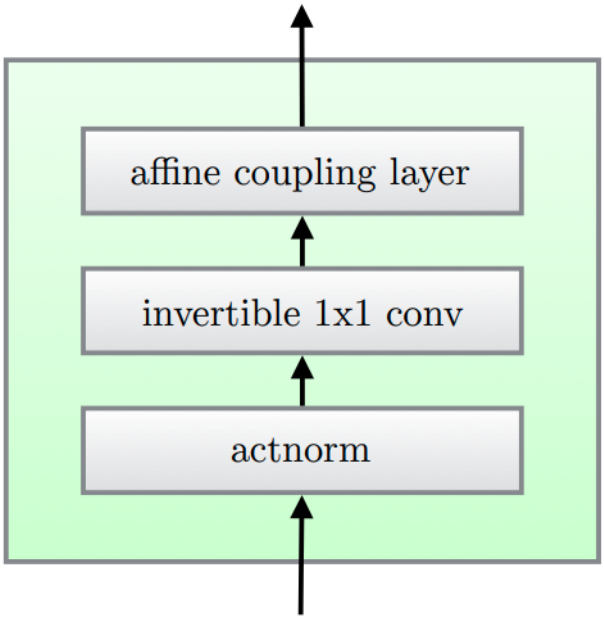
4.46 AGM - Advanced Topics in Normalizing Flows - 1x1 convolution

Filled notebook:
Authors: Cyril Hsu

4.46.1 Introduction

The Glow, a flow-based generative model extends the previous invertible generative models, NICE and RealNVP, and simplifies the architecture by replacing the reverse permutation operation on the channel ordering with **Invertible 1x1 Convolutions**. Glow is famous for being the one of the first flow-based models that works on high resolution images and enables manipulation in latent space. Let's have a look at the interactive demonstration from OpenAI.

Glow consists of a series of steps of flow. Each step of flow comprises **Actnorm** followed by an **Invertible 1×1 Convolution**, and finally a **Coupling Layer**.



Actnorm performs an affine transformation with a scale and bias parameter per channel, similar to that of batch normalization, but works on mini-batch size 1. The statistics (mean and std), however, are only calculated once to initialize the scale and bias parameters.

Invertible 1×1 Convolution with equal number of input and output channels is a generalization of any permutation of the channel ordering. Recall the operation between layers of the RealNVP flow, the ordering of channels is switched so that all the data dimensions have a chance to be mixed. 1x1 convolution is proposed to replace this fixed permutation with a learned invertible operation.

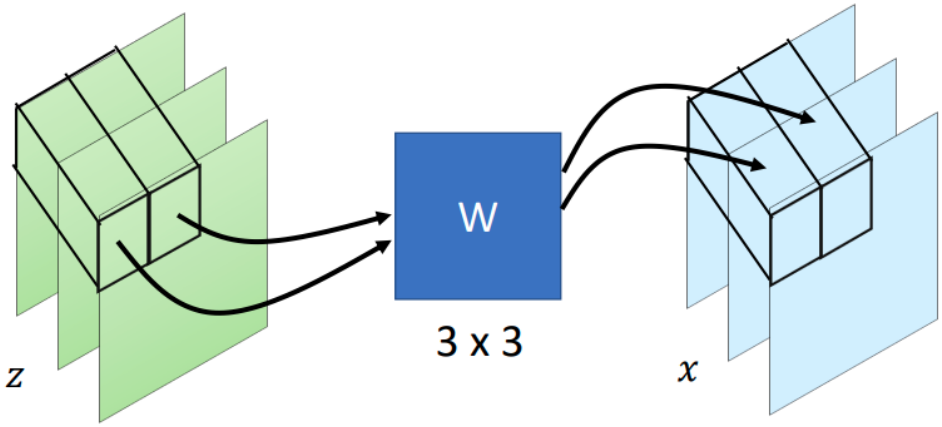
Coupling Layer is a powerful reversible transformation where the forward function, the reverse function and the logdeterminant are computationally efficient. The design is the same as in RealNVP.

Description	Function	Reverse Function	Log-determinant
Actnorm.	$\forall i,j : \mathbf{y}_{i,j} = \mathbf{s} \odot \mathbf{x}_{i,j} + \mathbf{b}$	$\forall i,j : \mathbf{x}_{i,j} = (\mathbf{y}_{i,j} - \mathbf{b})/\mathbf{s}$	$h \cdot w \cdot \texttt{sum}(\log \lvert\mathbf{s}\rvert)$
Invertible 1×1 convolution. $\mathbf{W} : [c \times c]$.	$\forall i,j : \mathbf{y}_{i,j} = \mathbf{W}\mathbf{x}_{i,j}$	$\forall i,j : \mathbf{x}_{i,j} = \mathbf{W}^{-1}\mathbf{y}_{i,j}$	$h \cdot w \cdot \log \lvert \det(\mathbf{W}) \rvert$ or $h \cdot w \cdot \texttt{sum}(\log \lvert\mathbf{s}\rvert)$
Affine coupling layer.	$\mathbf{x}_a, \mathbf{x}_b = \texttt{split}(\mathbf{x})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{x}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{y}_a = \mathbf{s} \odot \mathbf{x}_a + \mathbf{t}$ $\mathbf{y}_b = \mathbf{x}_b$ $\mathbf{y} = \texttt{concat}(\mathbf{y}_a, \mathbf{y}_b)$	$\mathbf{y}_a, \mathbf{y}_b = \texttt{split}(\mathbf{y})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{y}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{x}_a = (\mathbf{y}_a - \mathbf{t})/\mathbf{s}$ $\mathbf{x}_b = \mathbf{y}_b$ $\mathbf{x} = \texttt{concat}(\mathbf{x}_a, \mathbf{x}_b)$	$\texttt{sum}(\log(\lvert\mathbf{s}\rvert))$

In this tutorial, we will be focusing on the implementation of invertible 1x1 convolution layer.

4.46.2 Invertible 1x1 convolution

Given an input of shape $H \times W \times C$ applied with a 1x1 convolution with C filters, meaning the output tensor shape is also going to be $H \times W \times C$. Thus, each layer has a set of weights W with $C \times C$ values. The forward operation acts just like a typical convolution, while the inverse operation can be computed by simply applying a convolution with W^{-1} weights.



Enough descriptions! Now let's take a look at the code.

[14]:
```
import torch
from torch import nn
from torch.nn import functional as F

class InvConv2d(nn.Module):
    def __init__(self, in_channel):
        super().__init__()

        weight = torch.randn(in_channel, in_channel)
        # use the Q matrix from QR decomposition as the initial weight to make sure it's␣
↪invertible
        q, _ = torch.qr(weight)
```

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```
        weight = q.unsqueeze(2).unsqueeze(3)
        self.weight = nn.Parameter(weight)

    def forward(self, input, logdet, reverse=False):
        _, _, height, width = input.shape

        # You can also use torch.slogdet(self.weight)[1] to summarize the operations␣
↪below\n",
        dlogdet = (
            height * width * torch.log(torch.abs(torch.det(self.weight.squeeze())))
        )

        if not reverse:
            out = F.conv2d(input, self.weight)
            logdet = logdet + dlogdet

        else:
            out = F.conv2d(input, self.weight.squeeze().inverse().unsqueeze(2).
↪unsqueeze(3))
            logdet = logdet - dlogdet

        return out, logdet
```

Note that to calculate the determinant of W could be computationally expensive, thus there's also an implementation which utilizes LU decomposition to speed up, as suggested in the Glow paper.

The idea is to parameterizing W directly in its LU decomposition:

$$W = PL(U + \text{diag}(s)),$$

where P is a permutation matrix, L is a lower triangular matrix with ones on the diagonal, U is an upper triangular matrix with zeros on the diagonal, and s is a vector.

The log-determinant is then simply:

$$\log|\det(W)| = \sum(\log|s|)$$

Please check out the link above for the implementation.

A small pitfall

As you might notice, there's an inverse operation for the weight W involved when the **1x1 convolution** is forwarding reversely. As a result, an error can occur when the weight W is not invertible, even though it seldom happens.

To our best knowledge, there's no elegant solution to address this, but an easy way to workaround: If this happens unfortunately during the training, one can try to restart from the recent checkpoint.

A complete flow block

Now we have the **Invertible 1x1 Convolution**. Together with the aforementioned **Actnorm** and **Coupling Layer**, we are ready to try out the power of the Glow by plugging the block into the model we had in the NFs tutorial!

[21]:
```
class ActNorm(nn.Module):
    def __init__(self, in_channel):
        super().__init__()

        self.loc = nn.Parameter(torch.zeros(1, in_channel, 1, 1))
        self.log_scale = nn.Parameter(torch.zeros(1, in_channel, 1, 1))
        self.register_buffer("initialized", torch.tensor(0, dtype=torch.uint8))

    def initialize(self, input):

        with torch.no_grad():
            flatten = input.permute(1, 0, 2, 3).contiguous().view(input.shape[1], -1)
            mean = (
                flatten.mean(1)
                .unsqueeze(1)
                .unsqueeze(2)
                .unsqueeze(3)
                .permute(1, 0, 2, 3)
            )
            std = (
                flatten.std(1)
                .unsqueeze(1)
                .unsqueeze(2)
                .unsqueeze(3)
                .permute(1, 0, 2, 3)
            )

            self.loc.data.copy_(-mean)
            self.log_scale.data.copy_(-std.clamp_(min=1e-6).log())

    def forward(self, input, logdet, reverse=False):
        _, _, height, width = input.shape

        if self.initialized.item() == 0:
            self.initialize(input)
            self.initialized.fill_(1)

        dlogdet = height * width * torch.sum(self.log_scale)

        if not reverse:
            logdet += dlogdet
            return self.log_scale.exp() * (input + self.loc), logdet

        else:
            dlogdet *= -1
            logdet += dlogdet
            return input / self.log_scale.exp() - self.loc, logdet
```

A sample code for **Actnorm** is provided above.

As for **Coupling Layer**, please refer to the one in the NFs tutorial.

4.46.3 Conclusion

We've learned an advanced flow-based layer from the Glow model, an **Invertible 1x1 convolution**, which is adapted from the typical 1x1 convolution layers.

References

- Glow: Generative Flow with Invertible 1x1 Convolutions
- Glow: Better Reversible Generative Models
- https://github.com/rosinality/glow-pytorch
- Materials from NTU Speech Lab

4.47 HDL - Introduction to HyperParameter Tuning

Filled notebook:
Hyper-parameter tuning repository:
Authors: Samuele Papa

4.47.1 Introduction

This tutorial is meant as a description of the structure and features of the template GitHub repository to perform large scale hyperparameter tuning on a SLURM-based cluster using a combination of Pytorch Lightning, Hydra, Ax, MLFlow and Submitit.

The template is not meant to be the definitive way hyperparameter tuning should be performed. Instead, it is meant to be a very good example from which to pick the elements and the structure that make most sense for your own future projects. For example, MLFlow is not very good at comparing images from multiple runs, and if a qualitative evaluation is necessary, then it would be a good idea to include Tensorboard as an additional logging library. The use of SLURM was dictated by the popularity of the system and the fact that it is in use on the surfsara cluster, but the same template would work for other systems. Many more considerations and adaptations could be made at the discretion of the researcher.

4.47.2 The structure

```
.
├── hyperparameter_searcher
│   ├── __init__.py
│   ├── config
│   │   ├── data
│   │   │   └── mnist_config.py
│   │   ├── launcher
│   │   │   └── launcher_config.py
│   │   ├── logging
│   │   │   └── logging_config.py
```

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```
│   │   ├── model
│   │   │   └── mnist_module_config.py
│   │   ├── sweeper
│   │   │   └── sweeper_config.py
│   │   ├── trainer
│   │   │   └── trainer_config.py
│   │   ├── train_bayesian_config.py
│   │   └── train_grid_config.py
│   ├── data
│   │   ├── __init__.py
│   │   ├── dataloaders.py
│   │   └── mnist_datamodule.py
│   ├── loggers
│   │   ├── __init__.py
│   │   ├── loggers.py
│   │   └── mlflow_utils.py
│   ├── networks
│   │   ├── __init__.py
│   │   ├── components
│   │   │   ├── __init__.py
│   │   │   └── simple_dense_net.py
│   │   └── mnist_lightning_module.py
│   ├── utils
│   │   ├── __init__.py
│   │   └── io_utils.py
│   └── training_pipeline.py
├── scripts
│   ├── README.md
│   ├── hyperparameter_blueprint_bayesian.sh
│   └── hyperparameter_blueprint_grid.sh
├── tests
│   ├── __init__.py
│   └── tests_utils
│       ├── __init__.py
│       └── test_io_utils.py
├── environment.yml
├── .env
└── train.py
```

The main file of the whole repository is `train.py` in the root folder. From here the training procedure can run, and this is also the primary point that will be used for debugging the code. In the `tests` folder the eventual tests for the code being written will be placed, the `scripts` folder contains the scripts that we will be using for the hyperparameter search, and the `hyperparameter-searcher` folder is where the source code for all our experiments resides.

In this template, the source code for the experiments is divided into Python modules, that can be thought of as building components used to run the entire thing. Besides the modules, there is a file called `training_pipeline.py` which is where the training is defined, and that will be the only entry point to use the various modules from. In this template, only this file is present, however, often we will want to perform some additional analysis to our models after training, say creating nice visualizations with samples if we have a generative model, or computing a downstream task using the representations obtained. When this is the case, we will just need to add a new file, e.g. called `evaluation.py`, that will benefit from the already-defined modules and be used to load the model and run the evaluation.

The modules. In the experiment source code we have several modules. We can think of them as independent (as much as reasonable) packages that are used to perform a specific and complex task that can be re-used more than once or that

is completely logically separate from other modules. This modular approach that separates based on function and not based on experiment, forces us to think of code that can be used immediately by all experiments we will be running, and is easier to maintain in the future.

Next, we will be discussing the different components that we are using for config management, logging and hyperparameter tuning.

4.47.3 Hydra

Hydra configurations are usually defined through `.yaml` files. However, we can also define them manually using Python. By using Python-based config files we have more freedom in the definition of the configurations and in the re-usability of the code. The trade-off is more complexity in the management of the code, as all the configuration needs to be defined manually.

Hydra interfaces with your scripts using a decorator to the main function. This defines where to get the configs from, and which primary config file should be used to parse the arguments. In the case of this repository, the configuration is done through Python, so we don't need the `config_path`:

```
@hydra.main(config_path=None, config_name=os.environ["MAIN_CONFIG"])
```

The primary config file is the entry point for your configuration. Here, you define the command line parameters that you support and which default configurations are to be used. A default configuration, as the name suggests, is a file that contains some default arguments. In our case, these will be handy for defining default configurations of the various datasets and models that we support.

From command line, all already-define parameters can be changed, as well as new ones added. By default, you need to explicitly ask for an argument to be added, if this is not already defined in the config.

Overall, using Hydra is a very straightforward way to neatly organize you configurations and get closer to reproducible results.

Some observations

Hydra is used to manage the configuration of your experiments. All command line arguments and their processing can be handled through it. The are several advantages over using the traditional argument parser from Python. The first one is that we can more easily store and restore argument configurations. Another is that target classes can be defined directly in the configuration. A target class can then be initialized with the arguments given in the configuration. Think of what would happen if you wanted to switch between using `model_A` and `model_B` which are defined with the class `ModelA` and `ModelB`. From the config, you would say `model=model_A` and then in the code you would need a long if statement chain to select which class to launch with the given configuration, which in this case would be `ModelA`. Then, there would be several default parameters for this class that we would want to use, but would be hidden in the code. Instead, with Hydra you can more simply define the target class directly in the config file, which will be automatically selected when `model=model_A` is called in the command line. This will come automatically with all the parameters defined explicitly in the config file.

This only makes sense because the modular approach to config management allows for simple parameter switching when testing different models, datasets or when running different experiments entirely. Having modular configuration management simplifies the entire file structure as well, removing the need for separating different experiments in different folders, which can quickly become difficult to maintain as time goes on. Instead, each part of your project can be seen as a different packages, one dedicated for data handling, one for model definition, one for the logging, another for visualization and maybe also one for all the metrics that you want to test your models with. Such modularity would be very difficult without also having modular configurations, which Hydra handles very easily.

One thing that is important to highlight is that Hydra is not some magical wand that we can use to solve all our problems. Instead, Hydra takes its root in the elegant configuration management that Omegaconf already provides. Hydra is a handy extension of Omegaconf, with some features tailored for machine learning. When more complicated things need

to be done, do not hesitate to put your hands on what Hydra is doing and add your own code to make your workflow faster. Often, trying to work around the issue and use only the features available in the library slows you down more than you think.

4.47.4 MLFlow

MLFlow is a logging library, which is characterized by centralization of the logging, as to ease the process when multiple nodes are being used. Additionally, it provides a simplified way to compare the parameters that have been changed between runs, to get a quick overview of which change has made the most decise impact in the performance of the model.

MLFlow interfaces with the code through PyTorch Lightning. When the `Trainer` is instantiated, among the loggers passed is MLFlow. In the code, this will seem a bit opaque, as the initialization of the loggers is done through Hydra's instantiate (in file `training_pipeline.py`):

```
mlflow_logger = hydra.utils.instantiate(logger)
loggers.append(mlflow_logger)
```

Another important aspect is the **checkpoint**, which allows to store useful information and the model's weights through MLFlow as well. Using MLFlow in the checkpointing process is useful to centralize all the information (in file `training_pipeline.py`):

```
callbacks.append(
    hydra.utils.instantiate(callback, mlflow_logger=mlflow_logger)
)
```

Some observations

MLFlow is an excellent logging tool to keep track of your experiments. Where MLFlow shines is in its ability to quickly compare multiple runs of an hyperparameter search. Also, it centralizes everything, putting all of the things you need in a single location, which is extremely handy when running large scale experiments.

There are a few downsides to MLFlow, as it is not excellent with image logging and is overall lacking in the ability to compare different metrics and the qualitative performance of different models. When this is necessary for your models (which is the often the case for computer vision tasks) MLFlow needs to be supported by additional loggers, such as Tensorboard. This is easily done with Pythorch Lightning, just asking for multiple loggers in the Trainer.

4.47.5 Hyperparameter Search

Here, we will be using **Hydra** (with the Ax plugin) and **Submitit** to generate the jobs and submit them to the SLURM cluster.

These are the most fundamental parameters that need to be configured based on how many resources you have available to perform the search, that will be defined from the `.sh` script (code from `launcher_config.py` file):

```
@dataclass
class SlurmConfig(SlurmQueueConf):
    partition: str = "gpu_titanrtx_shared"
    gpus_per_node: int = 1
    tasks_per_node: int = 1
    cpus_per_task: int = 6
    mem_gb: int = 60
```

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```
    nodes: int = 1
    timeout_min: int = 1200  # how long can the job run
    array_parallelism: int = 2  # how many jobs can run simultaneously
```

The actual parameter search itself can be done in a *grid* or *bayesian* form. In the grid form, all combinations of the parameters are searched through, while in the bayesian form, the **Ax** sweeper will look for the best parameters to optimize a given metric, defined in the `optimized_metric` parameter. The syntax for defining what parameters should be *sweep*ed can be found in this Hydra documentation. The most fundamental ones are the following:

Choice. Select one between different options (here the example is different activation functions):

```
activation=choice(linear,relu)
```

Range. Sweeps the defined range based on the given step (here the example is a different lambda weight for regularization):

```
lambda=range(start=0,stop=10,step=2)  # 0,2,4,6,8
```

Some observations

Hyperparameter tuning is a task that requires an incredible amounts of resources. Always consider the computing time and available resources before starting large computational studies. Try with smaller tests, trying to understand if the model is working and what is the rough range of parameters before continuing.

4.47.6 Conclusion

We have seen how we have used a combination of Hydra, MLFlow, SubmitIt, and the Ax plugin in Hydra to perform bayesian or grid hyperparameter searches in a SLURM-based cluster. We have seen how it interfaces with a simple project and have observed some of the strength and pitfalls of the methods.

It is crucial to remember that this setup is meant as a guide, to introduce the useful tools that you may want to use and how they interface together. Ultimately, the best fit for any case will be determined by the specific circumstances that you are facing.

References

Reference Repository. https://github.com/NKI-AI/hyperparameter-search-template

Hydra. https://hydra.cc/

MLFlow. https://www.mlflow.org/docs/latest/index.html

Pytorch Lightning. https://www.pytorchlightning.ai/

Ax Sweeper. https://hydra.cc/docs/next/plugins/ax_sweeper/=

4.48 HDL - Introduction to Multi GPU Programming

Filled notebook:
Tutorial script files:
Recordings:
Authors: Samuele Papa

4.48.1 Introduction

Using multiple GPUs is a central part in scaling models to large datasets and obtain state of the art performance.

We have seen that, to control multiple GPUs, we need to understand the concepts of distributed computing. The core problem in distributed computing is the communication between nodes, which requires synchronization. Luckily, we are equipped with very limited communication tools, that minimize the chance that problems arise (the specifics are outside the scope of this course, to get more insight into the possible issues, look into concurrent programming, race conditions, deadlocks, resource starvation, semaphores and barriers, and the book Operating Systems Internals and Design Principles).

Tutorial content. To better understand the primitives of communication in a distributed environment, we will begin by looking at some very basic exercises where simple operations are performed. Then, we will look at a more realistic scenario, the computation of the loss in a one-layer classifier (*more* realistic, but still *very* simple). Finally, we will learn how to run full-scale training on multiple GPUs and multiple nodes using PyTorch Lightning.

Running the code

The code in these cells is not meant to be run with this notebook. Instead, the files provided should be used in an environment where multiple GPUs are available. This step is not required (all the outputs and explanation of the code are available here), but highly encouraged, as getting familiar with these concepts, especially the more simple primitives, will help when more cryptic errors start appearing in big projects.

Running the scripts can be done, for example, on the GPU partition of the LISA cluster (General Knowledge on how to use the cluster). After getting access using `ssh` (use WSL on Windows), we can setup the conda environment, by using the `module` package to load the correct anaconda version and then creating the environment based on the `environment.yml` file.

To upload the code, the `rsync` command can be used (on single files, it is possible to do it on folders by adding the `-r` option):

```
rsync file account@lisa-gpu.surfsara.nl:~/file
```

Then, the Anaconda module can be loaded and the environment created using:

```
module load 2021
module load Anaconda3/2021.05
conda env create -f environment.yml
```

It will take some time to download the necessary packages.

The main code to run is the following:

```
srun  -p gpu_shared -n 1 --ntasks-per-node 1 --gpus 2 --cpus-per-task 2 -t 1:00:00 --pty␣
↪/bin/bash
```

where with `-p gpu_shared` we ask for the shared partition where there are GPUs available (other gpu partitions available are listed here), then, we specify that we will be running only 1 task in this node, we want 2 GPUs and we use 2 CPUs as well, for 1 hour. The run consists of executing the command `/bin/bash` which starts a bash console on the node that we have been assigned. This allows for input of the necessary commands.

Once inside, we can activate the correct anaconda environment and start running the scripts. We need to make sure that both GPUs are exposed to the script, with the following syntax:

```
python my_script.py
```

For these examples we will make use of the straightforward interface provided by PyTorch, a good summary is available at the documentation page, where all the details of the functions are shown.

Some useful utilities

The following code will help in the running of the experiments, with some plotting functions and setup of the distributed environment.

```
import torch
import torch.distributed as dist
import matplotlib.pyplot as plt
import numpy as np
from pathlib import Path
from typing import Optional


def rank_print(text: str):
    """
    Prints a statement with an indication of what node rank is sending it
    """
    rank = dist.get_rank()
    # Keep the print statement as a one-liner to guarantee that
    # one single process prints all the lines
    print(f"Rank: {rank}, {text}.")


def disk(
    matrix: torch.Tensor,
    center: tuple[int, int] = (1, 1),
    radius: int = 1,
    value: float = 1.0,
):
    """
    Places a disk with a certain radius and center in a matrix. The value given to the␣
↪disk must be defined.
    Something like this:
    0 0 0 0 0
    0 0 1 0 0
    0 1 1 1 0
    0 0 1 0 0
    0 0 0 0 0

    Arguments:
```

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```
     - matrix: the matrix where to place the shape.
     - center: a tuple indicating the center of the disk
     - radius: the radius of the disk in pixels
     - value: the value to write where the disk is placed
    """
    device = matrix.get_device()
    shape = matrix.shape

    # genereate the grid for the support points
    # centered at the position indicated by position
    grid = [slice(-x0, dim - x0) for x0, dim in zip(center, shape)]
    x_coords, y_coords = np.mgrid[grid]
    mask = torch.tensor(
        ((x_coords / radius) ** 2 + (y_coords / radius) ** 2 <= 1), device=device
    )
    matrix = matrix * (~mask) + mask * value

    return matrix, mask


def square(
    matrix: torch.tensor,
    topleft: tuple[int, int] = (0, 0),
    length: int = 1,
    value: float = 1.0,
):
    """
    Places a square starting from the given top-left position and having given side␣
↪length.
    The value given to the disk must be defined.
    Something like this:
    0 0 0 0 0
    0 1 1 1 0
    0 1 1 1 0
    0 1 1 1 0
    0 0 0 0 0

    Arguments:
     - matrix: the matrix where to place the shape.
     - topleft: a tuple indicating the top-left-most vertex of the square
     - length: the side length of the square
     - value: the value to write where the square is placed
    """
    device = matrix.get_device()
    shape = matrix.shape
    grid = [slice(-x0, dim - x0) for x0, dim in zip(topleft, shape)]
    x_coords, y_coords = np.mgrid[grid]
    mask = torch.tensor(
        (
            (x_coords <= length)
            & (x_coords >= 0)
            & (y_coords >= 0)
```

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```
            & (y_coords <= length)
        ),
        device=device,
    )
    matrix = matrix * (~mask) + mask * value

    return matrix, mask


def plot_matrix(
    matrix: torch.Tensor,
    rank: int,
    title: str = "Matrix",
    name: str = "image",
    folder: Optional[str] = None,
    storefig: bool = True,
):
    """
    Helper function to plot the images more easily. Can store them or visualize them␣
↪right away.
    """
    plt.figure()
    plt.title(title)
    plt.imshow(matrix.cpu(), cmap="tab20", vmin=0, vmax=19)
    plt.axis("off")
    if folder:
        folder = Path(folder)
        folder.mkdir(exist_ok=True, parents=True)
    else:
        folder = Path(".")

    if storefig:
        plt.savefig(folder / Path(f"rank_{rank}_{name}.png"))
    else:
        plt.show()
    plt.close()
```

When starting the distributed environment, we need to decide a backend between `gloo`, `nccl` and `mpi`. The support for these libraries needs to be already available. The `nccl` backend should be already available from a GPU installation of PyTorch (CUDA Toolkit is required). On a Windows environment, only `gloo` works, but we will be running these scripts on a Unix environment.

The second fundamental aspect is how the information is shared between nodes. The method we choose is through a shared file, that is accessible from all the GPUs. It is important to remember that access to this file should be quick for all nodes, so on LISA we will put it in the `scratch` folder.

The other two parameters are the `rank` and `world_size`. The rank refers to the identifier for the current device, while the world size is the number of devices available for computation.

When setting up the distributed environment, the correct GPU device should be selected. For simplicity, we select the GPU that has ID corresponding to the rank, but this is not necessary.

Computation nodes could reside in different nodes, when this happens, using a shared fil

```
def setup_distrib(
    rank: int,
    world_size: int,
    init_method: str = "file:///scratch/sharedfile",
    backend: str = "nccl",
):
    # select the correct device for this process
    torch.cuda.set_device(rank)

    # initialize the processing group
    torch.distributed.init_process_group(
        backend=backend, world_size=world_size, init_method=init_method, rank=rank
    )

    # return the current device
    return torch.device(f"cuda:{rank}")
```

Training a model on multiple GPUs is a clear example that we will keep in mind throughout this tutorial to contextualize how to make use of the available primitives of communication in distributed computing.

Initially, we want to give the current weights of the model to every GPU that we are using. To do so, we will **broadcast** the necessary tensors.

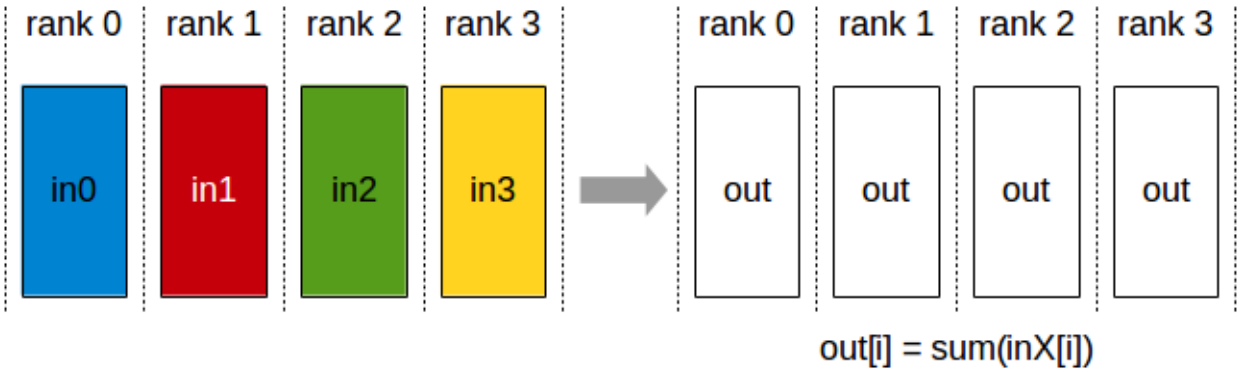
Then, each GPU will collect a subset of the full batch, lets say only 64 out of 256 samples, from memory and perform a forward pass of the model. At the end, we need to compute the loss over the entire batch of 256 samples, but no GPU can fit all of these. Here, the **reduction** primitive comes to the resque. The tensors that reside in different GPUs are collected and an operation is performed that will *reduce* the tensors to a single one. This allows for the result of the operation to still fit in memory. We may want to keep thisresult in a single GPU (using **reduce**) or send it to all of them (using **all_reduce**).

The operations that we can perform are determined by the backend that we are currently using. When using `nccl`, the list of available operations is the following: - `SUM` - `AVG` (only version 2.10 or higher) - `PRODUCT` - `MIN` - `MAX`

Communication Primitives

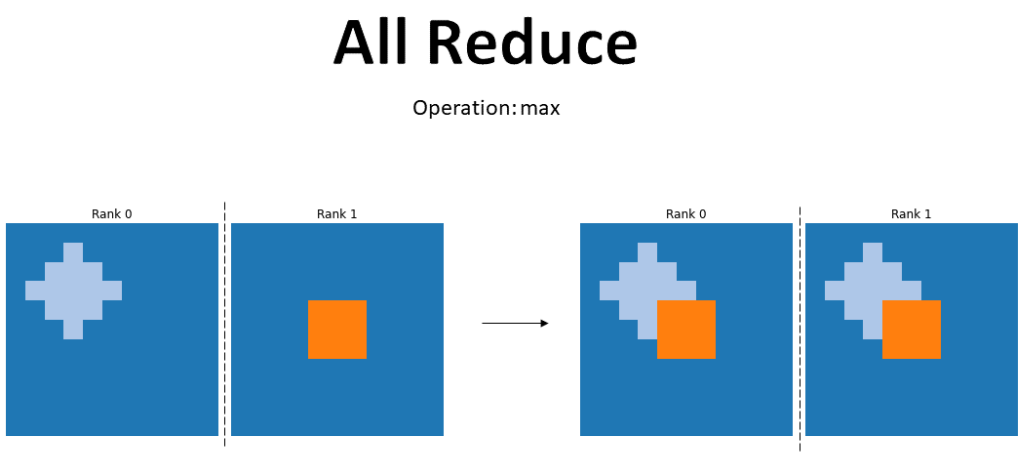
4.48.2 All Reduce

As we can see from the illustration, the **all reduce** primitive performs an operation between the tensors present in each GPU and replaces them with the result of the operation. The file to run is `all_reduce.py`.



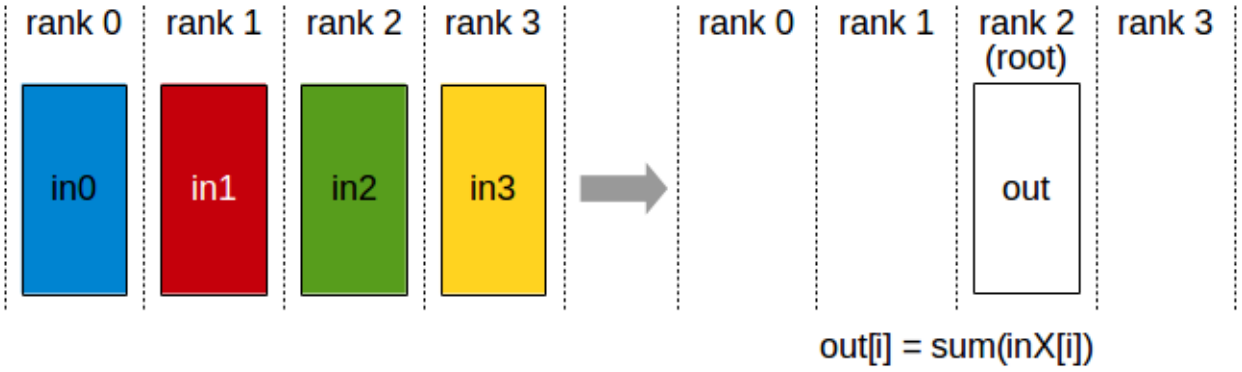
```
from utils import setup_distrib, disk, square, rank_print, plot_matrix
import torch.distributed as dist
import torch.multiprocessing as mp
import torch

# operation performed by the reduce
OPERATION = dist.ReduceOp.MAX


def main_process(rank:int, world_size:int=2):
    device = setup_distrib(rank, world_size)
    rank_print("test")
    image = torch.zeros((11,11), device=device)

    if rank == 0:
        rank_image, rank_mask = disk(image, (3,3), 2, rank+1)
    elif rank == 1:
        rank_image, rank_mask = square(image, (3,3), 2, rank+1)

    plot_matrix(rank_image, rank, title=f"Rank {rank} Before All Reduce", name="before_
↪all_reduce", folder="all_reduce")

    # The main operation
    dist.all_reduce(rank_image, op=OPERATION)
    plot_matrix(rank_image, rank, title=f"Rank {rank} After All Reduce Operation:
↪{OPERATION}", name="after_all_reduce", folder="all_reduce")

if __name__ == '__main__':
    mp.spawn(main_process, nprocs=2, args=())
```

The result of this operation is illustrated in the figure below. The operation is performed between the tensors stored in the different devices and the result is spread across all devices.



4.48.3 Reduce

As we can see from the illustration, the **reduce** primitive performs an operation between the tensors present in each GPU and sends the result only to the root rank. In Pytorch, we can define the destination rank. The file to run is `reduce.py`.




```
from utils import setup_distrib, disk, square, rank_print, plot_matrix
import torch.distributed as dist
import torch.multiprocessing as mp
import torch
DESTINATION_RANK = 0
OPERATION = dist.ReduceOp.MAX

def main_process(rank, world_size=2):
    device = setup_distrib(rank, world_size)

    image = torch.zeros((11,11), device=device)
```

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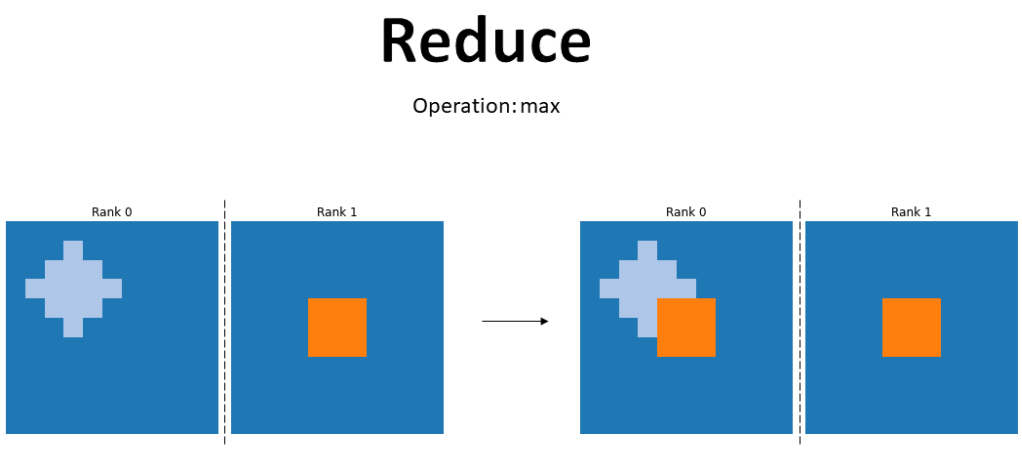
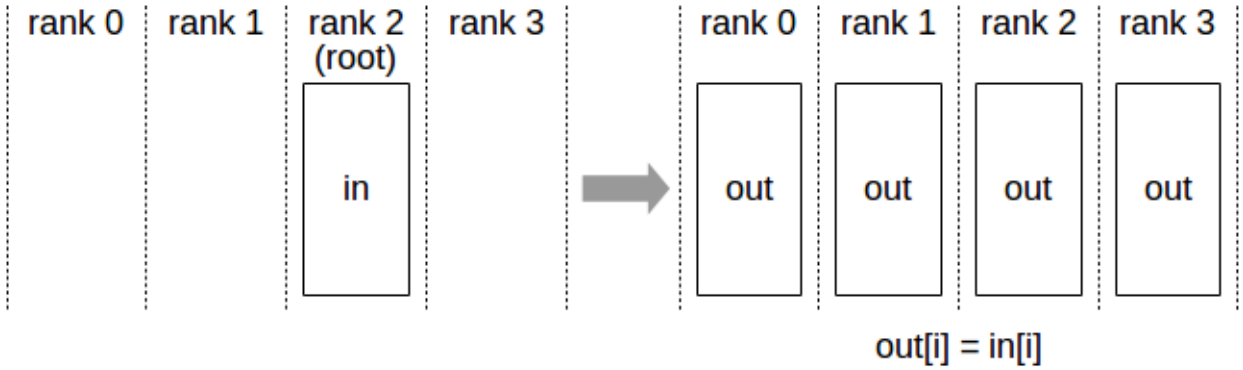
```
    if rank == 0:
        rank_image, rank_mask = disk(image, (4,5), 2, rank+1)
    elif rank == 1:
        rank_image, rank_mask = square(image, (3,3), 2, rank+1)

    plot_matrix(rank_image, rank, title=f"Rank {rank} Before Reduce", name="before_reduce
↪", folder="reduce")

    # The main operation
    dist.reduce(rank_image, dst=DESTINATION_RANK, op=OPERATION)
    plot_matrix(rank_image, rank, title=f"Rank {rank} After Reduce Operation: {OPERATION}
↪", name="after_reduce", folder="reduce")

if __name__ == '__main__':
    mp.spawn(main_process, nprocs=2, args=())
```

The results are shown below. We can see how only the rank 0, the one we selected, has the result of the operation. This helps in reducing the processing time, if the operation is executed in an asynchronous way, all other GPUs can keep processing while the root one is receiving the result.



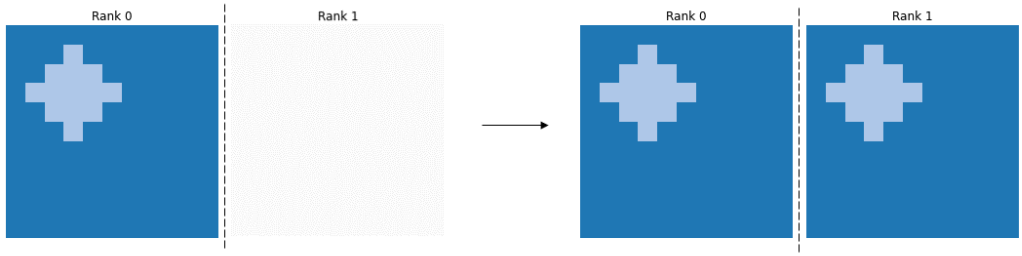
4.48.4 Broadcast

The **broadcast** operation is fundamental, as it allows to send (broadcast) data from one GPU to all others in the network. The file to run is `broadcast.py`.



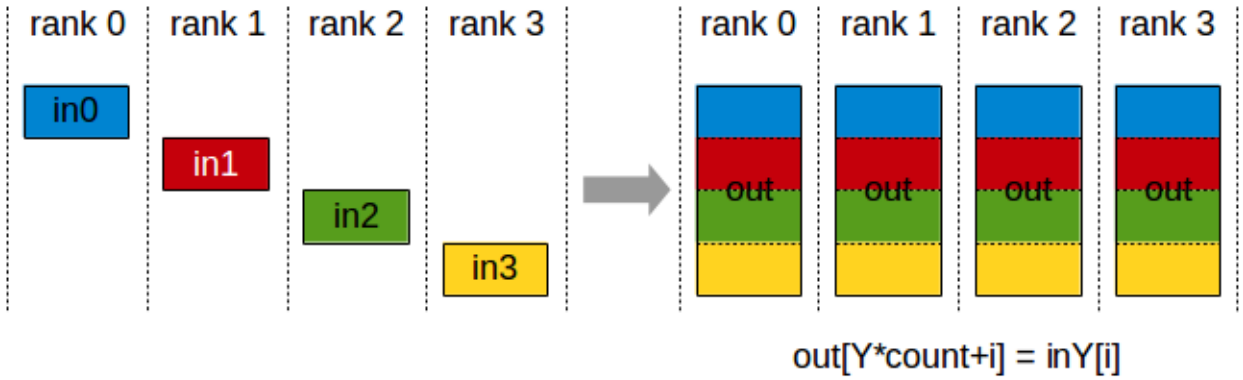

```
from utils import setup_distrib, disk, square, rank_print, plot_matrix
import torch.distributed as dist
import torch.multiprocessing as mp
import torch
SOURCE_RANK = 0
OPERATION = dist.ReduceOp.MAX

def main_process(rank, world_size=2):
    device = setup_distrib(rank, world_size)

    image = torch.zeros((11,11), device=device)

    if rank == 0:
        rank_image, rank_mask = disk(image, (4,5), 2, rank+1)
    elif rank == 1:
        rank_image, rank_mask = square(image, (3,3), 2, rank+1)

    plot_matrix(rank_image, rank, name="before_broadcast", folder="broadcast")

    # The main operation
    dist.broadcast(rank_image, src=SOURCE_RANK)
    plot_matrix(rank_image, rank, name="after_broadcast", folder="broadcast")


if __name__ == '__main__':
    mp.spawn(main_process, nprocs=2, args=())
```

In this illustration we see how, the rank 1 GPU gets the correct image after the broadcast is performed.



4.48.5 All Gather

The **all gather** operation allows for all GPUs to have access to all the data processed by the others. This can be especially useful when different operations need to be performed by each GPU, after a common operation has been performed on each subset of the data. It is important to note that the entirety of the data needs to fit in a single GPU, so here the bottleneck won't be the memory, instead, it will be the processing speed. The file to run is `all_gather.py`.




```
from utils import setup_distrib, disk, square, rank_print, plot_matrix
import torch.distributed as dist
import torch.multiprocessing as mp
import torch
def main_process(rank, world_size=2):
    device = setup_distrib(rank, world_size)

    image = torch.zeros((11,11), device=device)
```

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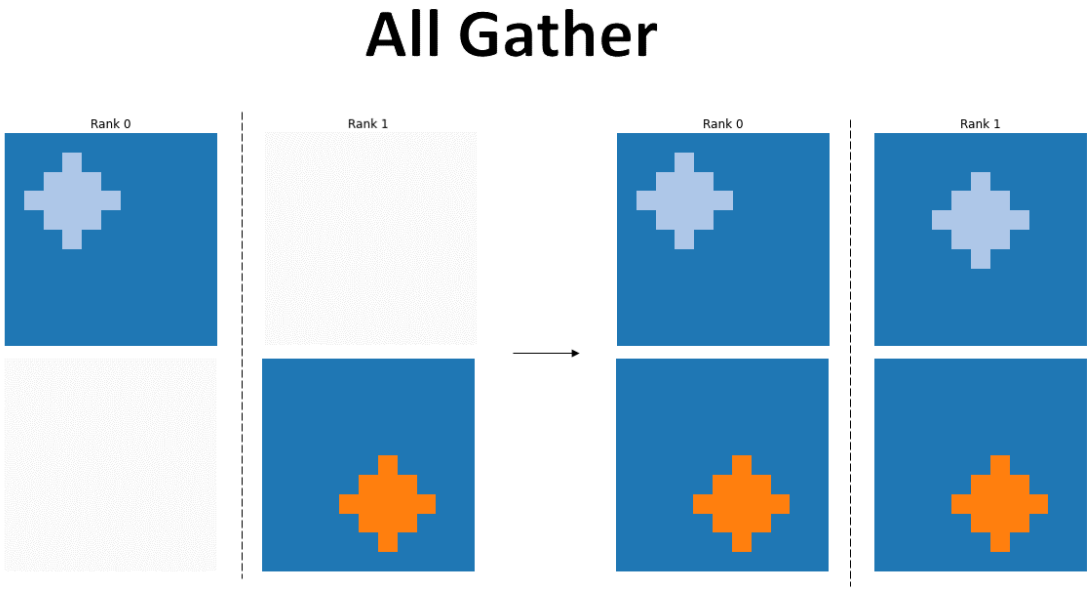
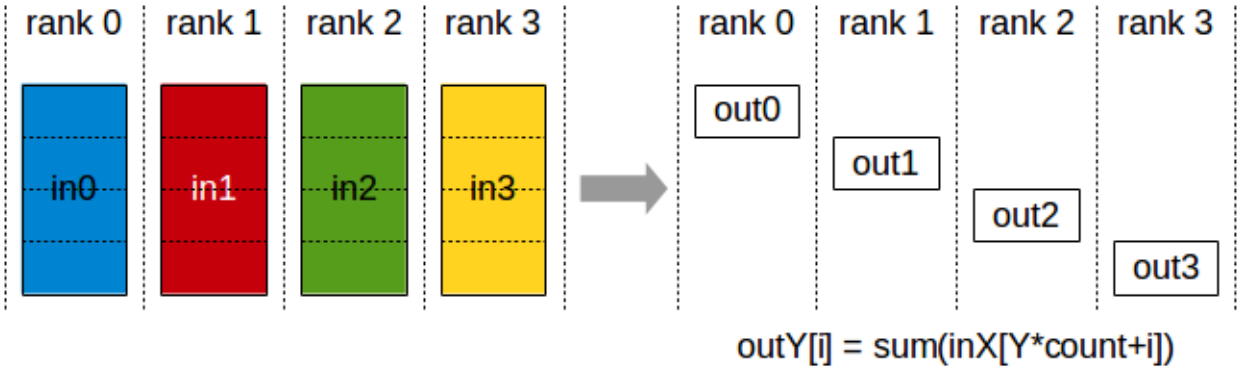
```
    rank_images = []

    if rank == 0:
        rank_images.append(disk(image, (4,5), 2, rank+1)[0])
    elif rank == 1:
        rank_images.append(disk(image, (7,6), 2, rank+1)[0])

    output_tensors = []
    for _ in range(world_size):
        output_tensors.append(torch.zeros_like(image, device=device))

    plot_matrix(output_tensors[0], rank, title=f"Rank {rank}", name="before_gather_0",␣
↪folder="all_gather")
    plot_matrix(output_tensors[1], rank, title=f"", name="before_gather_1", folder="all_
↪gather")

    # The main operation
    dist.all_gather(output_tensors, rank_images[0])
    plot_matrix(output_tensors[0], rank, title=f"Rank {rank}", name="after_gather_0",␣
↪folder="all_gather")
    plot_matrix(output_tensors[1], rank, title=f"", name="after_gather_1", folder="all_
↪gather")


if __name__ == '__main__':
    mp.spawn(main_process, nprocs=2, args=())
```

Here we can see the result of the **all_gather**. All GPUs now have access to the data that was initially only present in some of them.



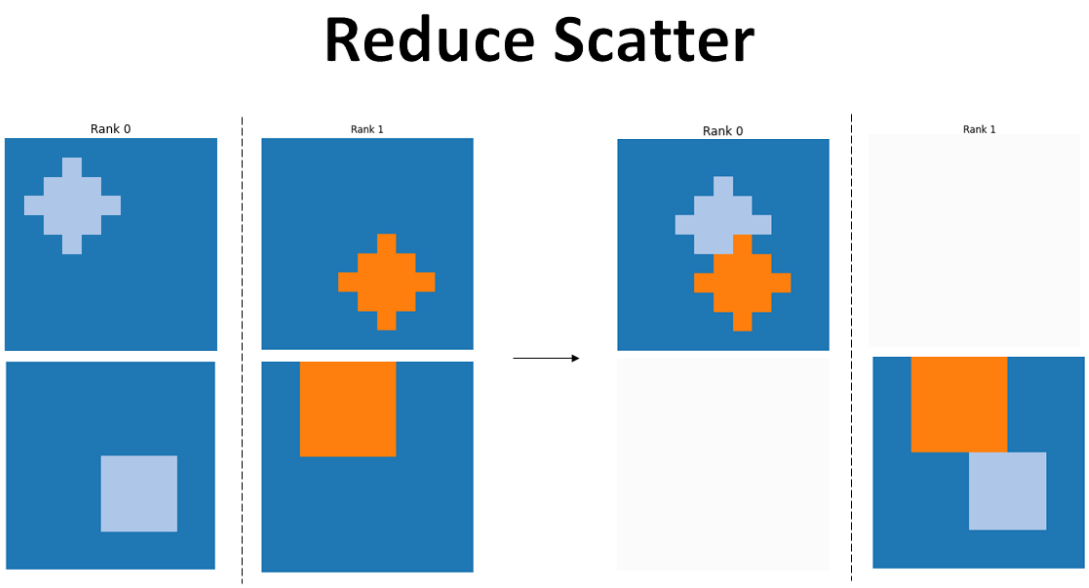
4.48.6 Reduce Scatter

With **reduce scatter** we can perform an operation on just a subset of the whole data and have each GPU have the partial results. The file to run is `reduce_scatter.py`.




```
from utils import setup_distrib, disk, square, rank_print, plot_matrix
import torch.distributed as dist
import torch.multiprocessing as mp
import torch
OPERATION = dist.ReduceOp.MAX
def main_process(rank, world_size=2):
    device = setup_distrib(rank, world_size)

    image = torch.zeros((11,11), device=device)

    input_tensors = []

    if rank == 0:
        input_tensors.append(disk(image, (4,5), 2, rank+1)[0])
        input_tensors.append(square(image, (5,5), 3, rank+1)[0])
    elif rank == 1:
        input_tensors.append(disk(image, (7,6), 2, rank+1)[0])
        input_tensors.append(square(image, (0,2), 4, rank+1)[0])

    output = torch.zeros_like(image, device=device)

    plot_matrix(input_tensors[0], rank, title=f"Rank {rank}", name="before_reduce_
↪scatter_0", folder="reduce_scatter")
    plot_matrix(input_tensors[1], rank, title=f"", name="before_reduce_scatter_1",␣
↪folder="reduce_scatter")
    plot_matrix(output, rank, title=f"", name="before_reduce_scatter", folder="reduce_
↪scatter")

    # The main operation
    dist.reduce_scatter(output, input_tensors, op=OPERATION)
    plot_matrix(output, rank, title=f"", name="after_reduce_scatter", folder="reduce_
↪scatter")


if __name__ == '__main__':
    mp.spawn(main_process, nprocs=2, args=())
```

In this figure we see that only one image is available at the end, allowing for the operation to be performed across GPUs while keeping the overall final memory footprint low.

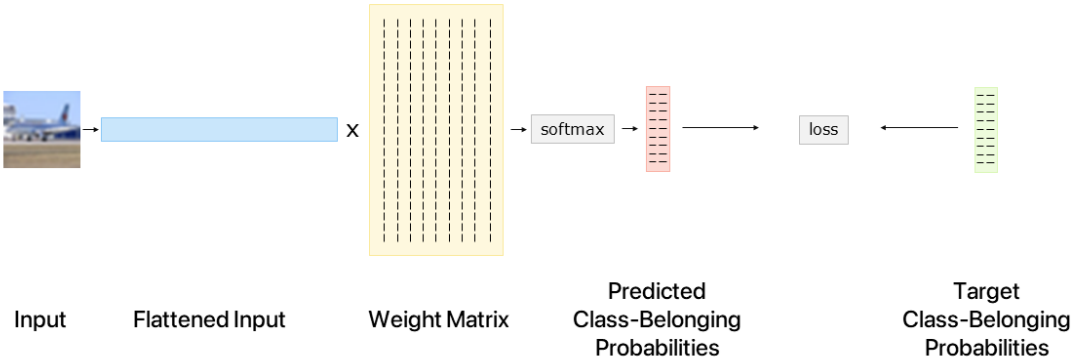


Exercise

An interesting thing to test, if you have access to a multi-GPU environment, is what are the physical limits of the system, and if the processing speed is the same with any number of tensors being loaded into the GPU. Is it more efficient to use a multiple of the number of cores that are processing the data in the GPU, or is the difference in performance negligible? You can investigate these topics through experimentation.

A more comprehensive example

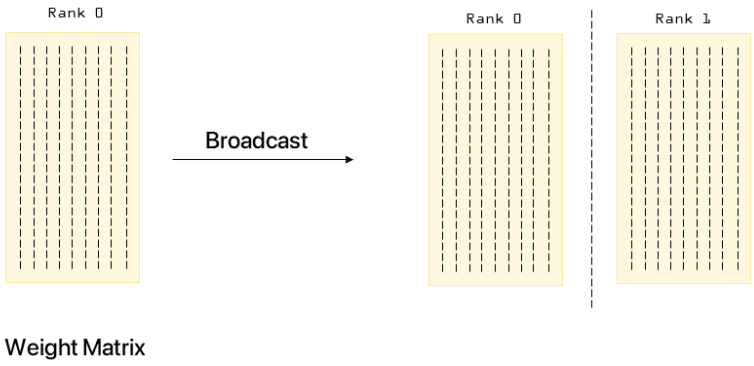
We will now look at a more realistic scenario (code in `single_layer.py`), the overall process is shown in the figure below.



The first thing we do is to spawn the two processes. In each, we begin by initializing the distributed processing environment.

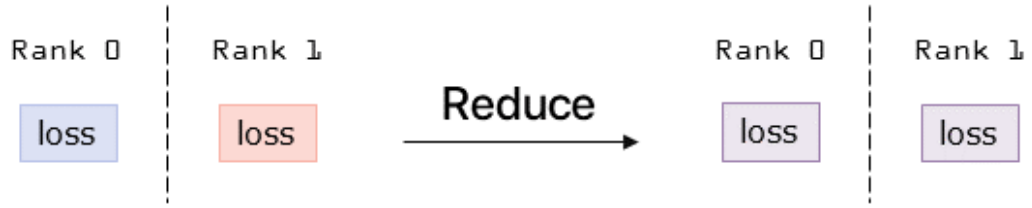
Then, the datasets needs to be downloaded. Here, I assume that it has not been downloaded yet, and I only let the GPU in rank 0 perform this operation. This avoids having two processes writing in the same file. In order to have the other process wait for the first one to download, a **barrier** is used. The working principle is very simple, when a barrier is reached in the code, the process waits for all other processes to also reach that point in the code. Here we see how this can be a very useful construct in parallel computing, all processes require the dataset to be downloaded before proceeding, so one of them starts the download, and all wait until it's done.

Then we initialize the weights, only in the rank 0 GPU, and **broadcast** them to all other GPUs. This broadcast operation is performed asynchronously, to allow for the rank 0 GPU to start loading images before the rank 1 has received the weights. This operation is akin to what DataParallel does, which is slowing the processing of the other GPUs down, waiting to receive the weights from the root GPU.



Each GPU will then load the images from disk, perform a product to find the activations of the next layer and calculate a softmax to get class-belonging probabilities.

Finally, the loss is computed by summing over the dimensions and a **reduction** with sum is performed to compute the overall loss over the entire batch.




```
import torch
import torch.distributed as dist
import torch.multiprocessing as mp
import torchvision
from torchvision import transforms
from utils import rank_print

DSET_FOLDER = "/scratch/"


def main_process(rank, world_size=2):
    print(f"Process for rank: {rank} has been spawned")
```

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```
    # Setup the distributed processing
    device = setup_distrib(rank, world_size)

    # Load the dataset in all processes download only in the first one
    if rank == 0:
        dset = torchvision.datasets.CIFAR10(DSET_FOLDER, download=True)

    # Make sure download has finished
    dist.barrier()

    # Load the dataset
    dset = torchvision.datasets.CIFAR10(DSET_FOLDER)

    input_size = 3 * 32 * 32  # [channel size, height, width]
    per_gpu_batch_size = 128
    num_classes = 10
    if dist.get_rank() == 0:
        weights = torch.rand((input_size, num_classes), device=device)
    else:
        weights = torch.zeros((input_size, num_classes), device=device)

    # Distribute weights to all GPUs
    handle = dist.broadcast(tensor=weights, src=0, async_op=True)
    rank_print(f"Weights received.")

    # Flattened images
    cur_input = torch.zeros((per_gpu_batch_size, input_size), device=device)

    # One-Hot encoded target
    cur_target = torch.zeros((per_gpu_batch_size, num_classes), device=device)
    for i in range(per_gpu_batch_size):
        rank_print(f"Loading image {i+world_size*rank} into GPU...")
        image, target = dset[i + world_size * rank]
        cur_input[i] = transforms.ToTensor()(image).flatten()
        cur_target[i, target] = 1.0

    # Compute the linear part of the layer
    output = torch.matmul(cur_input, weights)
    rank_print(f"\nComputed output: {output}, Size: {output.size()}.")

    # Define the activation function of the output layer
    logsoftm = torch.nn.LogSoftmax(dim=1)

    # Apply activation function to output layer
    output = logsoftm(output)
    rank_print(f"\nLog-Softmaxed output: {output}, Size: {output.size()}.")

    loss = output.sum(dim=1).mean()
    rank_print(f"Loss: {loss}, Size: {loss.size()}")

    # Here the GPUs need to be synched again
```

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```
    dist.reduce(tensor=loss, dst=0, op=dist.ReduceOp.SUM)

    rank_print(f"Final Loss: {loss/world_size}")


if __name__ == "__main__":
    mp.spawn(main_process, nprocs=2, args=())
```

PyTorch Lightning

When you have your Pytorch Lightning module defined, scaling to multiple GPUs and multi nodes is very straightforward (more details here):

```
trainer = Trainer(gpus=8, strategy="ddp")
```

Yes, seems impossible, but it's real. In most cases this is all you need to run multi GPU training.

Conclusion

We have seen how the basic collective primitives for communication work in a multi GPU environment. The reduction and broadcast operations are maybe the most important ones, allowing for delivery of data to all nodes and to perform mathematical operations on the data present in all the nodes.

We have seen how we can use these collectives to perform a calculation of the loss of a neural network, but the same can be extended to any type of parallelizable computation.

Finally, we saw how simple it is to set a PyTorch Lightning training to use multiple GPUs.

4.48.7 References

Pytorch Documentation on Distributed Communication. https://pytorch.org/docs/stable/distributed.html

NVIDIA NCCL Developer Guide. https://docs.nvidia.com/deeplearning/nccl/user-guide/docs/overview.html

PyTorch Lightning Multi-GPU Training. https://pytorch-lightning.readthedocs.io/en/stable/advanced/multi_gpu.html

Concurrent Programming and Operating Systems. Stallings, William. Operating Systems : Internals and Design Principles. Upper Saddle River, N.J. :Prentice Hall, 2001.

4.49 Tutorial 1: Bayesian Neural Networks with Pyro

Filled notebook: - Latest version (V04/23): this notebook

Empty notebook: - Latest version (V04/23):

Visit also the DL2 tutorial Github repo and associated Docs page.

Authors: Ilze Amanda Auzina, Leonard Bereska, Alexander Timans and Eric Nalisnick

4.49.1 Bayesian Neural Networks

A Bayesian neural network is a probabilistic model that allows us to estimate uncertainty in predictions by representing the weights and biases of the network as probability distributions rather than fixed values. This allows us to *incorporate prior knowledge* about the weights and biases into the model, and *update our beliefs* about them as we observe data.

Mathematically, a Bayesian neural network can be represented as follows:

Given a set of input data x, we want to predict the corresponding output y. The neural network represents this relationship as a function $f(x, \theta)$, where θ are the weights and biases of the network. In a Bayesian neural network, we represent the weights and biases as probability distributions, so $f(x, \theta)$ becomes a probability distribution over possible outputs:

$$p(y|x, \mathcal{D}) = \int p(y|x, \theta)p(\theta|\mathcal{D})d\theta$$

where $p(y|x, \theta)$ is the likelihood function, which gives the probability of observing y given x and θ, and $p(\theta|\mathcal{D})$ is the posterior distribution over the weights and biases given the observed data $\mathcal{D}$.

To make predictions, we use the posterior predictive distribution:

$$p(y^*|x^*, \mathcal{D}) = \int p(y^*|x^*, \theta)p(\theta|\mathcal{D})d\theta$$

where x^* is a new input and y^* is the corresponding predicted output.

To estimate the (intractable) posterior distribution $p(\theta|\mathcal{D})$, we can use either Markov Chain Monte Carlo (MCMC) or Variational Inference (VI).

4.49.2 Simulate data

Let's generate noisy observations from a sinusoidal function.

[3]:
```
import torch
import numpy as np
import matplotlib.pyplot as plt

# Set random seed for reproducibility
np.random.seed(42)

# Generate data
x_obs = np.hstack([np.linspace(-0.2, 0.2, 500), np.linspace(0.6, 1, 500)])
noise = 0.02 * np.random.randn(x_obs.shape[0])
y_obs = x_obs + 0.3 * np.sin(2 * np.pi * (x_obs + noise)) + 0.3 * np.sin(4 * np.pi * (x_
↪obs + noise)) + noise

x_true = np.linspace(-0.5, 1.5, 1000)
y_true = x_true + 0.3 * np.sin(2 * np.pi * x_true) + 0.3 * np.sin(4 * np.pi * x_true)

# Set plot limits and labels
xlims = [-0.5, 1.5]
ylims = [-1.5, 2.5]

# Create plot
fig, ax = plt.subplots(figsize=(10, 5))
ax.plot(x_true, y_true, 'b-', linewidth=3, label="True function")
```

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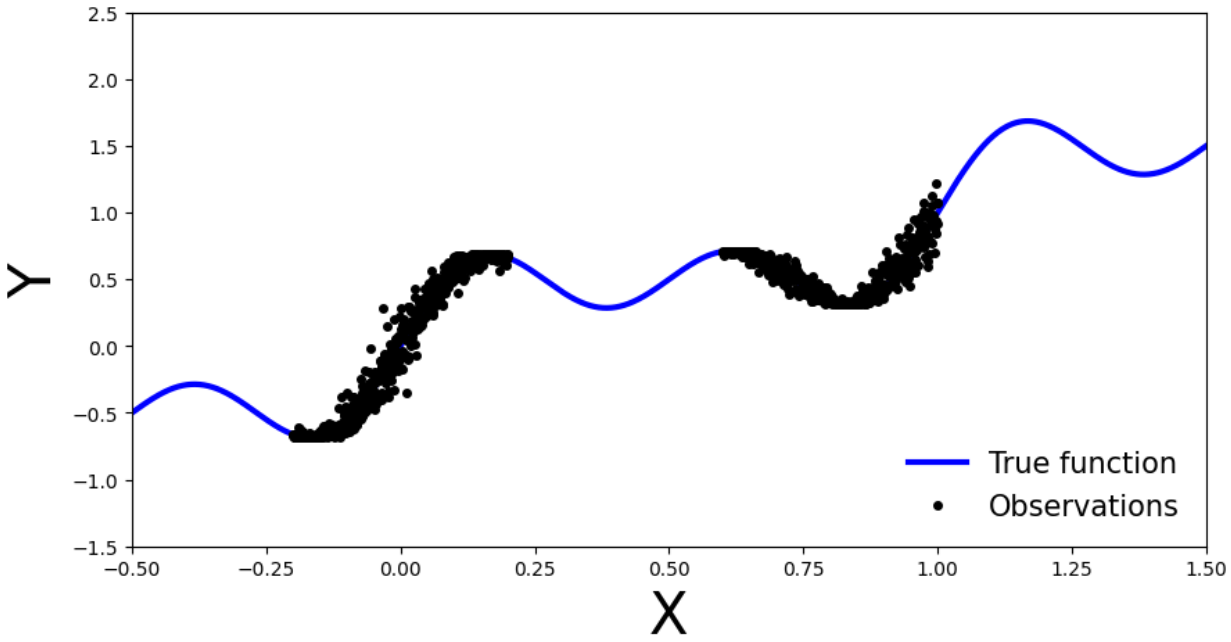
```
ax.plot(x_obs, y_obs, 'ko', markersize=4, label="Observations")
ax.set_xlim(xlims)
ax.set_ylim(ylims)
ax.set_xlabel("X", fontsize=30)
ax.set_ylabel("Y", fontsize=30)
ax.legend(loc=4, fontsize=15, frameon=False)

plt.show()
```



4.49.3 Getting started with Pyro

Let's install Pyro now. You may have to restart the runtime after this step.

[4]:
```
!pip install pyro-ppl
```

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/
↪public/simple/
Requirement already satisfied: pyro-ppl in /usr/local/lib/python3.9/dist-packages (1.8.4)
Requirement already satisfied: numpy>=1.7 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (1.22.4)
Requirement already satisfied: pyro-api>=0.1.1 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (0.1.2)
Requirement already satisfied: opt-einsum>=2.3.2 in /usr/local/lib/python3.9/dist-
↪packages (from pyro-ppl) (3.3.0)
Requirement already satisfied: torch>=1.11.0 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (2.0.0+cu118)
Requirement already satisfied: tqdm>=4.36 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (4.65.0)
Requirement already satisfied: networkx in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (3.1)
```

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```
Requirement already satisfied: filelock in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (3.11.0)
Requirement already satisfied: sympy in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (1.11.1)
Requirement already satisfied: typing-extensions in /usr/local/lib/python3.9/dist-
↪packages (from torch>=1.11.0->pyro-ppl) (4.5.0)
Requirement already satisfied: triton==2.0.0 in /usr/local/lib/python3.9/dist-packages␣
↪(from torch>=1.11.0->pyro-ppl) (2.0.0)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (3.1.2)
Requirement already satisfied: lit in /usr/local/lib/python3.9/dist-packages (from␣
↪triton==2.0.0->torch>=1.11.0->pyro-ppl) (16.0.1)
Requirement already satisfied: cmake in /usr/local/lib/python3.9/dist-packages (from␣
↪triton==2.0.0->torch>=1.11.0->pyro-ppl) (3.25.2)
Requirement already satisfied: MarkupSafe>=2.0 in /usr/local/lib/python3.9/dist-packages␣
↪(from jinja2->torch>=1.11.0->pyro-ppl) (2.1.2)
Requirement already satisfied: mpmath>=0.19 in /usr/local/lib/python3.9/dist-packages␣
↪(from sympy->torch>=1.11.0->pyro-ppl) (1.3.0)
```

4.49.4 Bayesian Neural Network with Gaussian Prior and Likelihood

Our first Bayesian neural network employs a Gaussian prior on the weights and a Gaussian likelihood function for the data. The network is a shallow neural network with one hidden layer.

To be specific, we use the following prior on the weights θ:

$p(\theta) = \mathcal{N}(\mathbf{0}, 10 \cdot \mathbb{I})$, where $\mathbb{I}$ is the identity matrix.

To train the network, we define a likelihood function comparing the predicted outputs of the network with the actual data points:

$p(y_i|x_i, \theta) = \mathcal{N}\big(NN_\theta(x_i), \sigma^2\big)$, with prior $\sigma \sim \Gamma(1, 1)$.

Here, y_i represents the actual output for the i-th data point, x_i represents the input for that data point, σ is the standard deviation parameter for the normal distribution and NN_θ is the shallow neural network parameterized by θ.

Note that we use σ^2 instead of σ in the likelihood function because we use a Gaussian prior on σ when performing variational inference and then want to avoid negative values for the standard deviation.

[5]:
```
import pyro
import pyro.distributions as dist
from pyro.nn import PyroModule, PyroSample
import torch.nn as nn


class MyFirstBNN(PyroModule):
    def __init__(self, in_dim=1, out_dim=1, hid_dim=5, prior_scale=10.):
        super().__init__()

        self.activation = nn.Tanh()  # or nn.ReLU()
        self.layer1 = PyroModule[nn.Linear](in_dim, hid_dim)  # Input to hidden layer
        self.layer2 = PyroModule[nn.Linear](hid_dim, out_dim)  # Hidden to output layer

        # Set layer parameters as random variables
```

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```
        self.layer1.weight = PyroSample(dist.Normal(0., prior_scale).expand([hid_dim, in_
↪dim]).to_event(2))
        self.layer1.bias = PyroSample(dist.Normal(0., prior_scale).expand([hid_dim]).to_
↪event(1))
        self.layer2.weight = PyroSample(dist.Normal(0., prior_scale).expand([out_dim,␣
↪hid_dim]).to_event(2))
        self.layer2.bias = PyroSample(dist.Normal(0., prior_scale).expand([out_dim]).to_
↪event(1))

    def forward(self, x, y=None):
        x = x.reshape(-1, 1)
        x = self.activation(self.layer1(x))
        mu = self.layer2(x).squeeze()
        sigma = pyro.sample("sigma", dist.Gamma(.5, 1))  # Infer the response noise

        # Sampling model
        with pyro.plate("data", x.shape[0]):
            obs = pyro.sample("obs", dist.Normal(mu, sigma * sigma), obs=y)
        return mu
```

4.49.5 Define and run Markov chain Monte Carlo sampler

To begin with, we can use MCMC to compute an *unbiased estimate* of $p(y|x, \mathcal{D}) = \mathbb{E}_{\theta \sim p(\theta|\mathcal{D})}\big[p(y|x, \theta)\big]$ through Monte Carlo sampling. Specifically, we can approximate $\mathbb{E}_{\theta \sim p(\theta|\mathcal{D})}\big[p(y|x, \theta)\big]$ as follows:

$$\mathbb{E}_{\theta \sim p(\theta|\mathcal{D})}\big[p(y|x, \theta)\big] \approx \frac{1}{N}\sum_{i=1}^{N} p(y|x, \theta_i),$$

where $\theta_i \sim p(\theta_i|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta)$ are samples drawn from the posterior distribution. Because the normalizing constant is intractable, we require MCMC methods like Hamiltonian Monte Carlo to draw samples from the non-normalized posterior.

Here, we use the No-U-Turn (NUTS) kernel.

[6]:
```
from pyro.infer import MCMC, NUTS

model = MyFirstBNN()

# Set Pyro random seed
pyro.set_rng_seed(42)

# Define Hamiltonian Monte Carlo (HMC) kernel
# NUTS = "No-U-Turn Sampler" (https://arxiv.org/abs/1111.4246), gives HMC an adaptive␣
↪step size
nuts_kernel = NUTS(model, jit_compile=False)  # jit_compile=True is faster but requires␣
↪PyTorch 1.6+

# Define MCMC sampler, get 50 posterior samples
mcmc = MCMC(nuts_kernel, num_samples=50)

# Convert data to PyTorch tensors
```

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```
x_train = torch.from_numpy(x_obs).float()
y_train = torch.from_numpy(y_obs).float()

# Run MCMC
mcmc.run(x_train, y_train)
```

```
Sample: 100%|| 100/100 [04:57,  2.98s/it, step size=3.40e-04, acc. prob=0.959]
```

We calculate and plot the predictive distribution.

[7]:
```
from pyro.infer import Predictive

predictive = Predictive(model=model, posterior_samples=mcmc.get_samples())
x_test = torch.linspace(xlims[0], xlims[1], 3000)
preds = predictive(x_test)
```

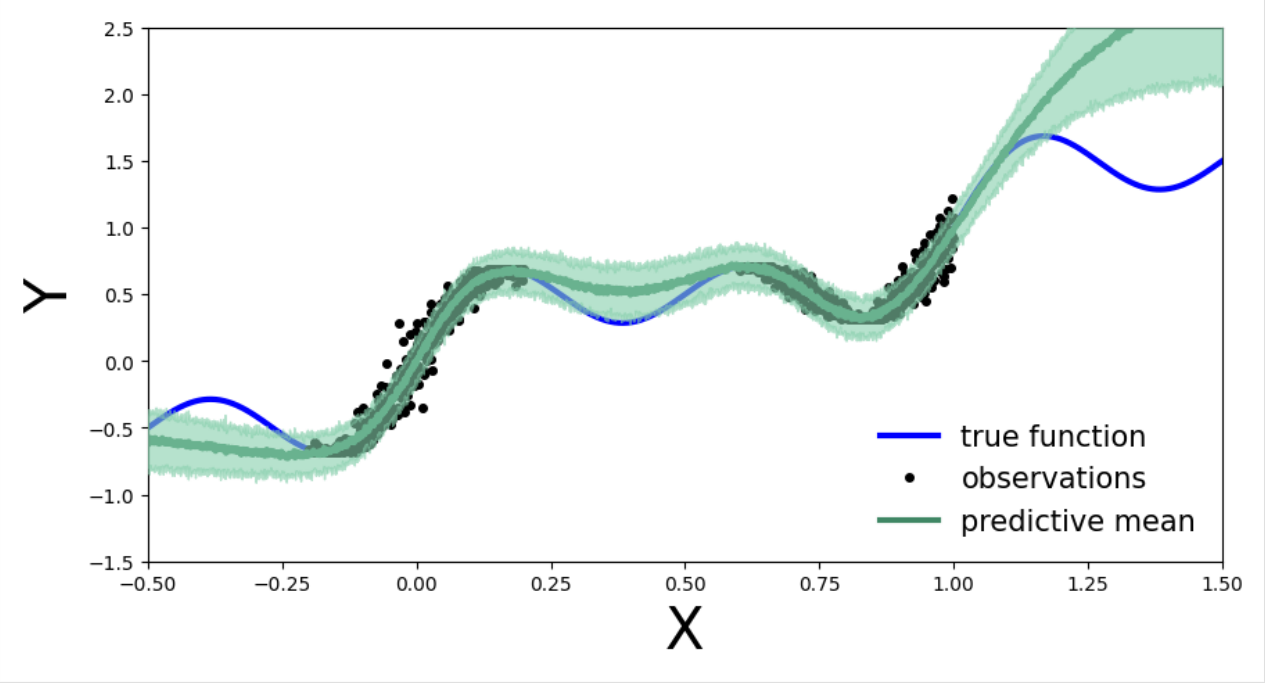
[8]:
```
def plot_predictions(preds):
    y_pred = preds['obs'].T.detach().numpy().mean(axis=1)
    y_std = preds['obs'].T.detach().numpy().std(axis=1)

    fig, ax = plt.subplots(figsize=(10, 5))
    xlims = [-0.5, 1.5]
    ylims = [-1.5, 2.5]
    plt.xlim(xlims)
    plt.ylim(ylims)
    plt.xlabel("X", fontsize=30)
    plt.ylabel("Y", fontsize=30)

    ax.plot(x_true, y_true, 'b-', linewidth=3, label="true function")
    ax.plot(x_obs, y_obs, 'ko', markersize=4, label="observations")
    ax.plot(x_obs, y_obs, 'ko', markersize=3)
    ax.plot(x_test, y_pred, '-', linewidth=3, color="#408765", label="predictive mean")
    ax.fill_between(x_test, y_pred - 2 * y_std, y_pred + 2 * y_std, alpha=0.6, color='
↪#86cfac', zorder=5)

    plt.legend(loc=4, fontsize=15, frameon=False)
```

[9]:
```
plot_predictions(preds)
```



4.49.6 Exercise 1: Deep Bayesian Neural Network

We can define a deep Bayesian neural network in a similar fashion, with Gaussian priors on the weights:

$p(\theta) = \mathcal{N}(\mathbf{0}, 5 \cdot \mathbb{I})$.

The likelihood function is also Gaussian:

$p(y_i|x_i, \theta) = \mathcal{N}\big(NN_\theta(x_i), \sigma^2\big)$, with $\sigma \sim \Gamma(0.5, 1)$.

> Implement the deep Bayesian neural network and run MCMC to obtain posterior samples. Compute and plot the predictive distribution. Use the following network architecture: Number of hidden layers: 5, Number of hidden units per layer: 10, Activation function: Tanh, Prior scale: 5.

[10]:
```
class BNN(PyroModule):
    def __init__(self, in_dim=1, out_dim=1, hid_dim=10, n_hid_layers=5, prior_scale=5.):
        super().__init__()

        self.activation = nn.Tanh()  # could also be ReLU or LeakyReLU
        assert in_dim > 0 and out_dim > 0 and hid_dim > 0 and n_hid_layers > 0  # make␣
↪sure the dimensions are valid

        # Define the layer sizes and the PyroModule layer list
        self.layer_sizes = [in_dim] + n_hid_layers * [hid_dim] + [out_dim]
        layer_list = [PyroModule[nn.Linear](self.layer_sizes[idx - 1], self.layer_
↪sizes[idx]) for idx in
                      range(1, len(self.layer_sizes))]
        self.layers = PyroModule[torch.nn.ModuleList](layer_list)

        for layer_idx, layer in enumerate(self.layers):
            layer.weight = PyroSample(dist.Normal(0., prior_scale * np.sqrt(2 / self.
↪layer_sizes[layer_idx])).expand(
```

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```
                [self.layer_sizes[layer_idx + 1], self.layer_sizes[layer_idx]]).to_
↪event(2))
            layer.bias = PyroSample(dist.Normal(0., prior_scale).expand([self.layer_
↪sizes[layer_idx + 1]]).to_event(1))

    def forward(self, x, y=None):
        x = x.reshape(-1, 1)
        x = self.activation(self.layers[0](x))  # input --> hidden
        for layer in self.layers[1:-1]:
            x = self.activation(layer(x))  # hidden --> hidden
        mu = self.layers[-1](x).squeeze()  # hidden --> output
        sigma = pyro.sample("sigma", dist.Gamma(.5, 1))  # infer the response noise

        with pyro.plate("data", x.shape[0]):
            obs = pyro.sample("obs", dist.Normal(mu, sigma * sigma), obs=y)
        return mu
```

Train the deep BNN with MCMC...

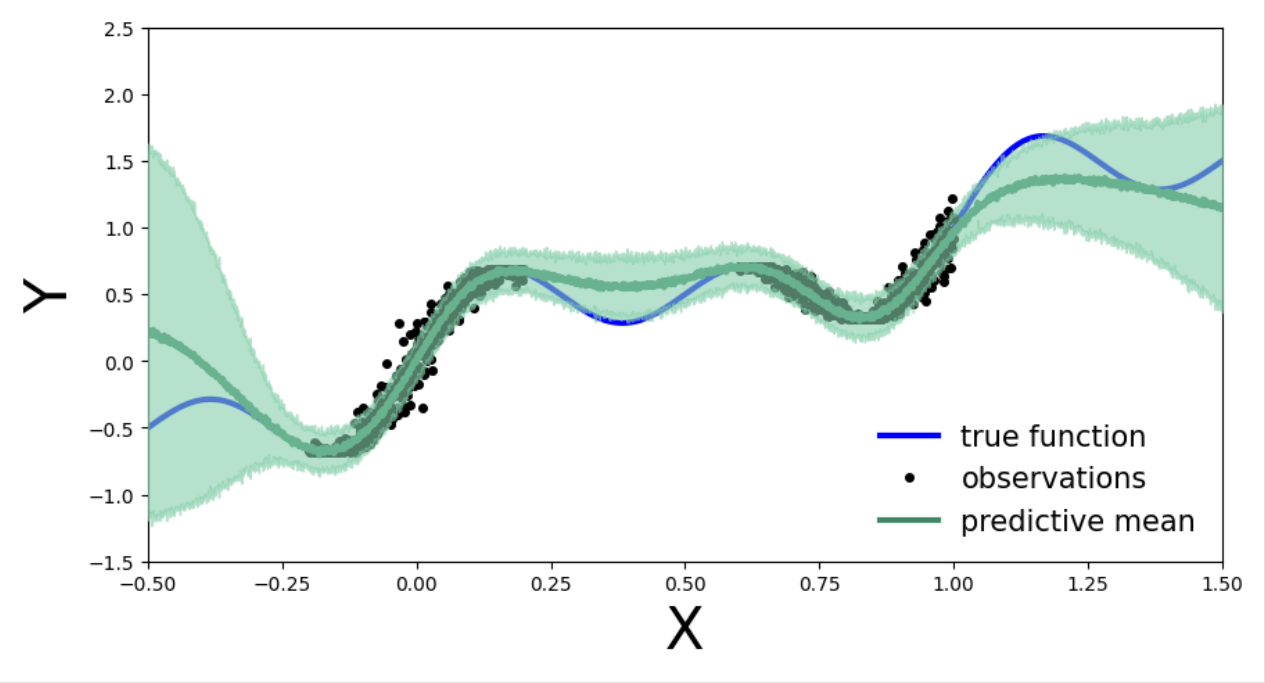
[11]:
```
# define model and data
model = BNN(hid_dim=10, n_hid_layers=5, prior_scale=5.)

# define MCMC sampler
nuts_kernel = NUTS(model, jit_compile=False)
mcmc = MCMC(nuts_kernel, num_samples=50)
mcmc.run(x_train, y_train)
```

```
Sample: 100%|| 100/100 [12:04,  7.24s/it, step size=6.85e-04, acc. prob=0.960]
```

Compute predictive distribution...

[12]:
```
predictive = Predictive(model=model, posterior_samples=mcmc.get_samples())
preds = predictive(x_test)
plot_predictions(preds)
```



4.49.7 Train BNNs with mean-field variational inference

We will now move on to variational inference. Since the normalized posterior probability density $p(\theta|\mathcal{D})$ is intractable, we approximate it with a tractable parametrized density $q_\phi(\theta)$ in a family of probability densities $\mathcal{Q}$. The variational parameters are denoted by ϕ and the variational density is called the "guide" in Pyro. The goal is to find the variational probability density that best approximates the posterior by minimizing the KL divergence

$$KL\big(q_\phi(\theta)||p(\theta|\mathcal{D})\big)$$

with respect to the variational parameters. However, directly minimizing the KL divergence is not tractable because we assume that the posterior density is intractable. To solve this, we use Bayes theorem to obtain

$$\log p(\mathcal{D}|\theta) = KL\big(q_\phi(\theta)||p(\theta|\mathcal{D})\big) + ELBO(q_\phi(\theta)),$$

where $ELBO(q_\phi(\theta))$ is the *Evidence Lower Bound*, given by

$$ELBO(q_\phi(\theta)) = \mathbb{E}_{\theta\sim q_\phi(\theta)}\big[\log p(y|x,\theta)\big] - KL\big(q_\phi(\theta)||p(\theta)\big).$$

By maximizing the ELBO, we indirectly minimize the KL divergence between the variational probability density and the posterior density.

Set up for stochastic variational inference with the variational density $q_\phi(\theta)$ by using a normal probability density with a diagonal covariance matrix:

[13]:
```
from pyro.infer import SVI, Trace_ELBO
from pyro.infer.autoguide import AutoDiagonalNormal
from tqdm.auto import trange
pyro.clear_param_store()

model = BNN(hid_dim=10, n_hid_layers=5, prior_scale=5.)
mean_field_guide = AutoDiagonalNormal(model)
```

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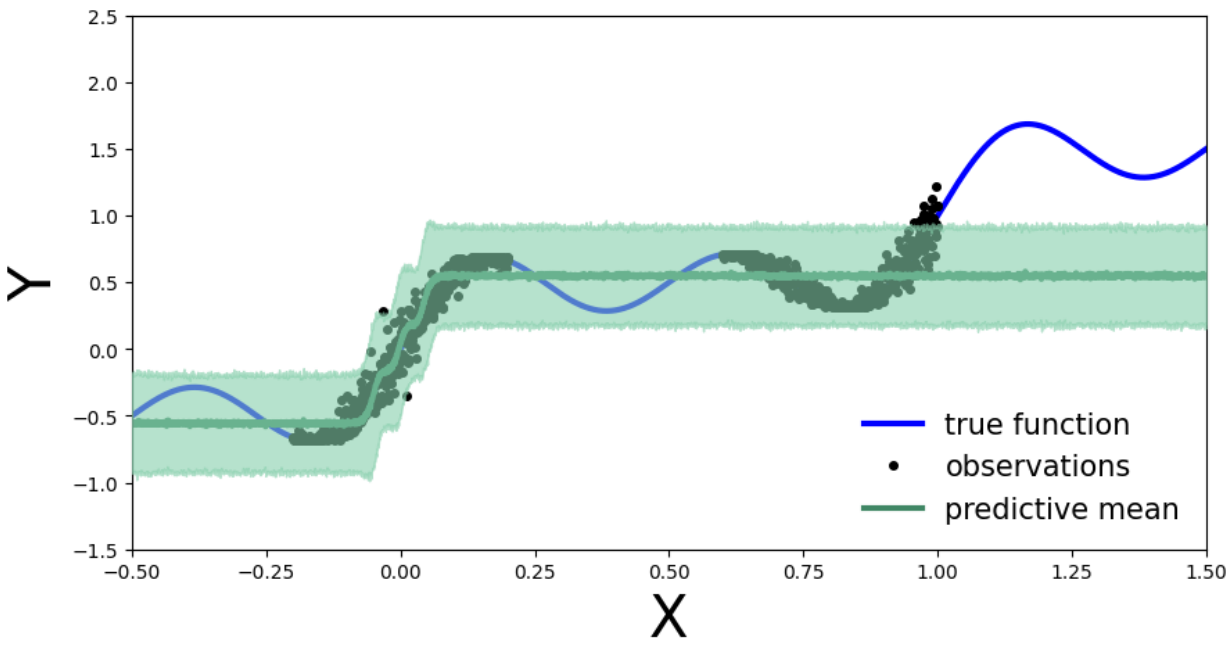
```
optimizer = pyro.optim.Adam({"lr": 0.01})

svi = SVI(model, mean_field_guide, optimizer, loss=Trace_ELBO())
pyro.clear_param_store()

num_epochs = 25000
progress_bar = trange(num_epochs)

for epoch in progress_bar:
    loss = svi.step(x_train, y_train)
    progress_bar.set_postfix(loss=f"{loss / x_train.shape[0]:.3f}")
```

```
  0%|          | 0/25000 [00:00<?, ?it/s]
```

As before, we compute the predictive distribution sampling from the trained variational density.

[14]:
```
predictive = Predictive(model, guide=mean_field_guide, num_samples=500)
preds = predictive(x_test)
plot_predictions(preds)
```



4.49.8 Exercise 2: Bayesian updating with variational inference

What happens if we obtain new data points, denoted as $\mathcal{D}'$, after performing variational inference using the observations $\mathcal{D}$?

[15]:
```
# Generate new observations
x_new = np.linspace(0.2, 0.6, 100)
noise = 0.02 * np.random.randn(x_new.shape[0])
y_new = x_new + 0.3 * np.sin(2 * np.pi * (x_new + noise)) + 0.3 * np.sin(4 * np.pi * (x_
↪new + noise)) + noise
```

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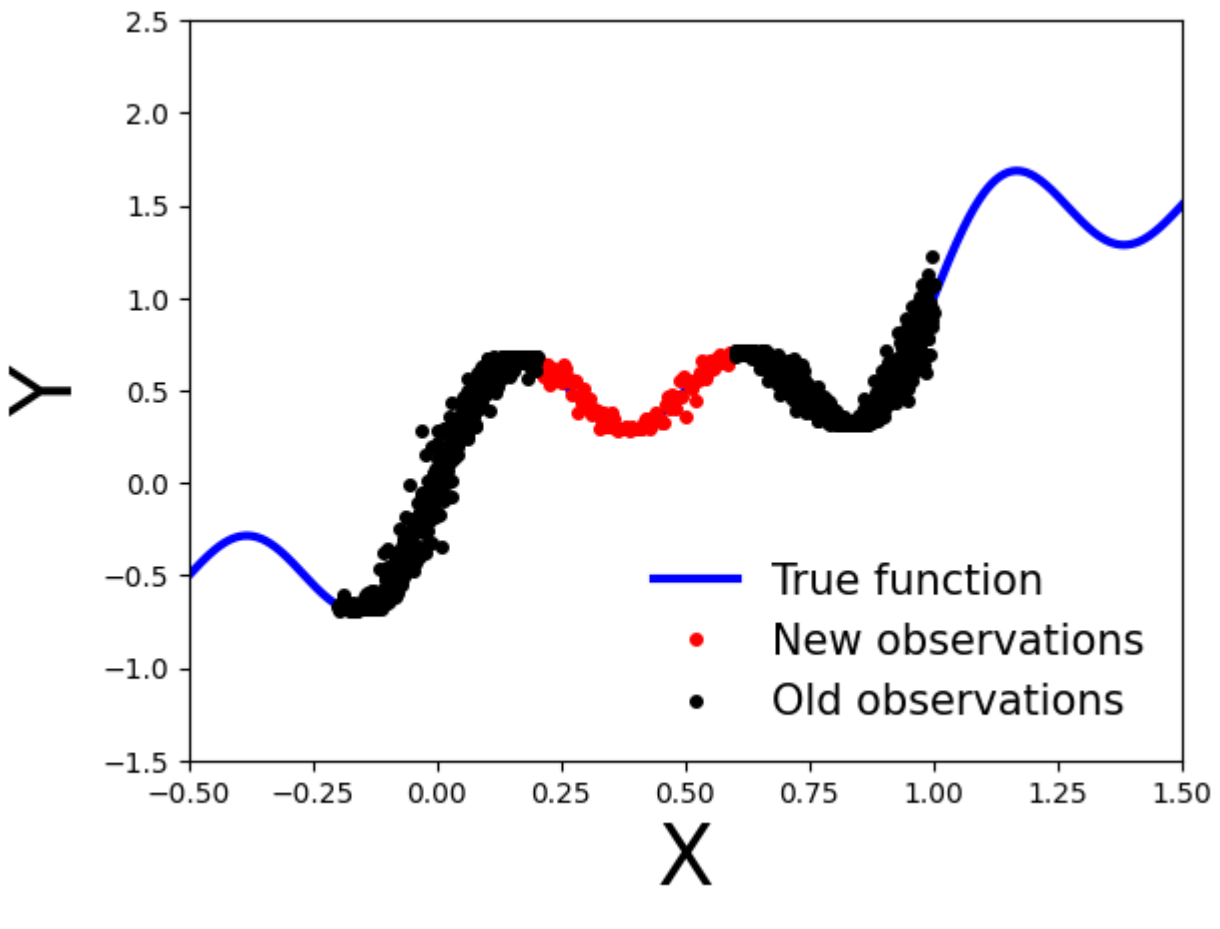
```
# Generate true function
x_true = np.linspace(-0.5, 1.5, 1000)
y_true = x_true + 0.3 * np.sin(2 * np.pi * x_true) + 0.3 * np.sin(4 * np.pi * x_true)

# Set axis limits and labels
plt.xlim(xlims)
plt.ylim(ylims)
plt.xlabel("X", fontsize=30)
plt.ylabel("Y", fontsize=30)

# Plot all datasets
plt.plot(x_true, y_true, 'b-', linewidth=3, label="True function")
plt.plot(x_new, y_new, 'ko', markersize=4, label="New observations", c="r")
plt.plot(x_obs, y_obs, 'ko', markersize=4, label="Old observations")
plt.legend(loc=4, fontsize=15, frameon=False)
plt.show()
```

```
<ipython-input-15-68b431b95167>:18: UserWarning: color is redundantly defined by the
↪'color' keyword argument and the fmt string "ko" (-> color='k'). The keyword argument␣
↪will take precedence.
  plt.plot(x_new, y_new, 'ko', markersize=4, label="New observations", c="r")
```



4.49.9 Bayesian update

How can we perform a Bayesian update on the model using variational inference when new observations become available?

We can use the previously calculated posterior probability density as the new prior and update the posterior with the new observations. Specifically, the updated posterior probability density is given by:

$$p(\theta|\mathcal{D}') = \frac{p(\mathcal{D}'|\theta)q_\phi(\theta)}{\int p(\mathcal{D}'|\theta)q_\phi(\theta)}$$

Note that we want to update our model using only the new observations $\mathcal{D}'$, relying on the fact that the variational density used as our new prior carries the necessary information on the old observations $\mathcal{D}$.

Implementation in Pyro

To implement this in Pyro, we can extract the variational parameters (mean and standard deviation) from the `guide` and use them to initialize the prior in a new model that is similar to the original model used for variational inference.

From the Gaussian `guide` we can extract the variational parameters (mean and standard deviation) as:

```
mu = guide.get_posterior().mean
sigma = guide.get_posterior().stddev
```

Exercise 2.1 Learn a model on the old observations

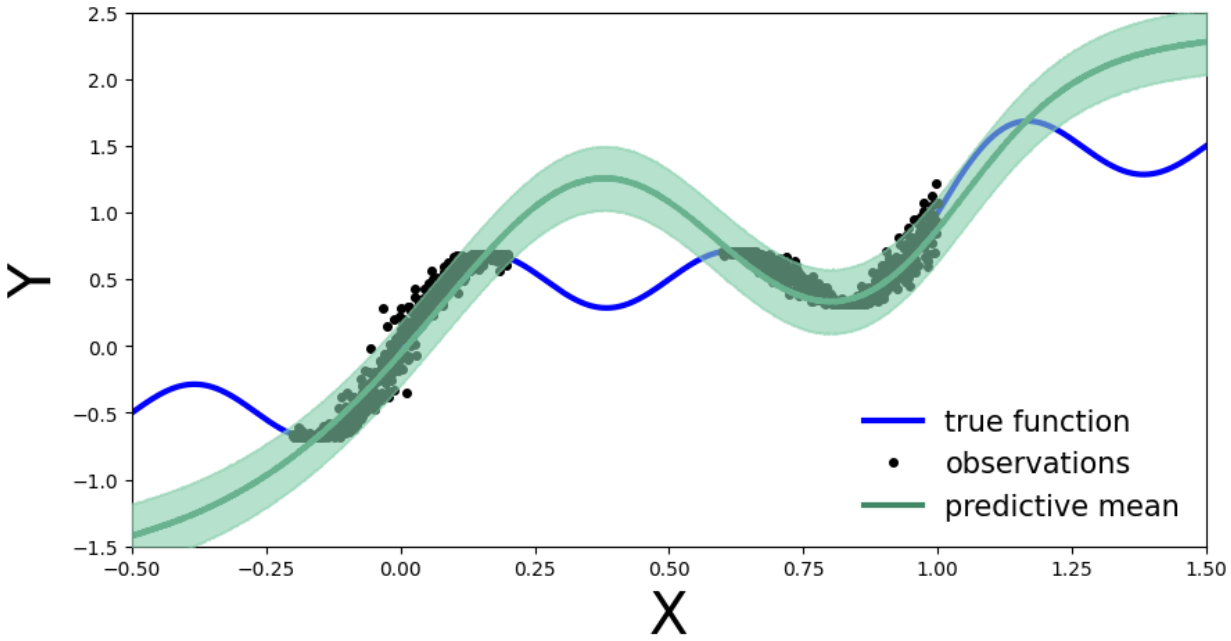
First, as before, we define a model using Gaussian prior $\mathcal{N}(\mathbf{0}, 10 \cdot \mathbb{I})$.

> Train a model `MyFirstBNN` on the old observations $\mathcal{D}$ using variational inference with `AutoDiagonalNormal()` as guide.

[16]:
```
from pyro.optim import Adam
pyro.set_rng_seed(42)
pyro.clear_param_store()

model = MyFirstBNN()
guide = AutoDiagonalNormal(model)
optim = Adam({"lr": 0.03})
svi = pyro.infer.SVI(model, guide, optim, loss=Trace_ELBO())

num_iterations = 10000
progress_bar = trange(num_iterations)

for j in progress_bar:
    loss = svi.step(x_train, y_train)
    progress_bar.set_description("[iteration %04d] loss: %.4f" % (j + 1, loss / len(x_
↪train)))
```

```
  0%|          | 0/10000 [00:00<?, ?it/s]
```

[17]:
```
predictive = Predictive(model, guide=guide, num_samples=5000)
preds = predictive(x_test)
plot_predictions(preds)
```



Next, we can extract the variational parameters (mean and standard deviation) from the `guide` and use them to initialize the prior in a new model that is similar to the original model used for variational inference.

[18]:
```
# Extract variational parameters from guide
mu = guide.get_posterior().mean.detach()
stddev = guide.get_posterior().stddev.detach()
```

[19]:
```
for name, value in pyro.get_param_store().items():
    print(name, pyro.param(name))
```

```
AutoDiagonalNormal.loc Parameter containing:
tensor([ 4.4192,  2.0755,  2.5186,  2.9757, -2.8465, -4.5504, -0.6823,  8.6747,
         8.4490,  1.4790,  1.2583,  5.1179,  0.9285, -1.8939,  4.3386,  1.2919,
        -1.0739], requires_grad=True)
AutoDiagonalNormal.scale tensor([1.4528e-02, 2.4028e-03, 2.1688e+00, 1.6080e+00, 4.6767e-
↪03, 1.4400e-02,
        1.4626e-03, 1.5972e+00, 8.8795e-01, 2.9016e-03, 6.1736e-03, 9.5345e-03,
        6.3799e-03, 5.4558e-03, 7.9139e-03, 5.9700e-03, 4.8264e-02],
       grad_fn=<SoftplusBackward0>)
```

Exercise 2.2 Initialize a second model with the variational parameters

Define a new model similar to `MyFirstBNN(PyroModule)`, that takes the variational parameters and uses them to initialize the prior.

[20]:
```
class UpdatedBNN(PyroModule):
    def __init__(self, mu, stddev, in_dim=1, out_dim=1, hid_dim=5):
        super().__init__()
        self.mu = mu
        self.stddev = stddev
```

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```
        self.activation = nn.Tanh()
        self.layer1 = PyroModule[nn.Linear](in_dim, hid_dim)
        self.layer2 = PyroModule[nn.Linear](hid_dim, out_dim)

        self.layer1.weight = PyroSample(dist.Normal(self.mu[0:5].unsqueeze(1), self.
↪stddev[0:5].unsqueeze(1)).to_event(2))
        self.layer1.bias = PyroSample(dist.Normal(self.mu[5:10], self.stddev[5:10]).to_
↪event(1))
        self.layer2.weight = PyroSample(dist.Normal(self.mu[10:15].unsqueeze(0), self.
↪stddev[10:15].unsqueeze(0)).to_event(2))
        self.layer2.bias = PyroSample(dist.Normal(self.mu[15:16], self.stddev[15:16]).to_
↪event(1))
        # 17th parameter is parameter sigma from the Gamma distribution

    def forward(self, x, y=None):
        x = x.reshape(-1, 1)
        x = self.activation(self.layer1(x))
        mu = self.layer2(x).squeeze()
        sigma = pyro.sample("sigma", dist.Gamma(.5, 1))

        with pyro.plate("data", x.shape[0]):
            obs = pyro.sample("obs", dist.Normal(mu, sigma * sigma), obs=y)
        return mu
```

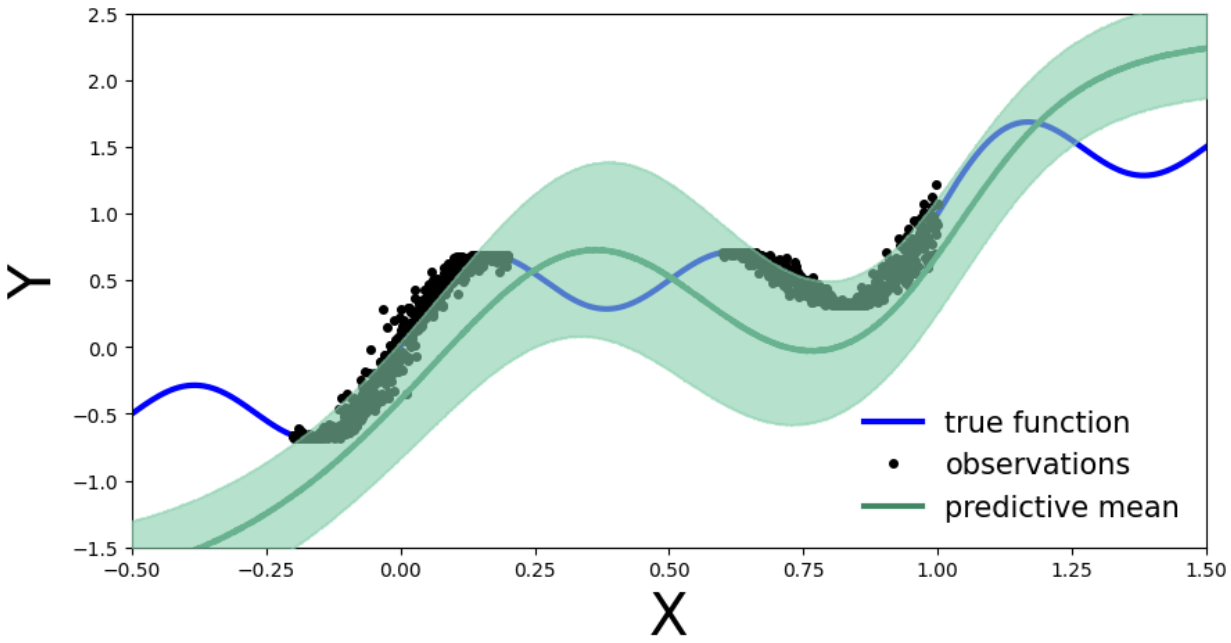
Exercise 2.3 Perform variational inference on the new model

Then perform variational inference on this new model using the new observations and plot the predictive distribution. What do you observe? How does the predictive distribution compare to the one obtained in Exercise 2.1?

[21]:
```
x_train_new = torch.from_numpy(x_new).float()
y_train_new = torch.from_numpy(y_new).float()

pyro.clear_param_store()
new_model = UpdatedBNN(mu, stddev)
new_guide = AutoDiagonalNormal(new_model)
optim = Adam({"lr": 0.01})
svi = pyro.infer.SVI(new_model, new_guide, optim, loss=Trace_ELBO())

num_iterations = 1000
progress_bar = trange(num_iterations)

for j in progress_bar:
    loss = svi.step(x_train_new, y_train_new)
    progress_bar.set_description("[iteration %04d] loss: %.4f" % (j + 1, loss / len(x_
↪train)))
```

```
  0%|          | 0/1000 [00:00<?, ?it/s]
```

[22]:
```
predictive = Predictive(new_model, guide=new_guide, num_samples=5000)
preds = predictive(x_test)
plot_predictions(preds)
```



4.50 Tutorial 2: Comparison to other methods of uncertainty quantification

Filled notebook: - Latest version (V04/23): this notebook

Empty notebook: - Latest version (V04/23):

Visit also the DL2 tutorial Github repo and associated Docs page.

Authors: Ilze Amanda Auzina, Leonard Bereska, Alexander Timans and Eric Nalisnick

---

In this tutorial we will investigate what are some benefits of Bayesian Neural Networks (BNN) over point estimate Neural Networks. We will also look at other uncertainty quantification methods, including conformal prediction.

Import standard libraries and setting random seeds for reproducibility.

[1]:
```
import torch
import torch.nn as nn
import numpy as np
import matplotlib.pyplot as plt
from tqdm.auto import trange, tqdm

torch.manual_seed(42)
np.random.seed(42)
```

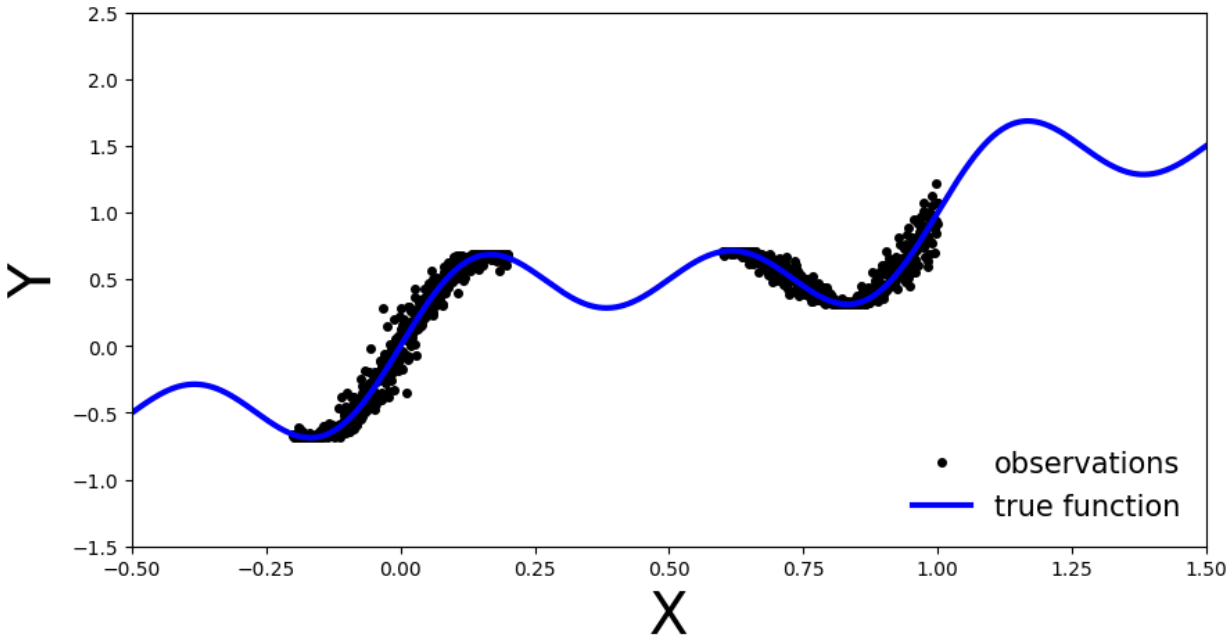
4.50.1 Simulate Data

Let's simulate a wiggly line and draw observations in separated regions...

[2]:
```
def get_simple_data_train():
    x = np.linspace(-.2, 0.2, 500)
    x = np.hstack([x, np.linspace(.6, 1, 500)])
    eps = 0.02 * np.random.randn(x.shape[0])
    y = x + 0.3 * np.sin(2 * np.pi * (x + eps)) + 0.3 * np.sin(4 * np.pi * (x + eps)) +␣
↪eps
    x_train = torch.from_numpy(x).float()[:, None]
    y_train = torch.from_numpy(y).float()
    return x_train, y_train
```

[3]:
```
def plot_generic(add_to_plot=None):
    fig, ax = plt.subplots(figsize=(10, 5))
    plt.xlim([-.5, 1.5])
    plt.ylim([-1.5, 2.5])
    plt.xlabel("X", fontsize=30)
    plt.ylabel("Y", fontsize=30)

    x_train, y_train = get_simple_data_train()

    x_true = np.linspace(-.5, 1.5, 1000)
    y_true = x_true + 0.3 * np.sin(2 * np.pi * x_true) + 0.3 * np.sin(4 * np.pi * x_true)

    ax.plot(x_train, y_train, 'ko', markersize=4, label="observations")
    ax.plot(x_true, y_true, 'b-', linewidth=3, label="true function")
    if add_to_plot is not None:
        add_to_plot(ax)

    plt.legend(loc=4, fontsize=15, frameon=False)
    plt.show()
```

[4]:
```
plot_generic()
```



As you can see, we have the true function in blue. The observations are observable in two regions of the function and there is some noise in their measurement. We will use this simple data to showcase the differences between BNNs and deterministic NNs.

4.50.2 Define non-Bayesian Neural Network

First let's create our point estimate neural network, in other words a standard fully connected MLP. We will define the number of hidden layers dynamically so we can reuse the same class for different depths. We will also add a *dropout* flag, this will allow us to easily use the same architecture for our BNN.

[5]:
```
class MLP(nn.Module):
    def __init__(self, input_dim=1, output_dim=1, hidden_dim=10, n_hidden_layers=1, use_
↪dropout=False):
        super().__init__()

        self.use_dropout = use_dropout
        if use_dropout:
            self.dropout = nn.Dropout(p=0.5)
        self.activation = nn.Tanh()

        # dynamically define architecture
        self.layer_sizes = [input_dim] + n_hidden_layers * [hidden_dim] + [output_dim]
        layer_list = [nn.Linear(self.layer_sizes[idx - 1], self.layer_sizes[idx]) for␣
↪idx in
                      range(1, len(self.layer_sizes))]
        self.layers = nn.ModuleList(layer_list)

    def forward(self, input):
        hidden = self.activation(self.layers[0](input))
        for layer in self.layers[1:-1]:
```

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```
            hidden_temp = self.activation(layer(hidden))

            if self.use_dropout:
                hidden_temp = self.dropout(hidden_temp)

            hidden = hidden_temp + hidden  # residual connection

        output_mean = self.layers[-1](hidden).squeeze()
        return output_mean
```

4.50.3 Train one deterministic NN

Training

Now let's train our MLP with the training data we generated above:

[6]:
```
def train(net, train_data):
    x_train, y_train = train_data
    optimizer = torch.optim.Adam(params=net.parameters(), lr=1e-3)
    criterion = nn.MSELoss()

    progress_bar = trange(3000)
    for _ in progress_bar:
        optimizer.zero_grad()
        loss = criterion(y_train, net(x_train))
        progress_bar.set_postfix(loss=f'{loss / x_train.shape[0]:.3f}')
        loss.backward()
        optimizer.step()
    return net
```

[7]:
```
train_data = get_simple_data_train()
x_test = torch.linspace(-.5, 1.5, 3000)[:, None]  # test over the whole range

net = MLP(hidden_dim=30, n_hidden_layers=2)
net = train(net, train_data)
y_preds = net(x_test).clone().detach().numpy()
```

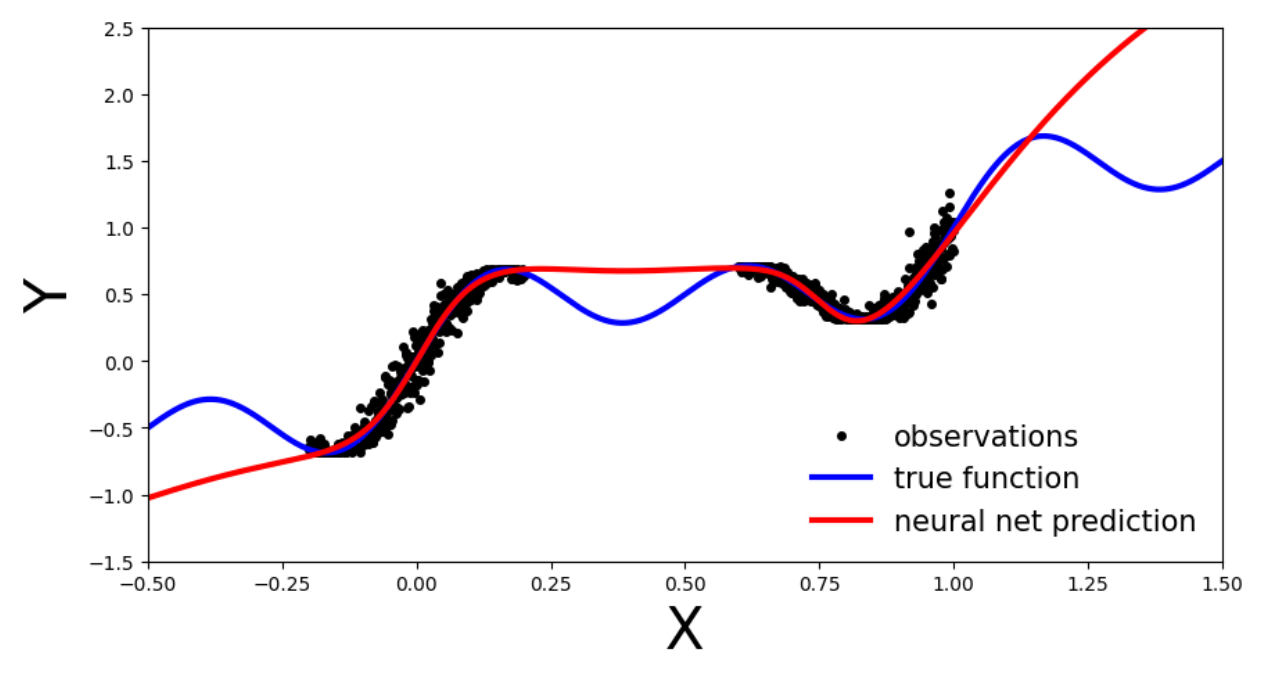
```
  0%|          | 0/3000 [00:00<?, ?it/s]
```

Evaluate

Let's investigate how our deterministic MLP generalizes over the entire domain of our input variable x (the model was only trained on the observations, now we will also pass in data outside this region)

[8]:
```
def plot_predictions(x_test, y_preds):
    def add_predictions(ax):
        ax.plot(x_test, y_preds, 'r-', linewidth=3, label='neural net prediction')

    plot_generic(add_predictions)
plot_predictions(x_test, y_preds)
```



We can see that our deterministic MLP (red line) has correctly learned the data distribution in the training regions, however, as the model has not learned the underlying sinusoidal wave function, it's predictions outside the training region are inaccurate. As our MLP is a point estimate NN we have no measure confidence in the predictions outside the training region. In the upcoming sections let's see how this compares to BNN.

4.50.4 Deep Ensemble

Deep ensembles were first introduced by Lakshminarayanan et al. (2017). As the name implies multiple point estimate NN are trained, *an ensemble*, and the final prediction is computed as an average across the models. From a Bayesian perspective the different point estimates correspond to modes of a Bayesian posterior. This can be interpreted as approximating the posterior with a distribution parametrized as multiple Dirac deltas:

$$q_\phi(\theta|D) = \sum_{\theta_i} \alpha_{\theta_i \theta_i}(\theta)$$

where α_{θ_i} are positive constants such that their sum is equal to one.

Training

We will reuse the MLP architecture introduced before, simply now we will train an ensemble of such models

[9]:
```
ensemble_size = 5
ensemble = [MLP(hidden_dim=30, n_hidden_layers=2) for _ in range(ensemble_size)]
for net in ensemble:
    train(net, train_data)
```

```
  0%|          | 0/3000 [00:00<?, ?it/s]
  0%|          | 0/3000 [00:00<?, ?it/s]
  0%|          | 0/3000 [00:00<?, ?it/s]
  0%|          | 0/3000 [00:00<?, ?it/s]
```

```
  0%|          | 0/3000 [00:00<?, ?it/s]
```

Evaluate

Same as before, let's investigate how our Deep Ensemble performs on the entire data domain of our input variable x.

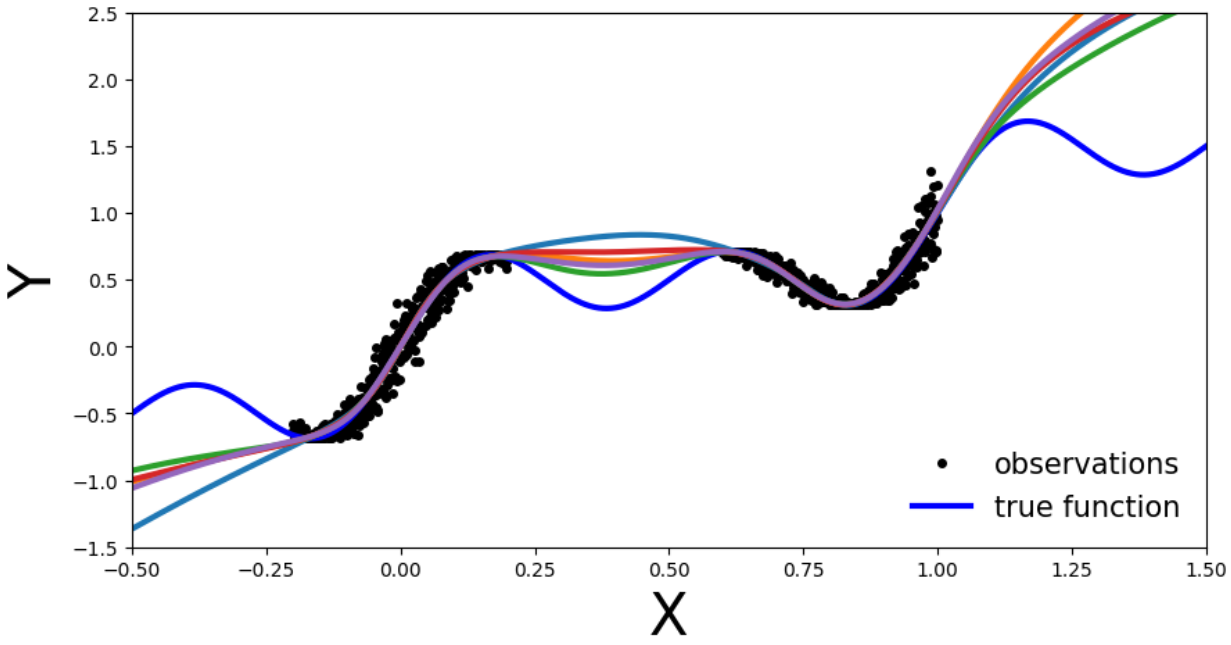
[10]:
```
y_preds = [np.array(net(x_test).clone().detach().numpy()) for net in ensemble]
```

Plot each ensemble member's predictive function.

[11]:
```
def plot_multiple_predictions(x_test, y_preds):
    def add_multiple_predictions(ax):
        for idx in range(len(y_preds)):
            ax.plot(x_test, y_preds[idx], '-', linewidth=3)

    plot_generic(add_multiple_predictions)
```

[12]:
```
plot_multiple_predictions(x_test, y_preds)
```



In this plot the benefit of an ensemble approach is not immediately clear. Still on the regions outside the training data each of the trained NN is inaccurate. So what is the benefit you might ask.

Well let's plot the above in a slightly different way: let's visualize the ensemble's **uncertainty bands**. > From a Bayesian perspective we want to quantify the model's uncertainty on its prediction. This is done via the marginal $p(y|x, D)$, which can be computed as:

$$In practice, for Deep Ensembles we approximate the above by computing the mean and standard deviation across the ensemble. Me$$

[13]:
```
def plot_uncertainty_bands(x_test, y_preds):
    y_preds = np.array(y_preds)
```

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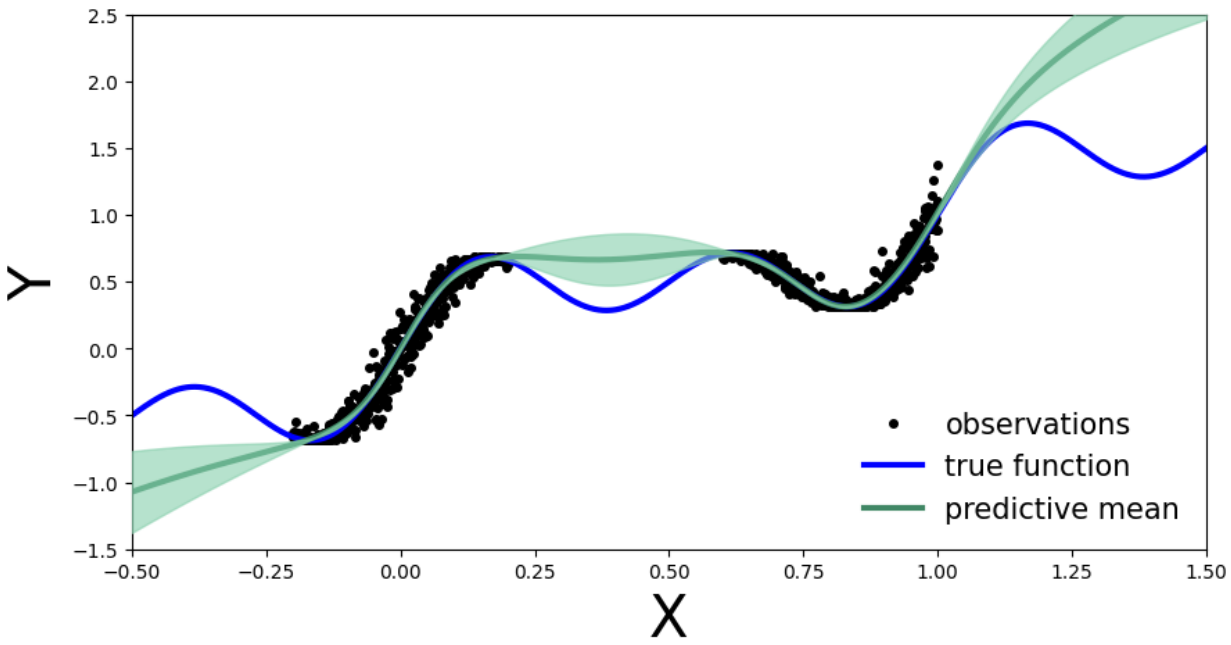
```
    y_mean = y_preds.mean(axis=0)
    y_std = y_preds.std(axis=0)

    def add_uncertainty(ax):
        ax.plot(x_test, y_mean, '-', linewidth=3, color="#408765", label="predictive mean
↪")
        ax.fill_between(x_test.ravel(), y_mean - 2 * y_std, y_mean + 2 * y_std, alpha=0.
↪6, color='#86cfac', zorder=5)

    plot_generic(add_uncertainty)
```

[14]:
```
plot_uncertainty_bands(x_test, y_preds)
```



Now we see the benefit of a Bayesian approach. Outside the training region we not only have the point estimate, but also model's uncertainty about its prediction.

4.50.5 Monte Carlo Dropout

First we create our MC-Dropout Network. As you can see in the code below, creating a dropout network is extremely simple: We can reuse our existing network architecture, the only alteration is that during the forward pass we randomly *switch off* (zero) some of the elements of the input tensor.

The Bayesian interpretation of MC-Dropout is that we can see each dropout configuration as a different sample from the approximate posterior distribution $\theta_i q(\theta|D)$.

Training

[15]:
```
net_dropout = MLP(hidden_dim=30, n_hidden_layers=2, use_dropout=True)
net_dropout = train(net_dropout, train_data)
```

```
  0%|          | 0/3000 [00:00<?, ?it/s]
```

Evaluate

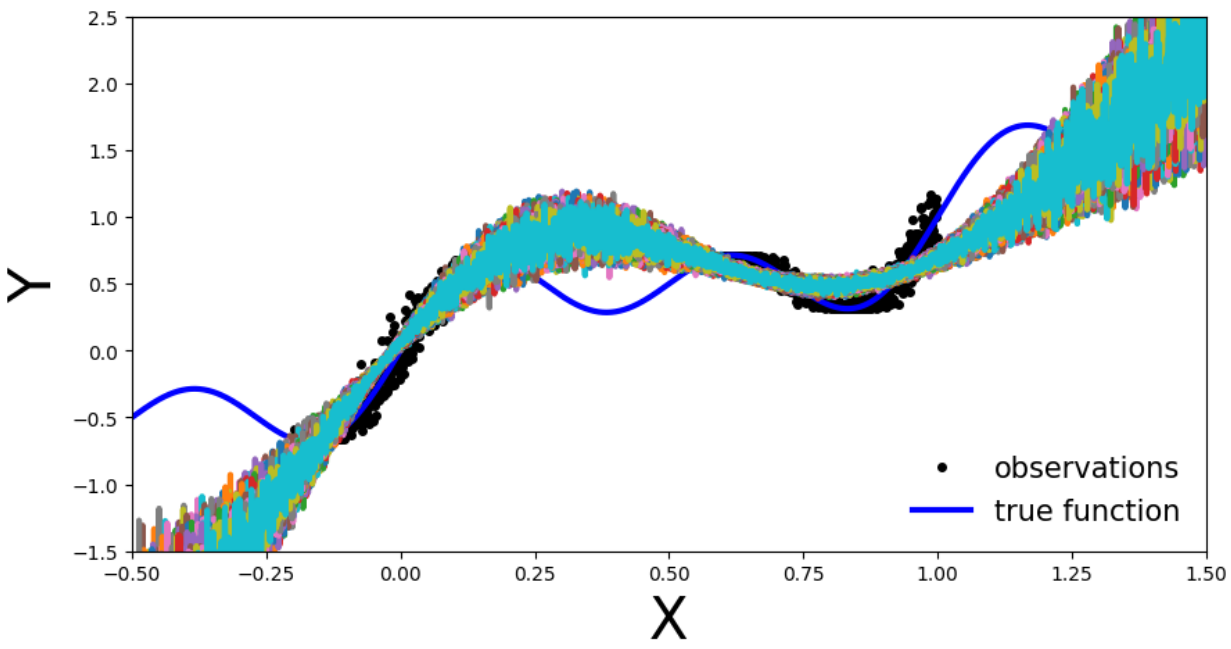
Similarly to Deep Ensembles, we pass the test data multiple times through the MC-Dropout network. We do so to obtain y_i at the different parameter settings, θ_i of the network, $y_i = f(x, \theta_i)$, governed by the dropout mask.

> This is the main difference compared to dropout implementation in a deterministic NN where it serves as a regularization term. In normal dropout application during test time the dropout is **not** applied. Meaning that all connections are present, but the weights are adjusted

[16]:
```
n_dropout_samples = 100

# compute predictions, resampling dropout mask for each forward pass
y_preds = [net_dropout(x_test).clone().detach().numpy() for _ in range(n_dropout_
↪samples)]
y_preds = np.array(y_preds)
```

[17]:
```
plot_multiple_predictions(x_test, y_preds)
```

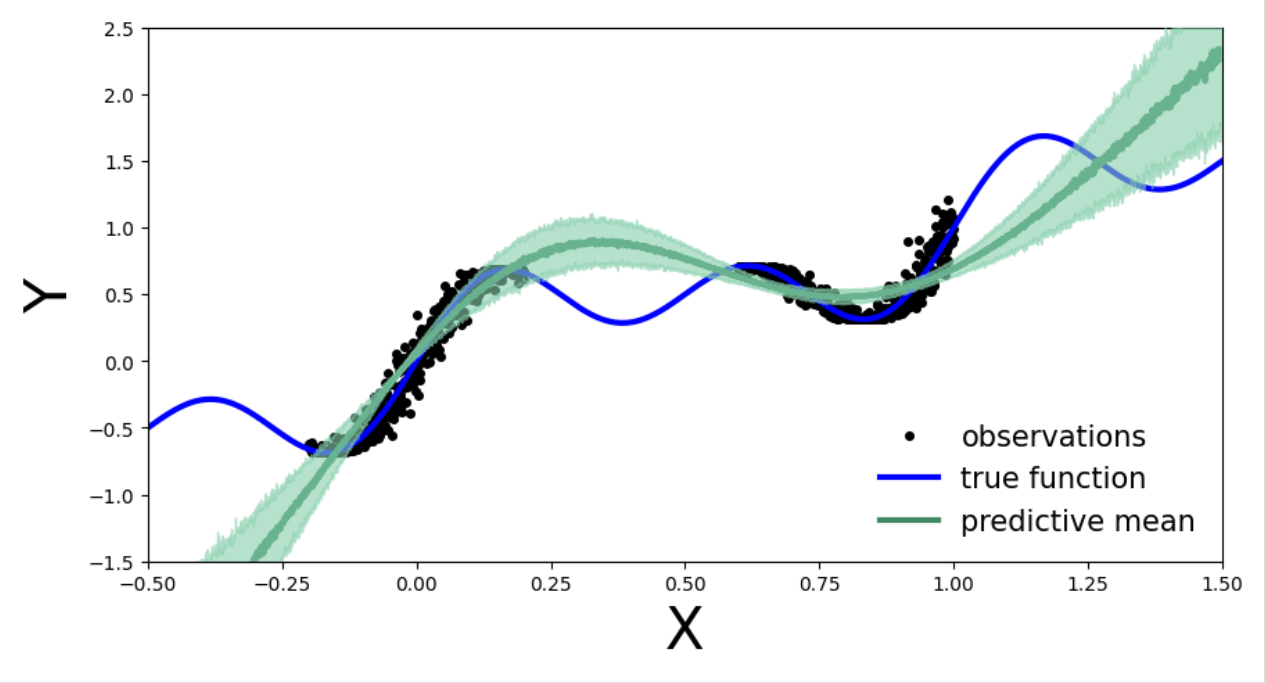


In the above plot each colored line (apart from blue) represents a different parametrization, θ_i, of our MC-Dropout Network.

Likewise to the Deep Ensemble Network, we can also compute the MC-dropout's **uncertainty bands**.

> The approach in practice is the same as before: we compute the mean and standard deviation across each dropout mask, which corresponds to the marginal estimation we discussed earlier.

[18]:
```
plot_uncertainty_bands(x_test, y_preds)
```



In the same way as Deep Ensembles, MC-Dropout allows us to have an uncertainty estimate next to our point wise predictions. However, for the given use-case this has come with the cost of an overall drop in the model's performance on the training regions. We observe this because at every pass through our network we randomly choose which nodes to keep, so one could argue that we hinder the networks optimal performance.

4.50.6 Conformal prediction

Conformal prediction is a statistical uncertainty quantification approach that has gained interest in the Machine Learning community more recently. Originally proposed by Vovk et al., it allows us to construct statistically rigorous uncertainty bands around our predictions, without requiring any modifications to our prediction model. This is achieved by comparing true and predicted values on out-of-sample data (more precisely we are looking at *inductive* conformal prediction), and computing an empirical quantile $\hat{q}$ based on these comparisons that defines the magnitude of the uncertainy bands. How we compare true and predicted values is a modelling decision, and there are different ways to do so. The comparison results are also called *(non)conformity scores*, hence the naming of the method.

If we follow the conformal recipe, with minimal assumptions our uncertainty bands will be statistically rigorous in the sense that they satisfy a nice property for any test sample (X_{n+1}, Y_{n+1}):

$$\mathbb{P}(Y_{n+1} \in \hat{C}(X_{n+1})) \geq 1 - \alpha,$$

i.e. with probability at least $1 - \alpha$, our computed uncertainty band $\hat{C}(X_{n+1})$ around our point estimate $\hat{Y}_{n+1}$ will contain the *true* unknown value Y_{n+1}. This is called a (marginal) coverage guarantee, and provides us with a measure of confidence in the quality of our uncertainty bands.

We will now see that the implementation of conformal prediction for our example is in fact very simple, which is part of its attractiveness.

Training

Firstly, we split our training samples into two different data sets, the true training set and a hold-out data set, which we call the calibration set (you can think of it as a specific kind of validation set). We will take 20% of our data for calibration. Usually this is a random sample, but for reproducebility we select them evenly spaced.

[19]:
```
# split data into training and calibration sets
x, y = get_simple_data_train()
cal_idx = np.arange(len(x), step=1/0.2, dtype=np.int64)
# cal_idx = np.random.choice(len(x), size=int(len(x) * 0.2), replace=False) # random␣
↪selection
mask = np.zeros(len(x), dtype=bool)
mask[cal_idx] = True
x_cal, y_cal = x[mask], y[mask]
x_train, y_train = x[~mask], y[~mask]
```

Then, we train a single standard (non-Bayesian) MLP on the true training set:

[20]:
```
net = MLP(hidden_dim=30, n_hidden_layers=2)
net = train(net, (x_train, y_train))
```

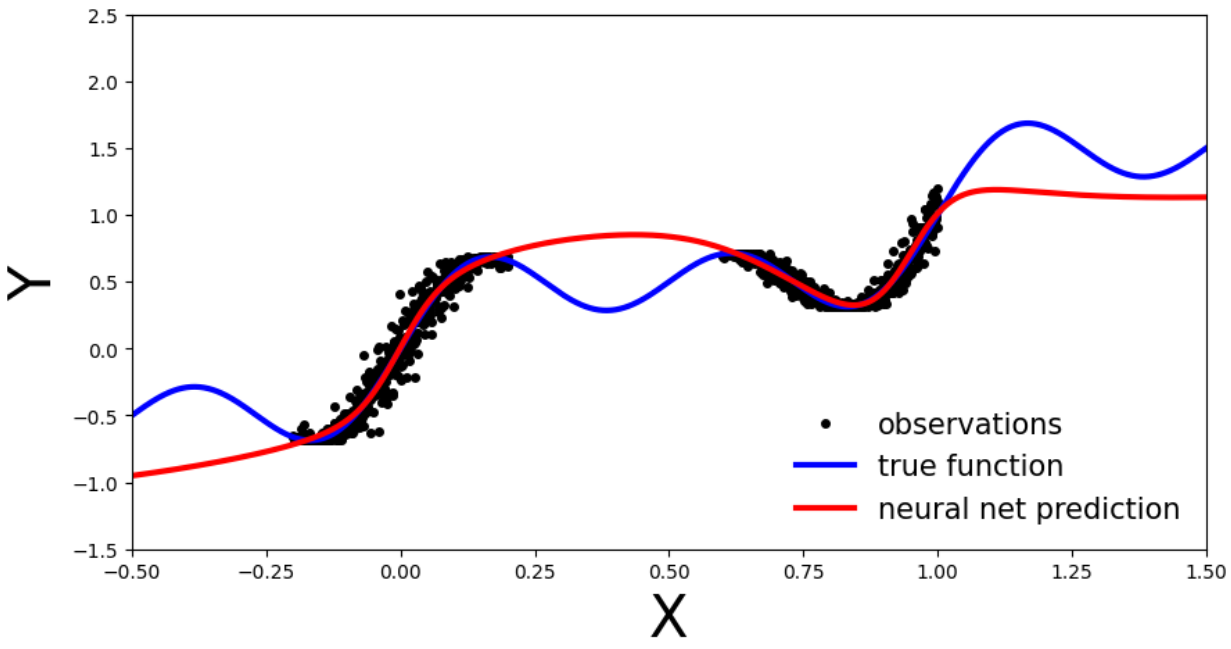
```
  0%|          | 0/3000 [00:00<?, ?it/s]
```

Evaluate

Same as before, we first visualize how the MLP performs on the entire data domain of our input variable x. We see that training it on only 80% instead of all available data did not notably change its performance.

[21]:
```
# compute predictions everywhere
x_test = torch.linspace(-.5, 1.5, 1000)[:, None]
y_preds = net(x_test).clone().detach().numpy()
```

[22]:
```
plot_predictions(x_test, y_preds)
```



We now perform the conformal prediction procedure to obtain our uncertainty bands. In the simplest case, our comparison of predicted and true values on the calibration data is achieved by simply looking at the residuals $|y - \hat{y}|$, which form our *conformity scores*. We then compute $\hat{q}$ as the $\left\lceil \frac{(n+1)(1-\alpha)}{n} \right\rceil$ empirical quantile of these residuals, and form our uncertainty bands for every test sample as $\hat{C}(X_{n+1}) = [\hat{f}(x_{n+1}) - \hat{q},\ \hat{f}(x_{n+1}) + \hat{q}]$. Our desired coverage rate is $(1 - \alpha) \in [0, 1]$, which we set to 90% (i.e. choose $\alpha = 0.1$).

[23]:
```
# compute calibration residuals
y_cal_preds = net(x_cal).clone().detach()
resid = torch.abs(y_cal - y_cal_preds).numpy()
```

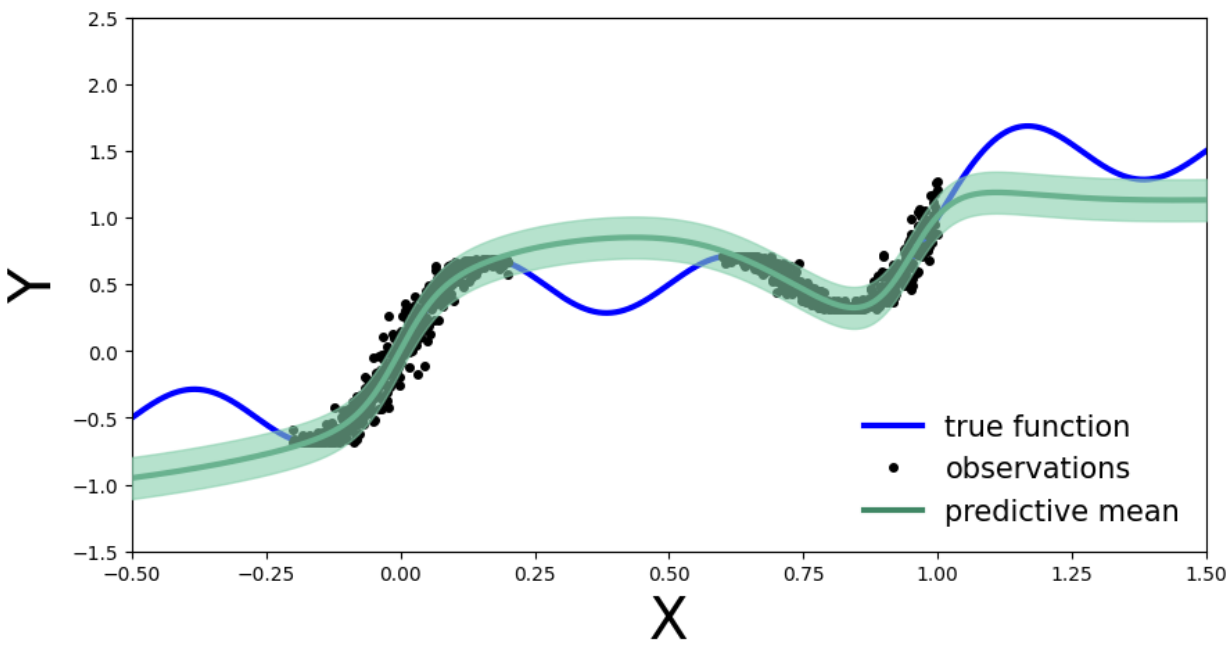
[24]:
```
# compute conformal quantile
alpha = 0.1
n = len(x_cal)
q_val = np.ceil((1 - alpha) * (n + 1)) / n
q = np.quantile(resid, q_val, method="higher")
```

[25]:
```
# true function
x_true = np.linspace(-.5, 1.5, 1000)
y_true = x_true + 0.3 * np.sin(2 * np.pi * x_true) + 0.3 * np.sin(4 * np.pi * x_true)

# generate plot
fig, ax = plt.subplots(figsize=(10, 5))
plt.xlim([-.5, 1.5])
plt.ylim([-1.5, 2.5])
plt.xlabel("X", fontsize=30)
plt.ylabel("Y", fontsize=30)

ax.plot(x_true, y_true, 'b-', linewidth=3, label="true function")
ax.plot(x, y, 'ko', markersize=4, label="observations")
ax.plot(x_test, y_preds, '-', linewidth=3, color="#408765", label="predictive mean")
ax.fill_between(x_test.ravel(), y_preds - q, y_preds + q, alpha=0.6, color='#86cfac',␣
↪zorder=5)

plt.legend(loc=4, fontsize=15, frameon=False);
```



We now obtain an uncertainty band around each test set prediction, which is informed by our performance on the calibration data (as quantified by the residuals). We can also compare our empirical coverage on the available test data

against our target coverage of 90%:

[26]:
```
# compute empirical coverage across whole test domain
cov = np.mean(((y_preds - q) <= y_true) * ((y_preds + q) >= y_true))
print(f"Empirical coverage: {cov:%}")
```

```
Empirical coverage: 49.100000%
```

We notice that the empirical coverage does not match our target coverage, suggesting that the conformal procedure is not working well for our given test samples (we are under-covering). This is mainly due to the fact that our calibration data, which is selected from available observations, is very localized and therefore not representative of the whole test domain. In other words, the information we get from the calibration data does not translate well to the whole test domain. Therefore the computed quantile $\hat{q}$ is inadequate on unseen sample spaces. Compare this to our empirical coverage for test samples from the domain of our calibration data:

[27]:
```
# compute empirical coverage only on previously observed test domain
mask = (x_true >= -.2) * (x_true < 0.2) + (x_true >= .6) * (x_true < 1)
cov = np.mean(((y_preds[mask] - q) <= y_true[mask]) * ((y_preds[mask] + q) >= y_
↪true[mask]))
print(f"Empirical coverage: {cov:%}")
```

```
Empirical coverage: 100.000000%
```

Here we are in fact over-covering, i.e. being overly conservative in the magnitude of our uncertainty bands. Note that the coverage guarantee only holds *marginally*, i.e. across *all possible* sets of calibration and test samples; this is particularly obvious in our case. Other factors playing a role in obtaining useful uncertainty bands are the choice of α, size of the calibration set and the predictive model's performance.

Exercise: Detecting Distribution Shift on MNIST

In this exercise we will compare Bayesian NNs with deterministic NNs on a distribution shift detection task. To do this, we'll monitor the predictive entropy as the distribution gradually shifts. A model with better uncertainty quantification should become less certain—that is, have a more entropic predictive distribution—as the input distribution shifts. Mathematically, our quantity of interest is:

$$\mathbb{H}[y|x^*, D] = -\sum_y p(y|x^*, D) \log p(y|x^*, D)$$

where $p(y|x^*, D)$ is the predictive distribution:

$$p(y|x^*, D) = \int_\theta p(y|x^*, \theta)\, p(\theta|D)\, d\theta.$$

The goal is to obtain something similar to Figure #4 from the paper Multiplicative Normalizing Flows for Variational Bayesian Neural Networks, comparing MC dropout, ensembles, and a Bayesian NN.

We will be using the well-known MNIST dataset, a set of 70,000 hand-written digit images, and we will generate a gradual distribution shift on the dataset by rotating the images. As such, the final plot will depict the change in the entropy of the predictive distribution (y-axis) as degree of rotation increases (x-axis). The paper above shows the result for one image. We, on the other hand, will average over multiple images to make a better comparison between models.

We'll use rotation to simulate a smooth shift. Here's how you can rotate a given image:

[28]:
```
from PIL import Image
from torchvision import datasets
from torch.nn.functional import softmax
from torchvision.transforms.functional import rotate
```

[29]:
```
def imshow(image):
    plt.imshow(image, cmap='gray', vmin=0, vmax=255)
    plt.show()
```

[30]:
```
def show_rotation_on_mnist_example_image():
    mnist_train = datasets.MNIST('../data', train=True, download=True)
    image = Image.fromarray(mnist_train.data[0].numpy())
    imshow(image)
    rotated_image = rotate(image, angle=90)
    imshow(rotated_image)
```

[31]:
```
show_rotation_on_mnist_example_image()
```

```
Downloading http://yann.lecun.com/exdb/mnist/train-images-idx3-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/train-images-idx3-ubyte.gz to ../data/MNIST/
↪raw/train-images-idx3-ubyte.gz
```

```
100%|| 9912422/9912422 [00:00<00:00, 104013908.09it/s]
```

```
Extracting ../data/MNIST/raw/train-images-idx3-ubyte.gz to ../data/MNIST/raw

Downloading http://yann.lecun.com/exdb/mnist/train-labels-idx1-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/train-labels-idx1-ubyte.gz to ../data/MNIST/
↪raw/train-labels-idx1-ubyte.gz
```

```
100%|| 28881/28881 [00:00<00:00, 108837101.37it/s]
```

```
Extracting ../data/MNIST/raw/train-labels-idx1-ubyte.gz to ../data/MNIST/raw

Downloading http://yann.lecun.com/exdb/mnist/t10k-images-idx3-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/t10k-images-idx3-ubyte.gz to ../data/MNIST/
↪raw/t10k-images-idx3-ubyte.gz
```

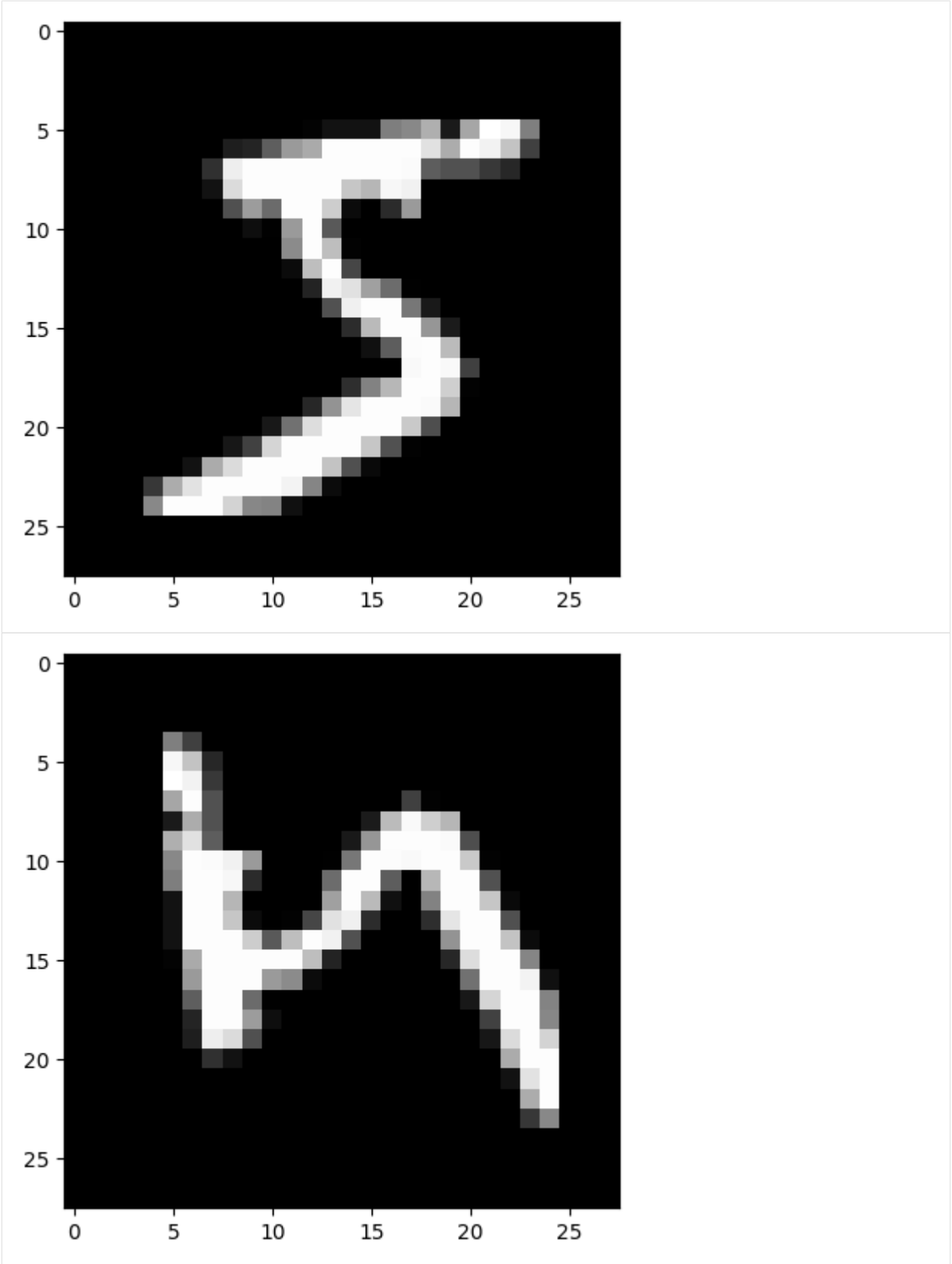
```
100%|| 1648877/1648877 [00:00<00:00, 25836124.81it/s]
```

```
Extracting ../data/MNIST/raw/t10k-images-idx3-ubyte.gz to ../data/MNIST/raw

Downloading http://yann.lecun.com/exdb/mnist/t10k-labels-idx1-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/t10k-labels-idx1-ubyte.gz to ../data/MNIST/
↪raw/t10k-labels-idx1-ubyte.gz
```

```
100%|| 4542/4542 [00:00<00:00, 15024076.32it/s]
```

```
Extracting ../data/MNIST/raw/t10k-labels-idx1-ubyte.gz to ../data/MNIST/raw
```


0
5
10
15
20
25
0
5
10
15
20
25
0
5
10
15
20
25
0
5
10
15
20
25

Let's setup the training and testing data:

[32]:
```
def get_mnist_data(train=True):
    mnist_data = datasets.MNIST('../data', train=train, download=True)
    x = mnist_data.data.reshape(-1, 28 * 28).float()
    y = mnist_data.targets
    return x, y

x_train, y_train = get_mnist_data(train=True)
x_test, y_test = get_mnist_data(train=False)
```

Now that we have the data, let's start training neural networks.

4.50.7 Deterministic Network

We will reuse our MLP network architecture with different hyperparameters:

[33]:
```
net = MLP(input_dim=784, output_dim=10, hidden_dim=30, n_hidden_layers=3)
```

Training

[34]:
```
def train_on_mnist(net):
    x_train, y_train = get_mnist_data(train=True)
    optimizer = torch.optim.Adam(params=net.parameters(), lr=1e-4)
    criterion = nn.CrossEntropyLoss()
    batch_size = 250

    progress_bar = trange(20)
    for _ in progress_bar:
        for batch_idx in range(int(x_train.shape[0] / batch_size)):
            batch_low, batch_high = batch_idx * batch_size, (batch_idx + 1) * batch_size
            optimizer.zero_grad()
            loss = criterion(target=y_train[batch_low:batch_high], input=net(x_
↪train[batch_low:batch_high]))
            progress_bar.set_postfix(loss=f'{loss / batch_size:.3f}')
            loss.backward()
            optimizer.step()
    return net
```

[35]:
```
net = train_on_mnist(net)
```

```
  0%|          | 0/20 [00:00<?, ?it/s]
```

Test

[36]:
```
def accuracy(targets, predictions):
  return (targets == predictions).sum() / targets.shape[0]
```

[37]:
```
def evaluate_accuracy_on_mnist(net):
    test_data = get_mnist_data(train=False)
    x_test, y_test = test_data
    net.eval()
    y_preds = net(x_test).argmax(1)
```

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```
    acc = accuracy(y_test, y_preds)
    print("Test accuracy is %.2f%%" % (acc.item() * 100))
```

[38]:
```
evaluate_accuracy_on_mnist(net)
```

```
Test accuracy is 92.53%
```

4.50.8 Rotating the images

Now let's compute predictive entropy on some rotated images...

First we will generate the rotated images with an increasing rotation angle from the test images. We use a subset of the MNIST test set for evaluation:

[39]:
```
def get_mnist_test_subset(n_test_images):
    mnist_test = datasets.MNIST('../data', train=False, download=True)
    x = mnist_test.data[:n_test_images].float()
    y = mnist_test.targets[:n_test_images]
    return x, y
```

[40]:
```
n_test_images = 100
x_test_subset, y_test_subset = get_mnist_test_subset(n_test_images=n_test_images)
```

[41]:
```
rotation_angles = [3 * i for i in range(0, 31)] # use angles from 0 to 90 degrees
rotated_images = [rotate(x_test_subset, angle).reshape(-1, 28 * 28) for angle in␣
↪rotation_angles]
```

Evaluate the trained MLP on the rotated images:

[42]:
```
y_preds_deterministic = [softmax(net(images), dim=-1) for images in rotated_images]
```

The information entropy H of a probability distribution p over a discrete random variable X with possible outcomes $x_1, \ldots, x_N$, occuring with probabilities $p(x_i) := p_i$ is given by:

$$H(p) = -\sum_{i=1}^{N} p_i \log p_i$$

The entropy quantifies the uncertainty of a probability distribution in the sense, that the more uncertain the outcome a hypothetical experiment with drawing from the distribution is the higher the entropy. Highest is for an equal distribution of probability mass over all possible outcomes. In our case the deterministic NN estimates a probability distribution over the ten digits as classes on MNIST for each image. For the rotated images we can thus calculate the entropy over the rotation angle.

1.1 How do you expect the entropy to behave with increasing rotation angle of the images?

1.2 Implement a function for calculating the entropy according to the formula above.

[43]:
```
def entropy(p):
  # return NotImplemented
  return (-p * np.log(p)).sum(axis=1)
```

Now we can calculate the accuracies and entropies for all rotated images and plot both:

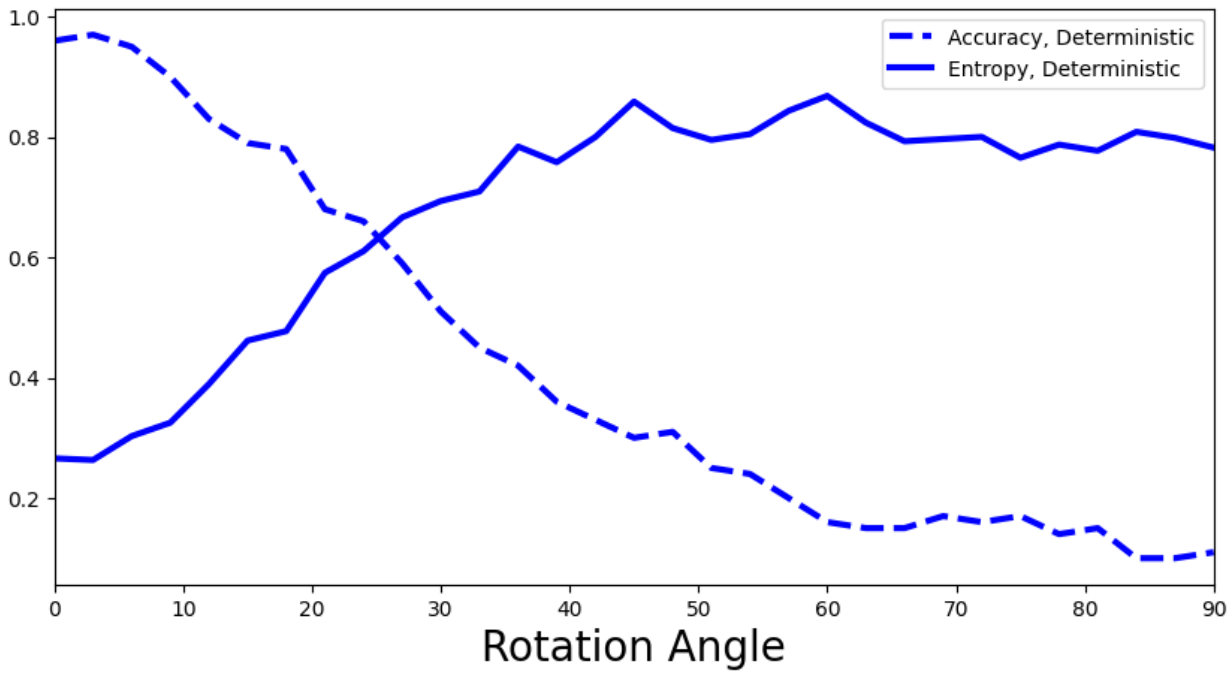
[44]:
```
def calculate_accuracies_and_entropies(y_preds):
    accuracies = [accuracy(y_test_subset, p.argmax(axis=1)) for p in y_preds]
    entropies = [np.mean(entropy(p.detach().numpy())) for p in y_preds]
    return accuracies, entropies
```

[45]:
```
def plot_accuracy_and_entropy(add_to_plot):
    fig, ax = plt.subplots(figsize=(10, 5))
    plt.xlim([0, 90])
    plt.xlabel("Rotation Angle", fontsize=20)

    add_to_plot(ax)

    plt.legend()
    plt.show()
```

[46]:
```
def add_deterministic(ax):
    accuracies, entropies = calculate_accuracies_and_entropies(y_preds_deterministic)
    ax.plot(rotation_angles, accuracies, 'b--', linewidth=3, label="Accuracy,␣
↪Deterministic")
    ax.plot(rotation_angles, entropies, 'b-', linewidth=3, label="Entropy, Deterministic
↪")
plot_accuracy_and_entropy(add_deterministic)
```



What is your interpretation of the plot above: Is the predictive entropy changing? If so, how would you explain this?

4.50.9 Monte Carlo Dropout Network

Let's create our Dropout Network. We keep the network depth and hidden layer size the same as for the MLP for a fair model comparison

[47]:
```
net_dropout = MLP(input_dim=784, output_dim=10, hidden_dim=30, n_hidden_layers=3, use_
↪dropout=True)
```

Training

[48]:
```
net_dropout = train_on_mnist(net_dropout)
```

```
  0%|          | 0/20 [00:00<?, ?it/s]
```

Test

[49]:
```
evaluate_accuracy_on_mnist(net_dropout)
```

```
Test accuracy is 92.46%
```

Evaluate on rotated images

2.1 Sample 100 different dropout masks and average the predictions over them.

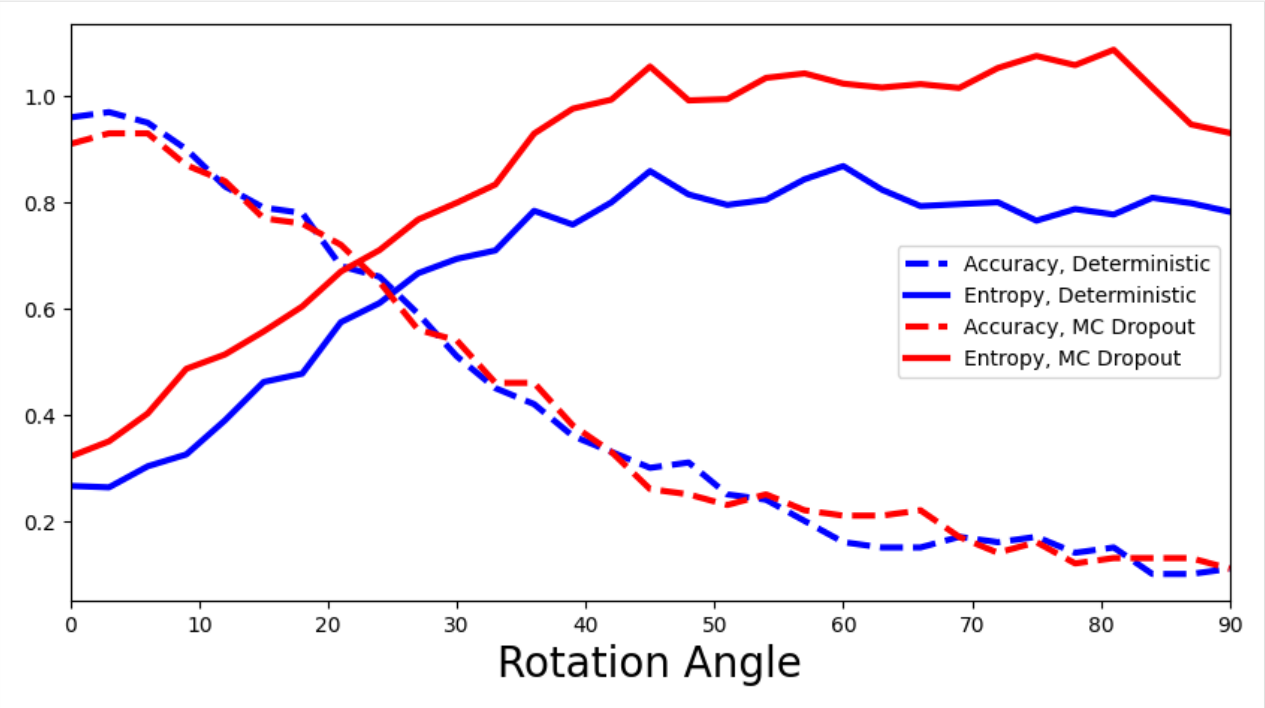
[50]:
```
n_dropout_samples = 100
net_dropout.train()  # we set the model to train to 'activate' the dropout layer

# y_preds_dropout = NotImplemented
y_preds_dropout = []
for image in rotated_images:
  y_preds = torch.zeros((n_test_images, 10))
  for idx in range(n_dropout_samples):
    y_preds += softmax(net_dropout(image), dim=1)
  y_preds_dropout.append(y_preds/n_dropout_samples)
```

2.2 What is the best way to average over the predictions? Should you first average the network output and then apply the softmax, or the other way around?

[51]:
```
def add_deterministic_and_dropout(ax):
    accuracies, entropies = calculate_accuracies_and_entropies(y_preds_deterministic)
    ax.plot(rotation_angles, accuracies, 'b--', linewidth=3, label="Accuracy,␣
↪Deterministic")
    ax.plot(rotation_angles, entropies, 'b-', linewidth=3, label="Entropy, Deterministic
↪")

    accuracies, entropies = calculate_accuracies_and_entropies(y_preds_dropout)
    ax.plot(rotation_angles, accuracies, 'r--', linewidth=3, label="Accuracy, MC Dropout
↪")
    ax.plot(rotation_angles, entropies, 'r-', linewidth=3, label="Entropy, MC Dropout")
plot_accuracy_and_entropy(add_deterministic_and_dropout)
```



How does MLP compare with MC-Dropout Network? (Are there any benefits of the Bayesian approach?)

4.50.10 Deep Ensemble

Now let's investigate Deep Ensemble performance. We will use the exact same network hyperparameters as for the MLP:

3.1 Define and train an ensemble of five MLPs with the same hyperparameters as above.

[52]:
```
ensemble_size = 5

# ensemble = NotImplemented
ensemble = []
for _ in range(ensemble_size):
  ensemble.append(MLP(input_dim=784, output_dim=10, hidden_dim=30, n_hidden_layers=3))
```

Training

[53]:
```
# ensemble = NotImplemented
for net in ensemble:
  train_on_mnist(net)
```

```
  0%|          | 0/20 [00:00<?, ?it/s]
  0%|          | 0/20 [00:00<?, ?it/s]
  0%|          | 0/20 [00:00<?, ?it/s]
  0%|          | 0/20 [00:00<?, ?it/s]
  0%|          | 0/20 [00:00<?, ?it/s]
```

Test

3.2 Evaluate the accuracy of the ensemble prediction. How do you aggregate best over the multiple different predictions given by the members of the ensemble? What is the difference to the regression setting above?

[54]:
```
# y_preds = NotImplemented
y_preds = []
for net in ensemble:
  net.eval()
  y_preds.append(net(x_test).argmax(dim=1))
y_preds = torch.stack(y_preds, dim=0).to(torch.float)
y_preds = torch.mean(y_preds, dim=0)

acc = accuracy(y_test, y_preds)
print("Test accuracy is %.2f%%" % (acc.item() * 100))
```

```
Test accuracy is 84.61%
```

Evaluate on rotated images

3.3 Again, average the predictions, but this time over the members of the ensemble.

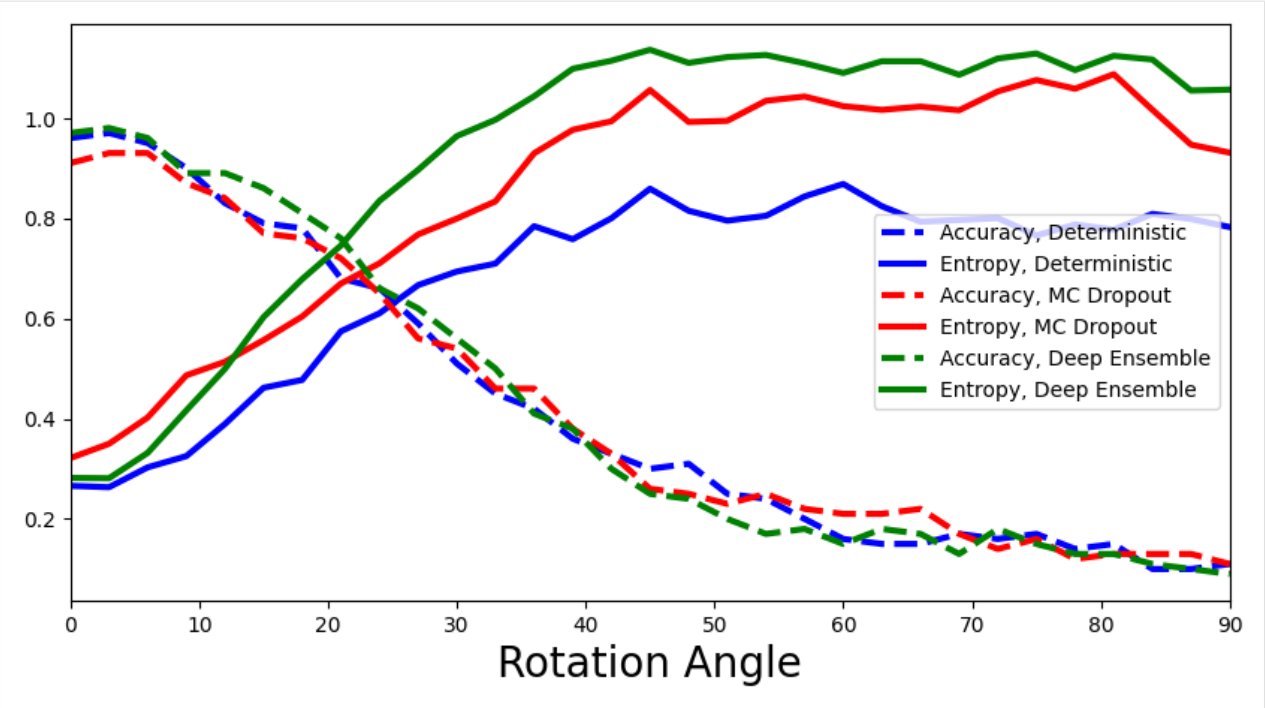
[55]:
```
# y_preds_ensemble = NotImplemented
y_preds_ensemble = []
for image in rotated_images:
  y_preds = torch.zeros((n_test_images, 10))
  for net in ensemble:
    y_preds += softmax(net(image), dim=1)
  y_preds_ensemble.append(y_preds/ensemble_size)
```

[56]:
```
def add_deep_ensemble(ax):
    accuracies, entropies = calculate_accuracies_and_entropies(y_preds_deterministic)
    ax.plot(rotation_angles, accuracies, 'b--', linewidth=3, label="Accuracy,␣
↪Deterministic")
    ax.plot(rotation_angles, entropies, 'b-', linewidth=3, label="Entropy, Deterministic
↪")

    accuracies, entropies = calculate_accuracies_and_entropies(y_preds_dropout)
    ax.plot(rotation_angles, accuracies, 'r--', linewidth=3, label="Accuracy, MC Dropout
↪")
    ax.plot(rotation_angles, entropies, 'r-', linewidth=3, label="Entropy, MC Dropout")

    accuracies, entropies = calculate_accuracies_and_entropies(y_preds_ensemble)
    ax.plot(rotation_angles, accuracies, 'g--', linewidth=3, label="Accuracy, Deep␣
↪Ensemble")
    ax.plot(rotation_angles, entropies, 'g-', linewidth=3, label="Entropy, Deep Ensemble
↪")
```

[57]:
```
plot_accuracy_and_entropy(add_deep_ensemble)
```



Are there any differences in the performance? Explain why you see or don't see any differences.

4.50.11 Bayesian Neural Network

First install pyro package:

[58]:
```
!pip install pyro-ppl
```

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/
↪public/simple/
Collecting pyro-ppl
  Downloading pyro_ppl-1.8.4-py3-none-any.whl (730 kB)
     730.7/730.7 kB 14.0 MB/s eta 0:00:00
Requirement already satisfied: numpy>=1.7 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (1.22.4)
Collecting pyro-api>=0.1.1
  Downloading pyro_api-0.1.2-py3-none-any.whl (11 kB)
Requirement already satisfied: opt-einsum>=2.3.2 in /usr/local/lib/python3.9/dist-
↪packages (from pyro-ppl) (3.3.0)
Requirement already satisfied: torch>=1.11.0 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (2.0.0+cu118)
Requirement already satisfied: tqdm>=4.36 in /usr/local/lib/python3.9/dist-packages␣
↪(from pyro-ppl) (4.65.0)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (3.1.2)
Requirement already satisfied: networkx in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (3.1)
Requirement already satisfied: sympy in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (1.11.1)
Requirement already satisfied: filelock in /usr/local/lib/python3.9/dist-packages (from␣
↪torch>=1.11.0->pyro-ppl) (3.11.0)
```

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```
Requirement already satisfied: typing-extensions in /usr/local/lib/python3.9/dist-
↪packages (from torch>=1.11.0->pyro-ppl) (4.5.0)
Requirement already satisfied: triton==2.0.0 in /usr/local/lib/python3.9/dist-packages␣
↪(from torch>=1.11.0->pyro-ppl) (2.0.0)
Requirement already satisfied: cmake in /usr/local/lib/python3.9/dist-packages (from␣
↪triton==2.0.0->torch>=1.11.0->pyro-ppl) (3.25.2)
Requirement already satisfied: lit in /usr/local/lib/python3.9/dist-packages (from␣
↪triton==2.0.0->torch>=1.11.0->pyro-ppl) (16.0.1)
Requirement already satisfied: MarkupSafe>=2.0 in /usr/local/lib/python3.9/dist-packages␣
↪(from jinja2->torch>=1.11.0->pyro-ppl) (2.1.2)
Requirement already satisfied: mpmath>=0.19 in /usr/local/lib/python3.9/dist-packages␣
↪(from sympy->torch>=1.11.0->pyro-ppl) (1.3.0)
Installing collected packages: pyro-api, pyro-ppl
Successfully installed pyro-api-0.1.2 pyro-ppl-1.8.4
```

[59]:
```
import pyro
import pyro.distributions as dist
from pyro.nn import PyroModule, PyroSample
from pyro.infer import Predictive
from pyro.infer import SVI, Trace_ELBO
from pyro.infer.autoguide import AutoDiagonalNormal
from pyro.distributions import Normal, Categorical
from torch.nn.functional import softmax
from tqdm.auto import trange, tqdm
```

4.1 Implement a Bayesian Neural Network for classifying MNIST digits. For orientation you can use the first tutorial.

As a backbone use the MLP architecture introduced in the beginning of the notebook. However, because we will implement a custom *guide()*, define every layer explicitly.

[60]:
```
class My_MLP(nn.Module):
  '''
  Implement a MLP with 3 hidden layers, Tanh activation, no dropout or residual␣
↪connections
  '''
  def __init__(self, in_dim=784, out_dim=10, hid_dim=200):
    super().__init__()
    assert in_dim > 0
    assert out_dim > 0
    assert hid_dim > 0
    # activation
    # self.act =
    self.act = nn.Tanh()

    #3 hidden layers
    # self.fc1 =
    # self.fc2 =
    # self.fc3 =
    # self.out =
    # raise NotImplemented
    self.fc1 = nn.Linear(in_dim, hid_dim)
```

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```
    self.fc2 = nn.Linear(hid_dim, hid_dim)
    self.fc3 = nn.Linear(hid_dim, hid_dim)
    self.out = nn.Linear(hid_dim, out_dim)

  def forward(self, x):
    # raise NotImplemented
    x = self.act(self.fc1(x))
    x = self.act(self.fc2(x))
    x = self.act(self.fc3(x))
    pred = self.out(x).squeeze()
    return pred
```

Initialize the network. You will have to access it's layers in your model and guide functions

[61]:
```
net = My_MLP()
```

[62]:
```
#confirm your layer names
for name, _ in net.named_parameters():
    print(name)
```

```
fc1.weight
fc1.bias
fc2.weight
fc2.bias
fc3.weight
fc3.bias
out.weight
out.bias
```

Define the model: > Probablistic models in Pyro are specified as *model()* functions. This function defines how the output data is generated. Within the model() function, first, the pyro module *random_module()* converts the paramaters of our NN into random variables that have prior probability distributions. Second, in pyro *sample* we define that the output of the network is categorical, while the pyro *plate* allows us to vectorize this function for computational efficiency.

> Hint: remember we are doing a classification instead of regression!

You can 'cheat' a little: to speed up the training and limit a bit more the number of paramters we need to optimize, implement a BNN where only the **last layer** is Bayesian!

[63]:
```
def model(x_data, y_data):
  # raise NotImplemented
  outw_prior = Normal(loc=torch.zeros_like(net.out.weight), scale=torch.ones_like(net.
↪out.weight)).to_event(2)
  outb_prior = Normal(loc=torch.zeros_like(net.out.bias), scale=torch.ones_like(net.out.
↪bias)).to_event(1)
  priors = {'out.weight': outw_prior, 'out.bias': outb_prior}
  # lift module parameters to random variables sampled from the priors
  lifted_module = pyro.random_module("module", net, priors)
  # sample a regressor (which also samples w and b)
  lifted_reg_model = lifted_module()
  with pyro.plate("data", x_data.shape[0]):
        yhat = softmax(lifted_reg_model(x_data), dim=1)
```

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```
        obs = pyro.sample("obs", dist.Categorical(yhat), obs=y_data)
```

implement the guide(), *variational distribution*: > the guide allows us to initialise a well behaved distribution which later we can optmize to approximate the true posterior

[64]:
```
softplus = torch.nn.Softplus()

def my_guide(x_data, y_data):
  # raise NotImplemented
  # Output layer weight distribution priors
  outw_mu_param = pyro.param("outw_mu", torch.randn_like(net.out.weight))
  outw_sigma_param = softplus(pyro.param("outw_sigma", torch.randn_like(net.out.weight)))
  outw_prior = Normal(loc=outw_mu_param, scale=outw_sigma_param).to_event(2)
  # Output layer bias distribution priors
  outb_mu_param = pyro.param("outb_mu", torch.randn_like(net.out.bias))
  outb_sigma_param = softplus(pyro.param("outb_sigma", torch.randn_like(net.out.bias)))
  outb_prior = Normal(loc=outb_mu_param, scale=outb_sigma_param).to_event(1)

  priors = {'out.weight': outw_prior, 'out.bias': outb_prior}
  lifted_module = pyro.random_module("module", net, priors)
  return lifted_module()
```

Initialize the stochastic variational inference (SVI)

[65]:
```
adam = pyro.optim.Adam({"lr": 1e-3})
# svi = raise NotImplemented
svi = SVI(model, my_guide, adam, loss=Trace_ELBO())
```

Training

[66]:
```
pyro.clear_param_store()
batch_size = 250
bar = trange(30)
for epoch in bar:
  for batch_idx in range(int(x_train.shape[0] / batch_size)):
    batch_low, batch_high = batch_idx * batch_size, (batch_idx+1) * batch_size
    loss = svi.step(x_train[batch_low:batch_high], y_train[batch_low:batch_high])
    bar.set_postfix(loss=f'{loss / batch_size:.3f}')
```

```
  0%|          | 0/30 [00:00<?, ?it/s]
```

```
/usr/local/lib/python3.9/dist-packages/pyro/primitives.py:491: FutureWarning: The␣
↪`random_module` primitive is deprecated, and will be removed in a future release. Use␣
↪`pyro.nn.Module` to create Bayesian modules from `torch.nn.Module` instances.
  warnings.warn(
```

Test

Use the learned *guide()* function to do predictions. Why? Because the *model()* function knows the **priors** for the weights and biases, **not** the learned posterior. The *guide()* contains the approximate posterior distributions of the parameter values, which we want to use to make the predictions.

[67]:
```
# y_preds = NotImplemented
num_samples = 10
def predict(x):
    sampled_models = [my_guide(None, None) for _ in range(num_samples)]
    yhats = [model(x).data for model in sampled_models]
    mean = torch.mean(torch.stack(yhats), 0)
    return mean
y_preds = predict(x_test).argmax(dim=1)


acc = accuracy(y_test, y_preds)
print("Test accuracy is %.2f%%" % (acc.item() * 100))
```

```
Test accuracy is 90.77%
```

Evaluate on rotated images

[68]:
```
# y_preds_bnn = NotImplemented

num_samples = 50
def predict_probability(x):
    sampled_models = [my_guide(None, None) for _ in range(num_samples)]
    yhats = [softmax(model(x).data, dim=1) for model in sampled_models]
    mean = torch.mean(torch.stack(yhats), 0)
    return mean

y_preds_bnn = []
for image in rotated_images:
  y_preds_bnn.append(predict_probability(image))
```

4.2 Show entropies for all four models. Which method is the best at detecting the distribution shift? How can you interpret this?

[69]:
```
#add the computed values for BNN
def add_bnn(ax):
  # raise NotImplemented
  accuracies, entropies = calculate_accuracies_and_entropies(y_preds_deterministic)
  ax.plot(rotation_angles, accuracies, 'b--', linewidth=3, label="Accuracy, Deterministic
↪")
  ax.plot(rotation_angles, entropies, 'b-', linewidth=3, label="Entropy, Deterministic")

  accuracies, entropies = calculate_accuracies_and_entropies(y_preds_dropout)
  ax.plot(rotation_angles, accuracies, 'r--', linewidth=3, label="Accuracy, MC Dropout")
  ax.plot(rotation_angles, entropies, 'r-', linewidth=3, label="Entropy, MC Dropout")

  accuracies, entropies = calculate_accuracies_and_entropies(y_preds_ensemble)
  ax.plot(rotation_angles, accuracies, 'g--', linewidth=3, label="Accuracy, Deep Ensemble
↪")
  ax.plot(rotation_angles, entropies, 'g-', linewidth=3, label="Entropy, Deep Ensemble")

  accuracies, entropies = calculate_accuracies_and_entropies(y_preds_bnn)
  ax.plot(rotation_angles, accuracies, 'y--', linewidth=3, label="Accuracy, BNN")
  ax.plot(rotation_angles, entropies, 'y-', linewidth=3, label="Entropy, BNN")
```

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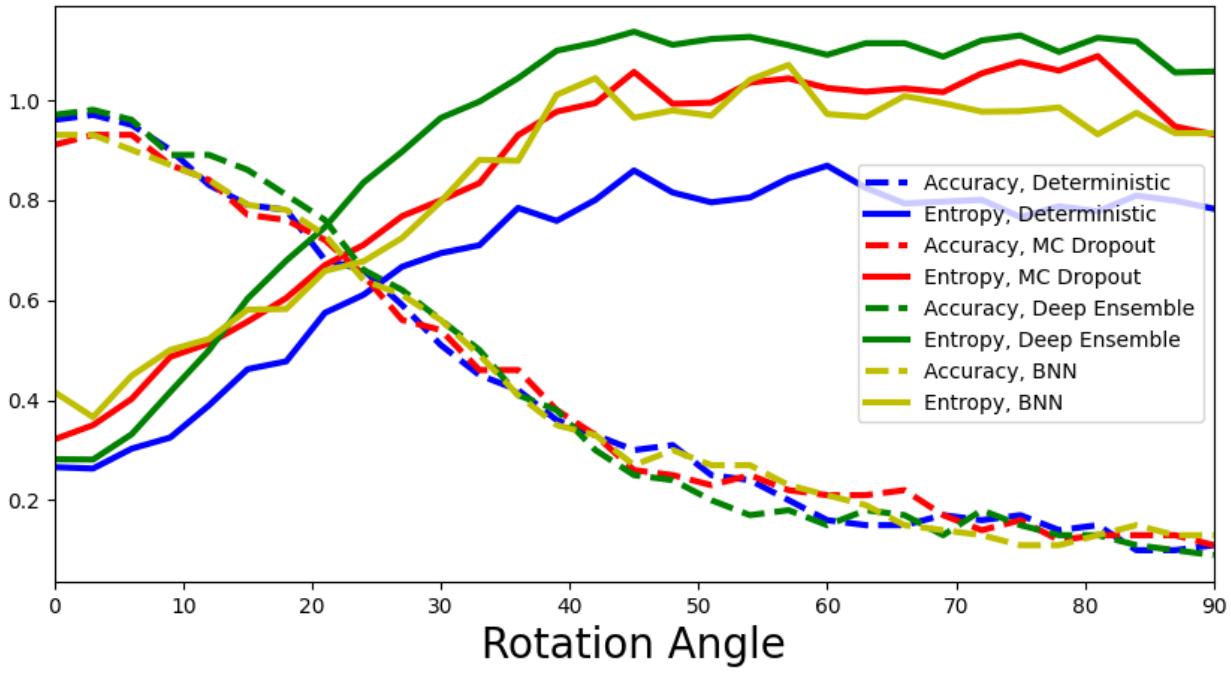
```
plot_accuracy_and_entropy(add_bnn)
```



4.50.12 Conformal prediction

In the previous example with simulated data, we used conformal prediction in the context of a regression task. Now, we are looking at a classification task. While the overall recipe is the same, there are differences in the specific design choices. In particular, our model outputs are now class probabilities $\hat{f}(x) \in [0,1]^K$, and our prediction sets are thus discrete sets $\hat{C}(X_{n+1}) \subseteq \{1,\dots,K\}$, where $K = 10$ in the case of MNIST. This is in contrast to the continuous uncertainty bands we obtained before, and influences how we design the comparison of true and predicted classes to obtain our *conformity scores*.

Since conformal prediction provides a measure of uncertainty via prediction sets *post-hoc*, i.e. without changes to model training procedure, we cannot directly compare conformal methods in terms of detecting distribution shift via entropy. Instead, we can look at empirical coverage and prediction set sizes.

> **5.1 How do you expect empirical coverage and prediction set size to behave as we increase the rotation angle?**
>
> A: The larger the rotation angle and thus distribution shift, the less information our calibration data provides for the test data. This distribution mismatch should be reflected in lower empirical coverage. Similarly, this mismatch results in higher predictive uncertainty, which should be reflected in larger prediction set sizes.

Training

As in the previous example, we split our training samples into two different data sets, the true training set and the calibration set. We take the last 5k samples from the MNIST training data as calibration samples. We take the first 55k images as true training samples.

[70]:
```
# split data into training and calibration sets
```

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```
# raise NotImplemented
# x_cal, y_cal =
# x_tr, y_tr =

cal_idx = np.arange(55000, 60000, step=1, dtype=np.int64)
mask = np.zeros(60000, dtype=bool)
mask[cal_idx] = True
x_cal, y_cal = x_train[mask], y_train[mask]
x_tr, y_tr = x_train[~mask], y_train[~mask]
```

We will reuse the deterministic MLP network architecture from the beginning of the exercise and train it on the true training set:

[71]:
```
mlp = MLP(input_dim=784, output_dim=10, hidden_dim=30, n_hidden_layers=3)
```

[72]:
```
# training
mlp_optimizer = torch.optim.Adam(params=mlp.parameters(), lr=1e-4)
mlp_criterion = nn.CrossEntropyLoss()
batch_size = 250

bar = trange(30)
for epoch in bar:
  for batch_idx in range(int(x_train.shape[0] / batch_size)):
    batch_low, batch_high = batch_idx * batch_size, (batch_idx+1) * batch_size
    mlp_optimizer.zero_grad()
    loss = mlp_criterion(target=y_tr[batch_low:batch_high], input=mlp(x_tr[batch_low:
↪batch_high]))
    bar.set_postfix(loss=f'{loss / batch_size:.3f}') #x.shape[0]
    loss.backward()
    mlp_optimizer.step()
```

```
  0%|          | 0/30 [00:00<?, ?it/s]
```

Test

We can then check the test accuracy, just to ensure that our model trained well.

[73]:
```
evaluate_accuracy_on_mnist(mlp)
```

```
Test accuracy is 93.09%
```

What can we conclude if we compare accuracies to the model trained on full data?

Conformal prediction for the classification setting

As previously mentioned, the choice of how to calculate the *conformity scores* is a modelling decision. We will look at three different choices proposed in the recent literature:

1. The naive softmax method studied by Sadinle et al. (2016)
2. The adaptive prediction sets (APS) method studied by Romano et al. (2020)
3. The regularized adaptive prediction sets (RAPS) method studied by Angelopoulos et al. (2021)

For an easy introduction it is recommended to read chapters 1 and 2 from A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification by Angelopoulos & Bates, which includes code snippets that have been adapted to our task.

We start by defining some basic functions to compute the conformal quantile, as well as mean prediction size and empirical coverage.

[74]:
```
def quantile(scores, alpha=0.1):
  # compute conformal quantile

  # raise NotImplemented
  # n =
  # q =
  # return np.quantile(...)

  n = len(scores)
  q_val = np.ceil((1 - alpha) * (n + 1)) / n
  return np.quantile(scores, q_val, method="higher")
```

[75]:
```
def mean_set_size(sets):
  # mean prediction set size
  return np.mean(np.sum(sets, axis=1), axis=0)
```

[76]:
```
def emp_coverage(sets, target):
  # empirical coverage
  return sets[np.arange(len(sets)), target].mean()
```

In this method, we define our *conformity scores* to be $s_i = 1 - \hat{\pi}_{x_i}(y_i)$ for some calibration sample (x_i, y_i), i.e. one minues the softmax output of the true (correct) class. Our prediction set for some test sample (x_{n+1}, y_{n+1}) is then constructed as $\hat{C}(x_{n+1}) = \{y' \in K : \hat{\pi}_{x_{n+1}}(y') \geq 1 - \hat{q}\}$, i.e. collect all classes for which the softmax score is above the threshold $1 - \hat{q}$. For examples on Imagenet, see here.

[77]:
```
# Calculate conformal quantile on calibration data
cal_smx = softmax(mlp(x_cal), dim=1).detach().numpy()
scores = 1 - cal_smx[np.arange(len(cal_idx)), y_cal.numpy()]
q = quantile(scores)
print(f"Softmax cut-off level: {1-q}")
```

```
Softmax cut-off level: 0.7470939755439758
```

[78]:
```
# Evaluate prediction sets on test data
test_smx = softmax(mlp(x_test), dim=1).detach().numpy()

# raise NotImplemented
# pred_sets =
pred_sets = test_smx >= (1-q)

print(f"Mean set size: {mean_set_size(pred_sets)}")
print(f"Empirical coverage: {emp_coverage(pred_sets, y_test.numpy())}")
```

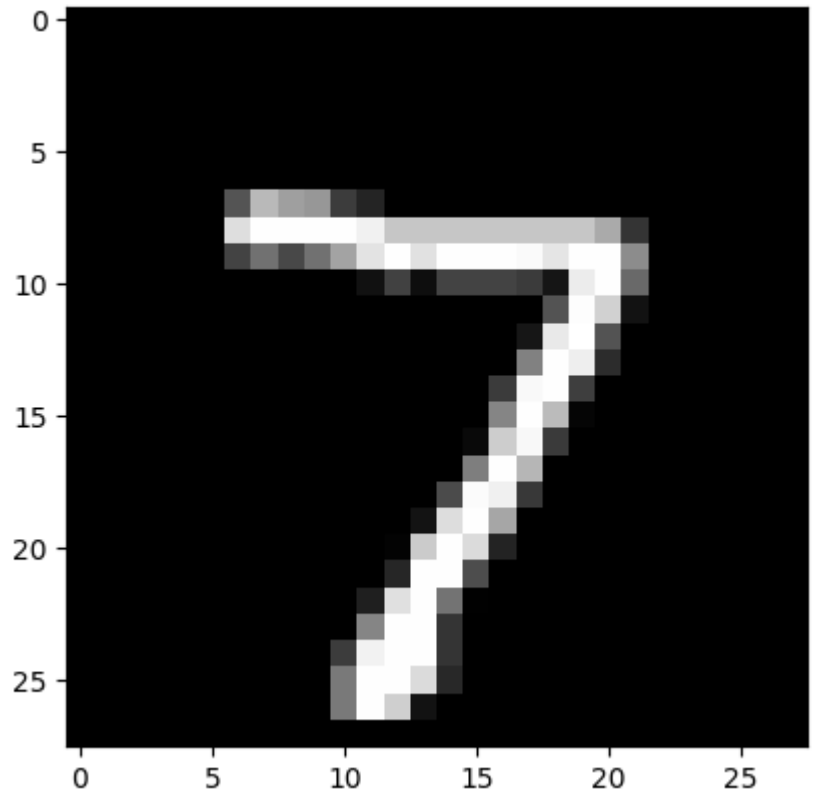
```
Mean set size: 0.8977
Empirical coverage: 0.8726
```

The empirical coverage is close to target coverage 90% but does not quite reach it. Perhaps unintuitive is that the mean set size is <1. This is because for some test samples, the constructed approach can return empty sets. This happens if no softmax score is above the threshold. While there are workarounds to exclude empty sets, we do not consider them here.

Visualize for some test sample…

[79]:
```
img_idx = 0 # compare e.g. img_idx = 4, 4000
plt.imshow(x_test[img_idx].reshape(28, 28), cmap='gray', vmin=0, vmax=255)
print(f"Prediction set: {pred_sets[img_idx].nonzero()[0].tolist()}")
```

```
Prediction set: [7]
```



Now let's compute accuracy, set size and empirical coverage on some of the rotated MNIST images...

[80]:
```
deter_pred_means = []
for image in rotated_images:
  deter_pred_means.append(softmax(mlp(image), dim=1))
```

[81]:
```
acc = [accuracy(y_test[:n_test_images], p.argmax(axis=1)) for p in deter_pred_means]
set_size = [mean_set_size(p.detach().numpy() >= (1-q)) for p in deter_pred_means]
cov = [emp_coverage(p.detach().numpy() >= (1-q), y_test[:n_test_images].numpy()) for p␣
↪in deter_pred_means]
```

[82]:
```
# generate plot

fig, ax = plt.subplots(figsize=(10, 5))
plt.xlim([0, 90])
plt.xlabel("Rotation Angle", fontsize=20)

ax.plot(rotation_angles, acc, 'b--', linewidth=3, label="Accuracy")
ax.plot(rotation_angles, set_size, 'b-', linewidth=3, label="Mean set size")
ax.plot(rotation_angles, cov, 'b:', linewidth=3, label="Emp. coverage")
```

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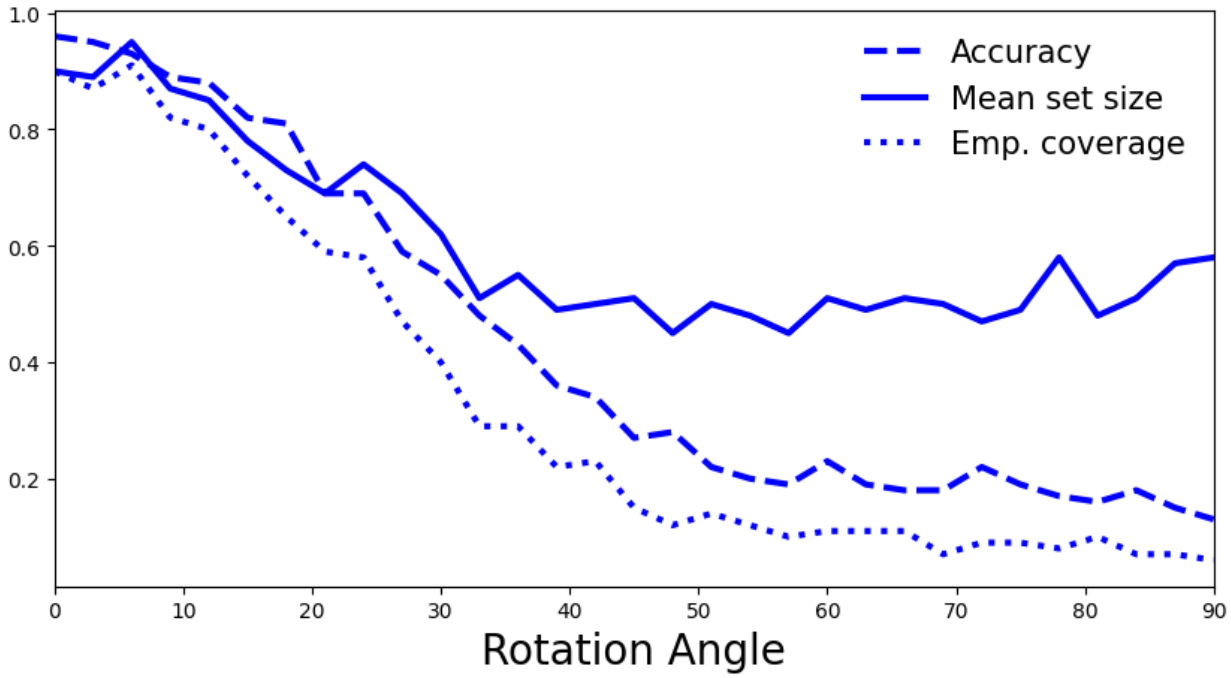
```
plt.legend(loc=1, fontsize=15, frameon=False);
```



5.2 How do you interpret the plot? Is it what you expected, or is there a surprising trend? If so, how could you try to explain it? (hint: empty sets)

A: As expected, with a higher rotation angle model's accuracy drops, and the empirical coverage also decreases. Perhaps counterintuitive is that the mean set size also decreases. This is based on the way we constructed our conformity scores, in particular that we only consider the softmax scores of the correct class when computing . As the distribution shift increases our model's uncertainty increases, which results in lower softmax scores for each class and thus less scores above the threshold. In that sense, the higher entropy is reflected in more empty sets, which pushes down mean set size.

In this method, we define our *conformity scores* to be $s_i = \sum_{y'=1}^{K} \hat{\pi}_{x_i}(y') \mathbb{1}_{\{\hat{\pi}_{x_i}(y') > \hat{\pi}_{x_i}(y)\}}$ for some calibration sample (x_i, y_i). In other words, we sum up the softmax probabilities of all classes until we reach the true class probability. In comparison to the previous method, this allows us to incorporate information not only on the true class, but also its relation to all other classes, and should lead to more adaptive prediction sets, at the cost of overall larger set sizes.

The prediction set for some test sample (x_{n+1}, y_{n+1}) is then constructed as $\hat{C}(x_{n+1}) = \{y_1, \ldots, y_k\}$, where $k = \sup\left\{k' : \sum_{y'=1}^{k'} \hat{\pi}_{x_{n+1}}(y') < \hat{q}\right\}$. In other words, sort all softmax scores by magnitude and include all classes in the prediction set until the sum of their softmax scores hits $\hat{q}$. For examples on Imagenet, see here.

[83]:
```
# Calculate conformal quantile on calibration data
cal_smx = softmax(mlp(x_cal), dim=1).detach().numpy()
cal_pi = cal_smx.argsort(axis=1)[:, ::-1]
cal_srt = np.take_along_axis(cal_smx, cal_pi, axis=1).cumsum(axis=1)
scores = np.take_along_axis(cal_srt, cal_pi.argsort(axis=1), axis=1)[range(len(cal_idx)),
↪ y_cal.numpy()]
q = quantile(scores)
print(f"Softmax cut-off level: {q}")
```

```
Softmax cut-off level: 0.998565137386322
```

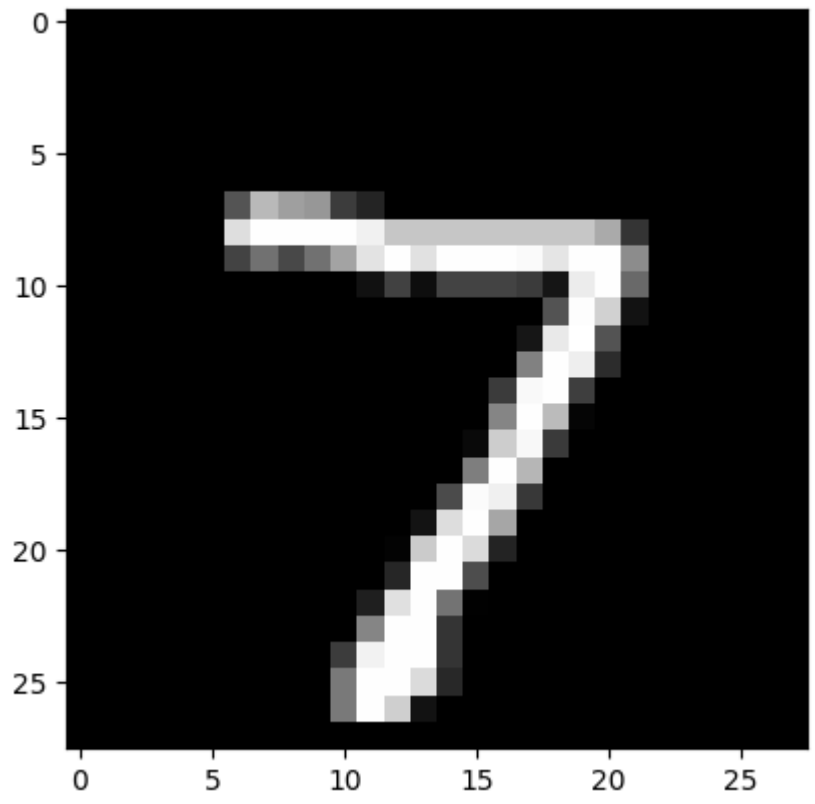
[84]:
```
# Evaluate prediction sets on test data
test_smx = softmax(mlp(x_test), dim=1).detach().numpy()
test_pi = test_smx.argsort(axis=1)[:, ::-1]
test_srt = np.take_along_axis(test_smx, test_pi, axis=1).cumsum(axis=1)

# raise NotImplemented
# pred_sets = np.take_along_axis(..., test_pi.argsort(axis=1), axis=1)
pred_sets = np.take_along_axis(test_srt <= q, test_pi.argsort(axis=1), axis=1)

print(f"Mean set size: {mean_set_size(pred_sets)}")
print(f"Empirical coverage: {emp_coverage(pred_sets, y_test.numpy())}")
```

```
Mean set size: 3.1416
Empirical coverage: 0.9157
```

Visualize for some test sample…

[85]:
```
img_idx = 0 # compare e.g. img_idx = 4, 4000
plt.imshow(x_test[img_idx].reshape(28, 28), cmap='gray', vmin=0, vmax=255)
print(f"Prediction set: {pred_sets[img_idx].nonzero()[0].tolist()}")
```

```
Prediction set: []
```



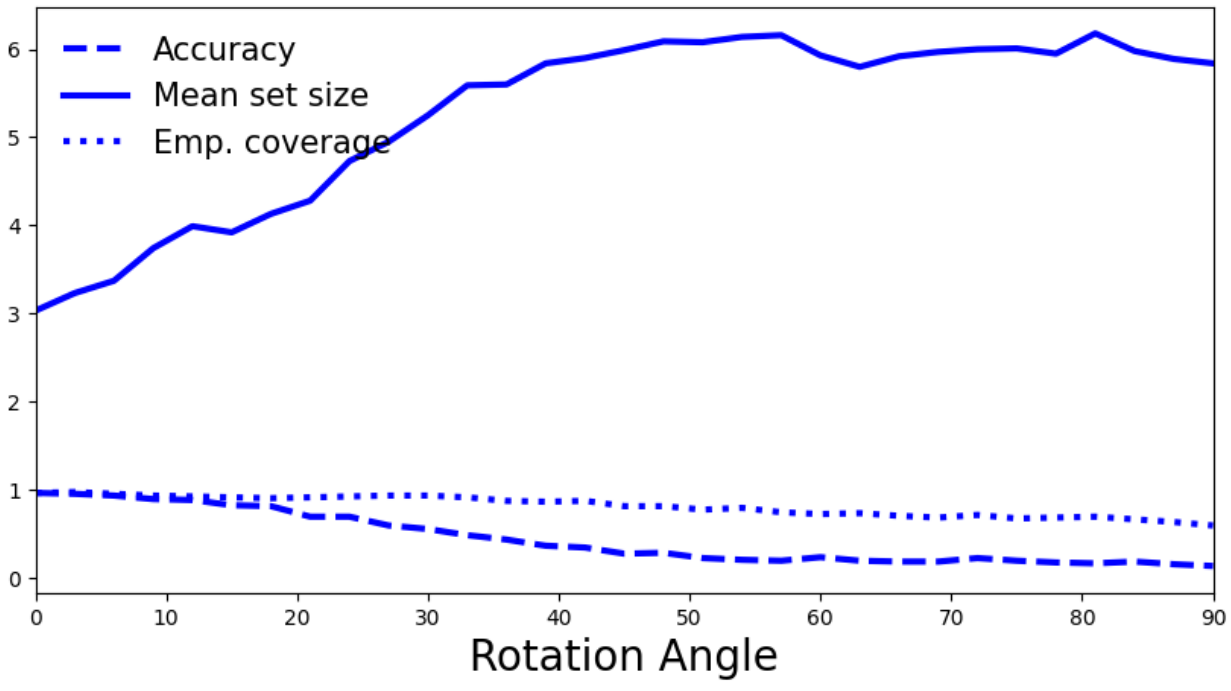
Now let's compute accuracy, set size and empirical coverage on some of the rotated MNIST images…

[86]:
```
deter_pred_means = []
for image in rotated_images:
  deter_pred_means.append(softmax(mlp(image), dim=1))
```

[87]:
```
acc = [accuracy(y_test[:n_test_images], p.argmax(axis=1)) for p in deter_pred_means]
```

[88]:
```
set_size, cov = [], []
for p in deter_pred_means:
  p = p.detach().numpy()
  p_pi = p.argsort(axis=1)[:, ::-1]
  p_srt = np.take_along_axis(p, p_pi, axis=1).cumsum(axis=1)
  pred_sets = np.take_along_axis(p_srt <= q, p_pi.argsort(axis=1), axis=1)
  set_size.append(mean_set_size(pred_sets))
  cov.append(emp_coverage(pred_sets, y_test[:n_test_images].numpy()))
```

[89]:
```
# generate plot

fig, ax = plt.subplots(figsize=(10, 5))
plt.xlim([0, 90])
plt.xlabel("Rotation Angle", fontsize=20)

ax.plot(rotation_angles, acc, 'b--', linewidth=3, label="Accuracy")
ax.plot(rotation_angles, set_size, 'b-', linewidth=3, label="Mean set size")
ax.plot(rotation_angles, cov, 'b:', linewidth=3, label="Emp. coverage")

plt.legend(loc=2, fontsize=15, frameon=False);
```



5.3 How do you interpret the plot? Is it what you expected?

A: As expected, with a higher rotation angle model's accuracy drops, as does its empirical coverage, although at a lower rate than before. By taking into account additional class information in the *conformity*

scores, the quantile $\hat{q}$ is somewhat more robust to changes. We also observe the anticipated trend for prediction set sizes. As the shift increases, higher predictive uncertainty is reflected in larger set sizes. Note that a set of size 6+ for our task with only 10 classes becomes very uninformative at high shift.

This method builds on APS and proposes an additional regularization term to decrease prediction set sizes, while maintaining the conformal coverage guarantee. This introduces additional parameters but strongly reduces set sizes, making it more useful in practice. The regularization term essentially adds probability mass as a "penalty" term λ_{reg} to all softmax scores after a defined threshold k_{reg} to reach the APS softmax threshold faster, resulting in smaller prediction sets. The general score construction is similar to APS. For further reading you can have a look at the paper (sections 2.1 and 2.2, see also Fig. 3). For examples on Imagenet, see here.

[90]:
```
# Set RAPS regularization parameters
smx_classes = 10

lam_reg = 0.01 # Effect?
k_reg = 3 # Effect?

disallow_zero_sets = False # Set this to False in order to see the coverage upper bound␣
↪hold
rand = True # Set this to True in order to see the coverage upper bound hold
reg_vec = np.array(k_reg * [0,] + (smx_classes - k_reg) * [lam_reg,])[None, :]
print(f"Probability mass penalty for each class: {reg_vec}")
```

```
Probability mass penalty for each class: [[0.   0.   0.   0.01 0.01 0.01 0.01 0.01 0.01␣
↪0.01]]
```

5.4 Try out different parameter settings. What effects do :math:`lambda_{reg}` and :math:`k_{reg}` have on regularization?

A: Larger λ_{reg} leads to smaller sets by imposing higher penalty mass, so the cutoff $\hat{q}$ is reached faster. Smaller k_{reg} leads to smaller sets by allowing more classes to be penalized, leading to a larger cumulative score which again reaches cutoff $\hat{q}$ faster.

[91]:
```
# Calculate conformal quantile on calibration data
cal_smx = softmax(mlp(x_cal), dim=1).detach().numpy()

cal_pi = cal_smx.argsort(axis=1)[:, ::-1]
cal_srt = np.take_along_axis(cal_smx, cal_pi, axis=1)
cal_srt_reg = cal_srt + reg_vec
cal_L = np.where(cal_pi == y_cal.numpy()[:, None])[1]
n = len(cal_idx)

scores = cal_srt_reg.cumsum(axis=1)[np.arange(n), cal_L] - np.random.rand(n) * cal_srt_
↪reg[np.arange(n), cal_L]
q = quantile(scores)
print(f"Softmax cut-off level: {q}")
```

```
Softmax cut-off level: 0.9008058661638462
```

[92]:
```
# Evaluate prediction sets on test data
test_smx = softmax(mlp(x_test), dim=1).detach().numpy()

test_pi = test_smx.argsort(1)[:, ::-1]
test_srt = np.take_along_axis(test_smx, test_pi, axis=1)
test_srt_reg = test_srt + reg_vec
```

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```
test_srt_reg_cumsum = test_srt_reg.cumsum(axis=1)

if rand:
  indicators = (test_srt_reg.cumsum(axis=1) - np.random.rand(len(test_smx), 1) * test_
↪srt_reg) <= q
else:
  indicators = (test_srt_reg.cumsum(axis=1) - test_srt_reg) <= q

if disallow_zero_sets:
  indicators[:, 0] = True

pred_sets = np.take_along_axis(indicators, test_pi.argsort(axis=1), axis=1)
print(f"Mean set size: {mean_set_size(pred_sets)}")
print(f"Empirical coverage: {emp_coverage(pred_sets, y_test.numpy())}")
```

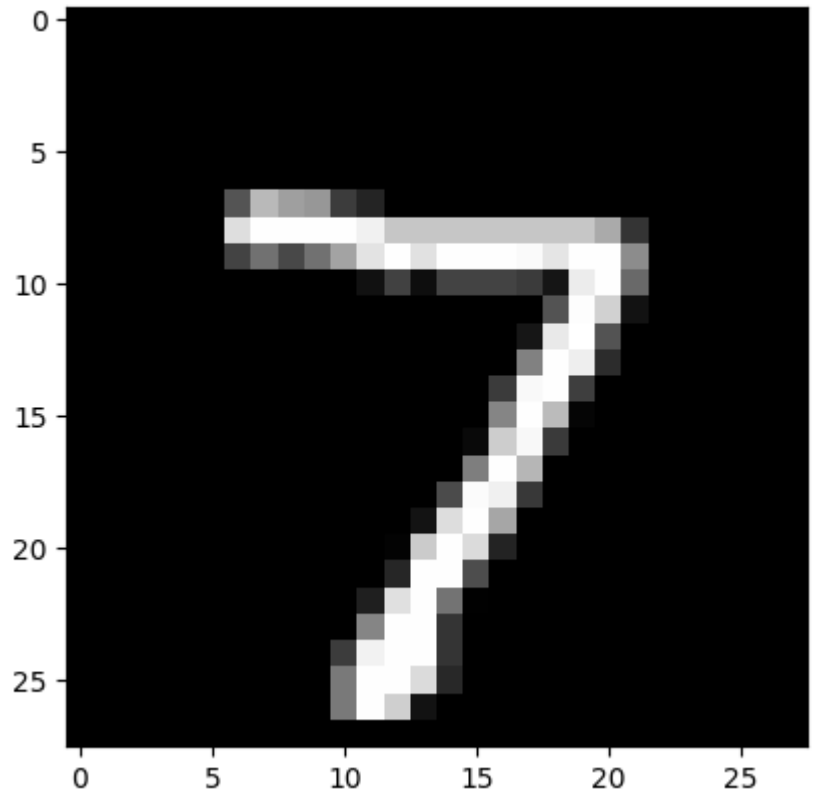
```
Mean set size: 1.1334
Empirical coverage: 0.9051
```

How do the metrics compare to those obtained using APS without regularization?

Visualize for some test sample…

[93]:
```
img_idx = 0 # compare e.g. img_idx = 4, 4000
plt.imshow(x_test[img_idx].reshape(28, 28), cmap='gray', vmin=0, vmax=255)
print(f"Prediction set: {pred_sets[img_idx].nonzero()[0].tolist()}")
```

```
Prediction set: [7]
```



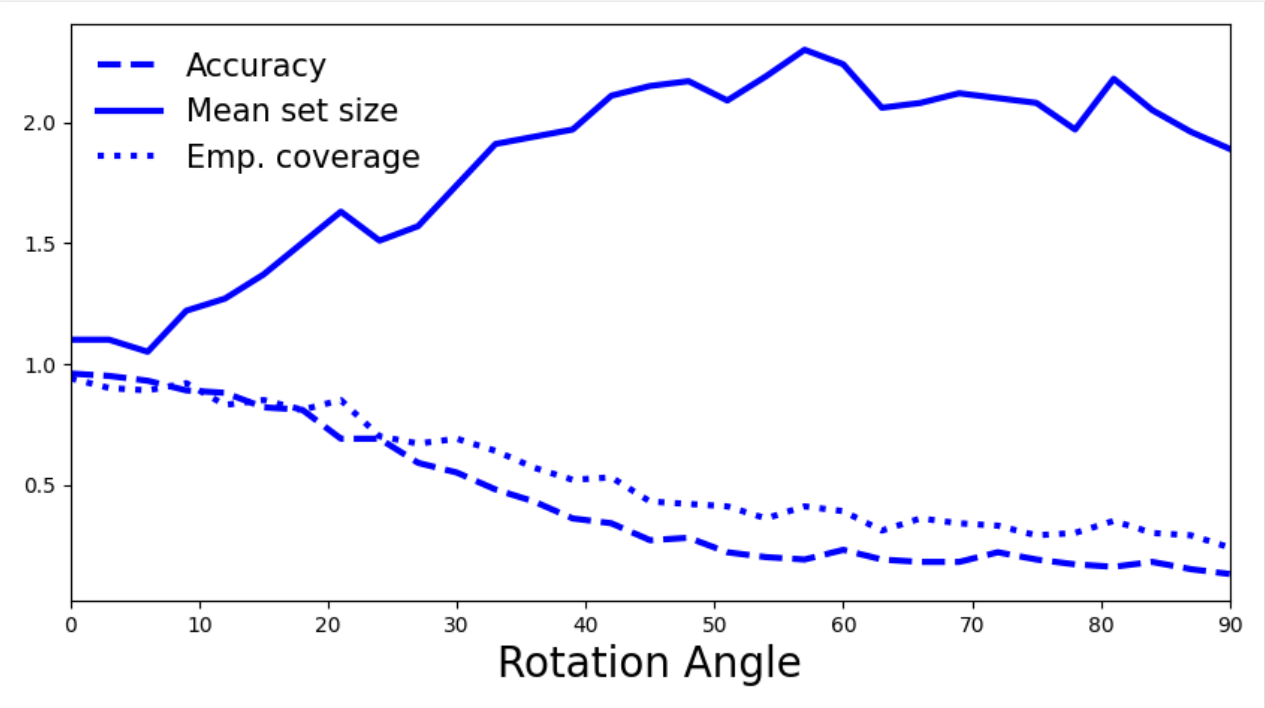
Now let's compute accuracy, set size and empirical coverage on some of the rotated MNIST images...

[94]:
```
deter_pred_means = []
for image in rotated_images:
  deter_pred_means.append(softmax(mlp(image), dim=1))
```

[95]:
```
acc = [accuracy(y_test[:n_test_images], p.argmax(axis=1)) for p in deter_pred_means]
```

[96]:
```
set_size, cov = [], []
for p in deter_pred_means:
  p = p.detach().numpy()
  p_pi = p.argsort(1)[:, ::-1]
  p_srt = np.take_along_axis(p, p_pi, axis=1)
  p_srt_reg = p_srt + reg_vec
  p_srt_reg_cumsum = p_srt_reg.cumsum(axis=1)

  if rand:
    indicators = (p_srt_reg.cumsum(axis=1) - np.random.rand(len(p), 1) * p_srt_reg) <= q
  else:
    indicators = (p_srt_reg.cumsum(axis=1) - p_srt_reg) <= q

  if disallow_zero_sets:
    indicators[:, 0] = True

  pred_sets = np.take_along_axis(indicators, p_pi.argsort(axis=1), axis=1)
  set_size.append(mean_set_size(pred_sets))
  cov.append(emp_coverage(pred_sets, y_test[:n_test_images].numpy()))
```

[97]:
```
# generate plot

fig, ax = plt.subplots(figsize=(10, 5))
plt.xlim([0, 90])
plt.xlabel("Rotation Angle", fontsize=20)

ax.plot(rotation_angles, acc, 'b--', linewidth=3, label="Accuracy")
ax.plot(rotation_angles, set_size, 'b-', linewidth=3, label="Mean set size")
ax.plot(rotation_angles, cov, 'b:', linewidth=3, label="Emp. coverage")

plt.legend(loc=2, fontsize=15, frameon=False);
```



5.5 How do you interpret the plot? Is it what you expected? How does it compare to APS without regularization?

A: We once again observe the same pattern as for APS: larger distribution shift is reflected in decreased accuracy and empirical coverage, and in increased prediction set sizes.

5.6 What do you conclude? Is conformal prediction able to identify the distribution shift caused by rotating the MNIST images?

A: We conclude that conformal prediction methods are also able to identify distribution shifts while relying on very different techniques and metrics in comparison to the presented (approximate) Bayesian uncertainty quantification approaches.

4.51 DNN - Tutorial 2 Part I: Physics inspired Machine Learning

Sparse Identification of Nonlinear Dynamical Systems (SINDy)

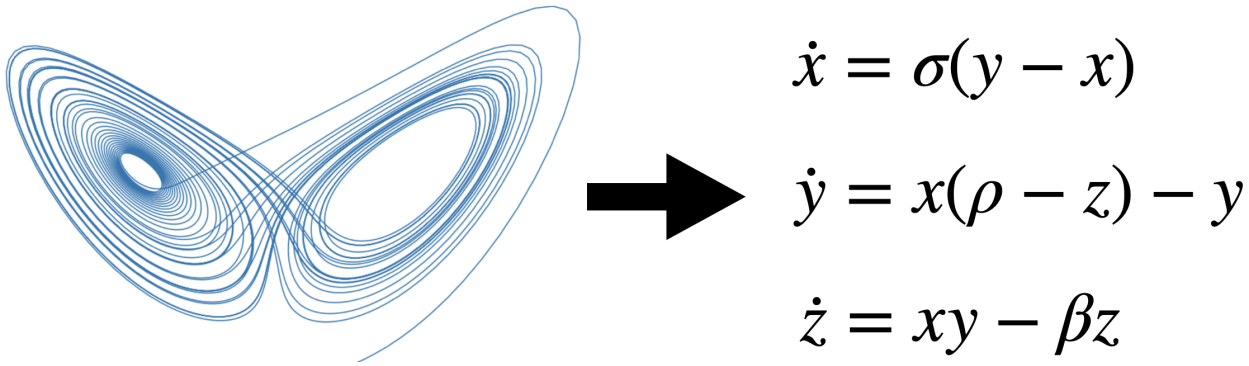
Filled notebook:
Authors: Leonard Bereska and Ilze Amanda Auzina

This section provides an overview of the Sparse Identification of Nonlinear Dynamical systems (SINDy) algorithm, which was first proposed in:

> Brunton, Steven L., Joshua L. Proctor, and J. Nathan Kutz. 2016. *"Discovering Governing Equations from Data by Sparse Identification of Nonlinear Dynamical Systems."* Proceedings of the National Academy of Sciences 113 (15): 3932–37. https://doi.org/10.1073/pnas.1517384113.

4.51.1 What do we mean by *identifying* nonlinear dynamics from data?

Suppose we have time-series data that originate from a (nonlinear) dynamical system.
- To identify a system means to infer the governing equations of that system based on the data. - That is, to find f for dynamical systems equations $\dot{\mathbf{x}} = f(\mathbf{x})$ (where $\mathbf{x}$ may be vector-valued).



For example for the Lorenz system, we want to learn the **equations** on the *right* from the time-series **data** visualized on the *left*.

4.51.2 Why do we want *sparsity*?

In this context, by sparse we mean a low number of terms in the governing equations. Sparsity is beneficial, because it is more: 1. **Interpretible**. Crucial, when understanding the variables and their interactions is needed, e.g. for applications with safety-critical guarantees. 2. **Generalizable**. If correct, the equations describe the dynamics accurately beyond the region of state space filled by the training data.

In general, one can think of the models identified by SINDy as equations from physics as opposed to big, opaque, deep neural networks.

4.51.3 SINDy Algorithm

SINDy tries to find the dynamical system f that suits the data $\dot{\mathrm{X}} = f(\mathrm{X})$. This function approximation problem is formulated as linear regression $\dot{\mathrm{X}} = \Theta(\mathrm{X})\Xi$, with coefficients Ξ and a library of regression terms $\Theta(X)$. The algorithm proceeds in three steps:

1. Generate data X from a dynamical system and compute derivatives $\dot{X}$.
2. Set up library of candidate terms $\Theta(X)$ as functions on X.
3. Sparsely regress the coefficients Ξ, that best describe the data.

1. SINDy assumes a time-series of n-dimensional data points $\mathbf{x} = (x_1, \dots x_n)$ measured at m time steps $t_1, \dots, t_m$, we define the data matrix X as and derivatives matrix $\dot{X}$:

$$X = \begin{bmatrix} x_1(t_1) & x_2(t_1) & \dots & x_n(t_1) \\ x_1(t_2) & x_2(t_2) & \dots & x_n(t_2) \\ \vdots & \vdots & & \vdots \\ x_1(t_m) & x_2(t_m) & \dots & x_n(t_m) \end{bmatrix}, \qquad \dot{X} = \begin{bmatrix} \dot{x_1}(t_1) & \dot{x_2}(t_1) & \dots & \dot{x_n}(t_1) \\ \dot{x_1}(t_2) & \dot{x_2}(t_2) & \dots & \dot{x_n}(t_2) \\ \vdots & \vdots & & \vdots \\ \dot{x_1}(t_m) & \dot{x_2}(t_m) & \dots & \dot{x_n}(t_m) \end{bmatrix}.$$

2. Next, we define the library matrix $\Theta(X)$, the columns of which are a set of basis functions $\{\theta_l\}_{l=1,\dots,L}$ applied to the data:

$$\Theta(X) = \begin{bmatrix} | & | & & | \\ \theta_1(X) & \theta_2(X) & \dots & \theta_\ell(X) \\ | & | & & | \end{bmatrix}.$$

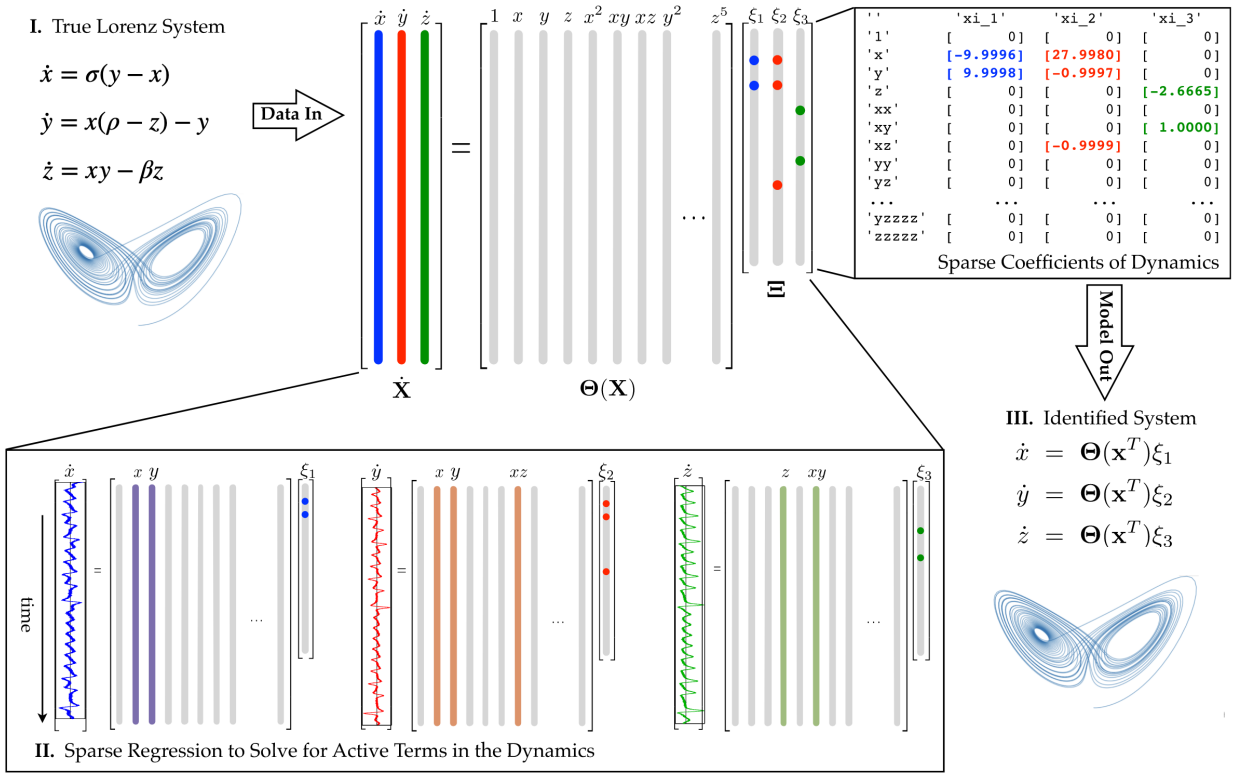
Simple examples are e.g. a basis of polynomials $x_1, x_2, x_1^2, x_2^2, x_1 x_2, x_1^3 \ldots$, such as in the *Taylor expansion*, or trigonometric functions $:nbsphinx-math:*sin* `(x_1), :nbsphinx-math:*cos* (x_1), :nbsphinx-math:*sin* `(2 x_1), :nbsphinx-math:`ldots `$, such as in a *Fourier expansion*. But, depending on the problem more complex basis may be appropriate, e.g. Bessel functions.

3. Lastly, we employ a sparse linear regression algorithm (such as e.g. LASSO) to find the coefficients Ξ,

$$\Xi = \begin{bmatrix} | & | & & | \\ \xi_1 & \xi_2 & \dots & \xi_n \\ | & | & & | \end{bmatrix},$$

such that

$$\dot{\mathrm{X}} = \Theta(\mathrm{X})\Xi.$$



4.51.4 Example: Linear Dynamical System

Suppose we measure a particle trajectory that is governed by the following dynamical system:

$$\frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -2x \\ y \end{pmatrix} = \begin{pmatrix} -2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}$$

With the initial conditions $x_0 = 3$ and $y_0 = \frac{1}{2}$, we construct the data matrix X:

[4]:
```
import numpy as np
import pysindy as ps

t = np.linspace(0, 1, 100)
x = 3 * np.exp(-2 * t)
y = 0.5 * np.exp(t)
X = np.stack((x, y), axis=-1)
```

When instantiating a SINDy model, we can choose the differentiation method, the library and the optimizer:

Let's first investigate a Fourier basis as a basis function

[18]:
```
model = ps.SINDy(
    differentiation_method=ps.FiniteDifference(order=2),
    feature_library=ps.FourierLibrary(),
    optimizer=ps.STLSQ(threshold=0.2),
    feature_names=["x", "y"]
)
model.fit(X, t=t)
```

[18]:
```
SINDy(differentiation_method=FiniteDifference(),
      feature_library=<pysindy.feature_library.fourier_library.FourierLibrary object at␣
↪0x137889100>,
      feature_names=['x', 'y'], optimizer=STLSQ(threshold=0.2))
```

After fitting the model can be inspected with the *print* member function.

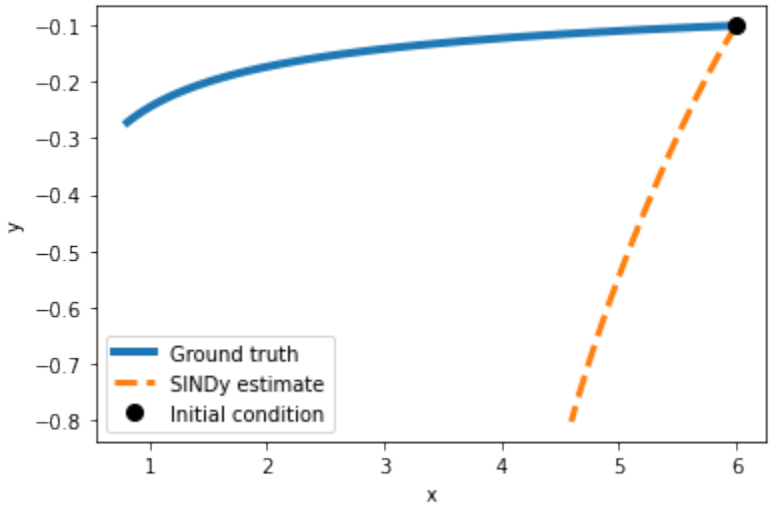
[19]:
```
model.print()
```

```
(x)' = 0.772 sin(1 x) + 2.097 cos(1 x) + -2.298 sin(1 y) + -3.115 cos(1 y)
(y)' = 1.362 sin(1 y) + -0.222 cos(1 y)
```

Let us verify this on some test data:

[20]:
```
import matplotlib.pyplot as plt
def plot_simulation(model, x0, y0):
    t_test = np.linspace(0, 1, 100)
    x_test = x0 * np.exp(-2 * t_test)
    y_test = y0 * np.exp(t_test)

    sim = model.simulate([x0, y0], t=t_test)

    plt.figure(figsize=(6, 4))
    plt.plot(x_test, y_test, label="Ground truth", linewidth=4)
    plt.plot(sim[:, 0], sim[:, 1], "--", label="SINDy estimate", linewidth=3)
    plt.plot(x0, y0, "ko", label="Initial condition", markersize=8)
    plt.xlabel("x")
    plt.ylabel("y")
    plt.legend()
    plt.show()
```

[21]:
```
x0 = 6
y0 = -0.1
plot_simulation(model, x0,y0)
```



As we may have expected, a Fourier basis is not optimal for this problem. Let's try a differetn basis function!

Exercise 1 Let's investigate what happens if we choose a different basis function.

Implement a Sindy algorithm class with a Fourier basis by initializing `ps.SINDy()` with the `feature_library` attribute set to `ps.PolynomialLibrary()`. Fit the instantiated algorithm with the `.fit(X, t=t)` method.

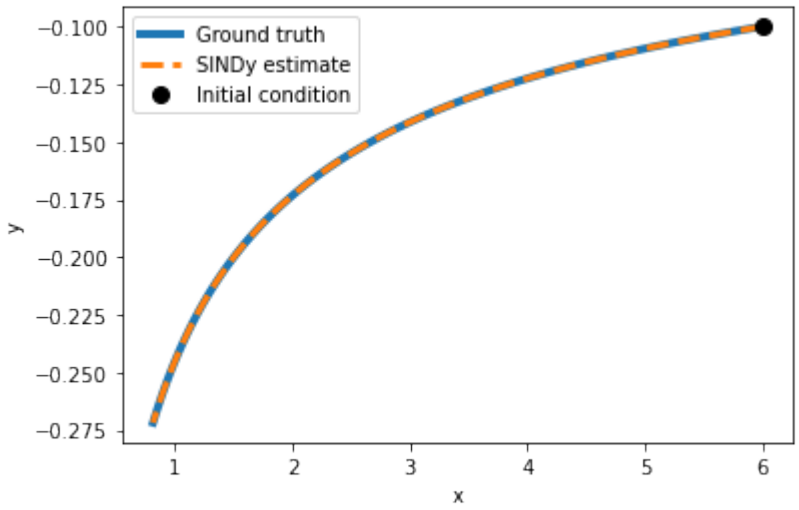
[103]:
```
model_1 = ps.SINDy(
    differentiation_method=ps.FiniteDifference(order=2),
    feature_library=ps.PolynomialLibrary(degree=1),
    optimizer=ps.STLSQ(threshold=0.2),
    feature_names=["x", "y"]
)
model_1.fit(X, t=t)
```

[103]:
```
SINDy(differentiation_method=FiniteDifference(),
      feature_library=PolynomialLibrary(degree=1), feature_names=['x', 'y'],
      optimizer=STLSQ(threshold=0.2))
```

[104]:
```
model_1.print()
```

```
(x)' = -2.000 x
(y)' = 1.000 y
```

[105]:
```
x0 = 6
y0 = -0.1
plot_simulation(model_1, x0,y0)
```



As we can see in this (simple) case, the model has perfectly identified the underlying equation by using polynomial basis functions.

Our problem was a first-order polynomial differential equation, so it is only natural that regression with exactly these model assumptions succeeds.

Exercise 1.1 At which degree is SINDy not able anymore to correctly identify the equation? At which degree do the predictions on a test set diverge? Test this by successively increasing the `degree` of the polynomial.

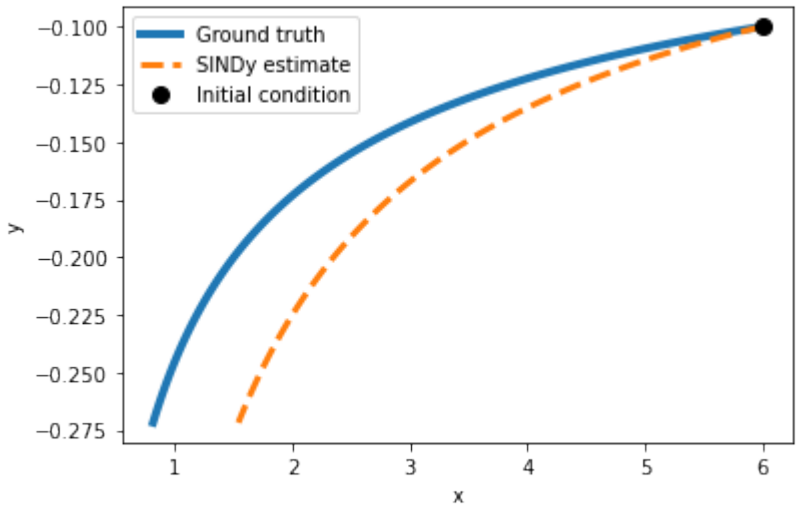
[106]:
```
model_1 = ps.SINDy(
    differentiation_method=ps.FiniteDifference(order=2),
    feature_library=ps.PolynomialLibrary(degree=4),
    optimizer=ps.STLSQ(threshold=0.2),
    feature_names=["x", "y"]
)
model_1.fit(X, t=t)
```

[106]:
```
SINDy(differentiation_method=FiniteDifference(),
      feature_library=PolynomialLibrary(degree=4), feature_names=['x', 'y'],
      optimizer=STLSQ(threshold=0.2))
```

[107]:
```
model_1.print()
```

```
(x)' = -1.280 x + -0.960 x^2 y^2
(y)' = 1.000 y
```

[108]:
```
x0 = 6
y0 = -0.1
plot_simulation(model_1, x0,y0)
```



Exercise 1.2 What happens if you set the threshold too low? What if it is too high?

STLSQ : Attempts to minimize the objective function $||y - Xw||_2^2 + \alpha||w||_2^2$ by iteratively performing least squares and masking out elements of the weight that are below a given threshold.

threshold : minimum magnitude for a coefficient in the weight vector. Coefficients with magnitude below the threshold are set to zero.

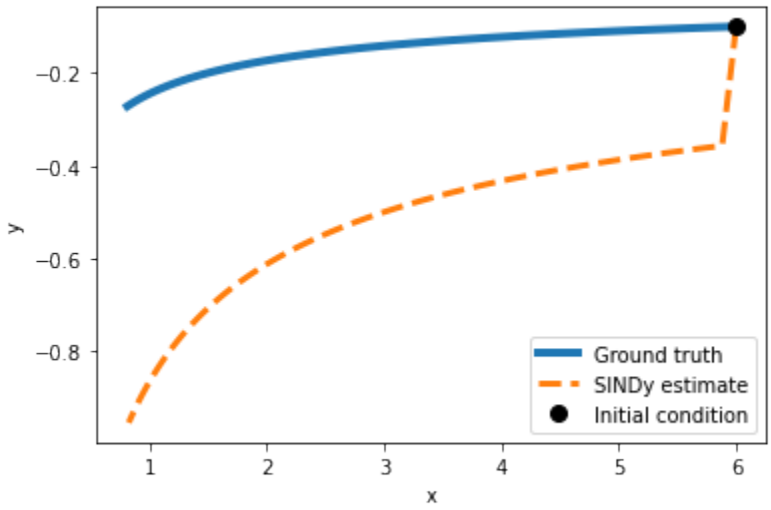
[109]:
```
model_1 = ps.SINDy(
    differentiation_method=ps.FiniteDifference(order=2),
    feature_library=ps.PolynomialLibrary(degree=4),
    optimizer=ps.STLSQ(threshold=0.1),
    feature_names=["x", "y"]
)
model_1.fit(X, t=t)
```

[109]:
```
SINDy(differentiation_method=FiniteDifference(),
      feature_library=PolynomialLibrary(degree=4), feature_names=['x', 'y'],
      optimizer=STLSQ())
```

[110]:
```
model_1.print()
```

```
(x)' = -1.277 x + 0.001 x^2 + -0.002 x y + -0.005 x^2 y + -0.958 x^2 y^2
(y)' = 3063674878.195 y + -4084899836.260 x y^3
```

[111]:
```
x0 = 6
y0 = -0.1
plot_simulation(model_1, x0,y0)
```



4.51.5 Example: Lorenz attractor

For testing SINDy on the Lorenz attractor we first simulate a trajectory from the ground truth equations:

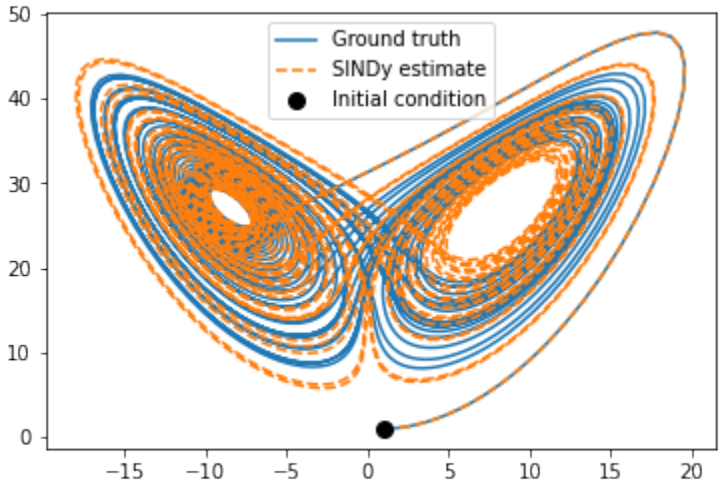
[112]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint
from mpl_toolkits.mplot3d import Axes3D

rho = 28.0
sigma = 10.0
beta = 8.0 / 3.0
dt = 0.01

def f(state, t):
    x, y, z = state
    return sigma * (y - x), x * (rho - z) - y, x * y - beta * z

state0 = [1.0, 1.0, 1.0]
time_steps = np.arange(0.0, 40.0, dt)

x_train = odeint(f, state0, time_steps)
```

[113]:
```
model = ps.SINDy(
    optimizer=ps.STLSQ(threshold=0.05),
    feature_library=ps.PolynomialLibrary(degree=2),
)

model.fit(x_train, t=dt)

x_sim = model.simulate(x_train[0], time_steps)
```

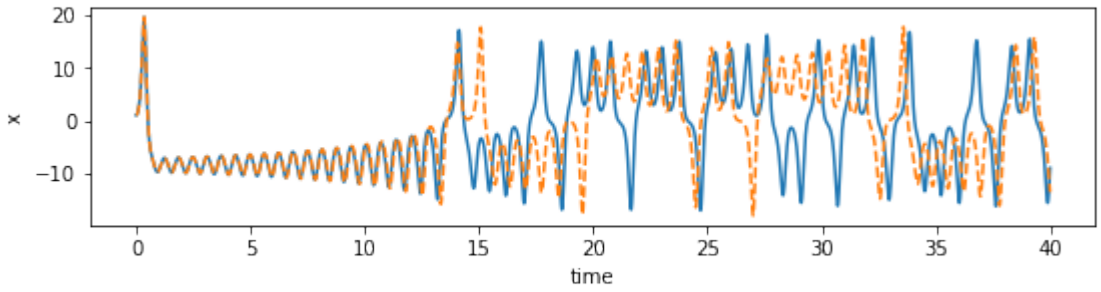
[114]:
```
model.print()
```

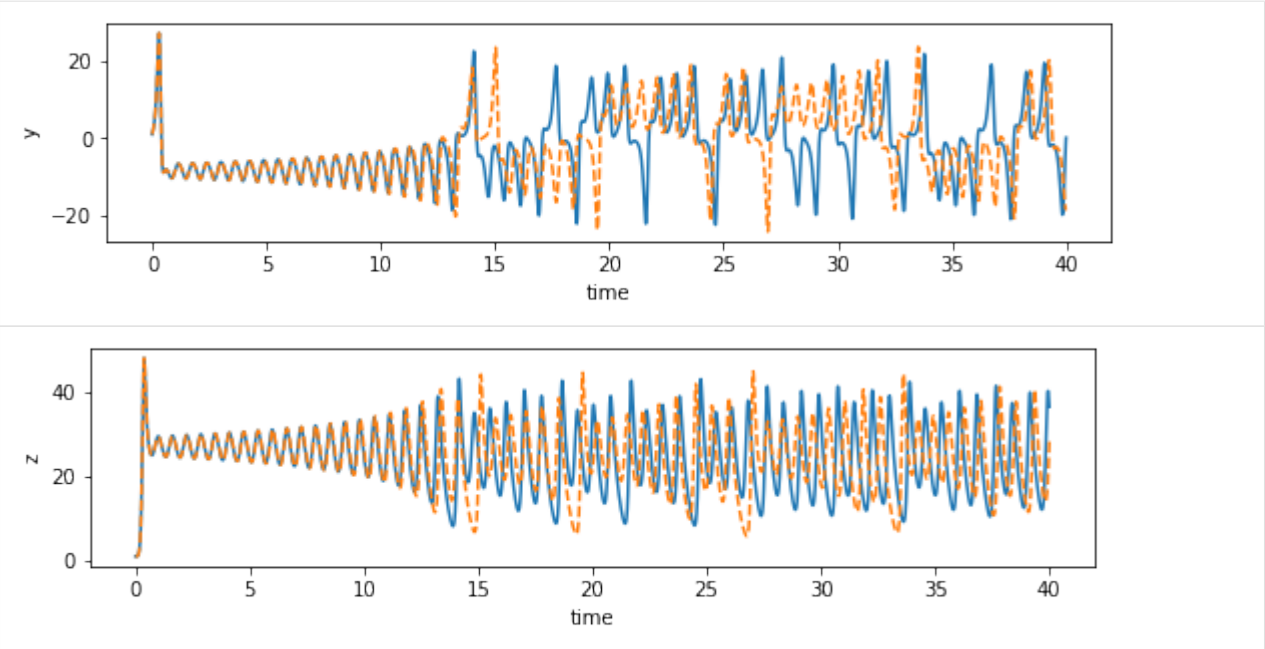
```
(x0)' = -9.977 x0 + 9.977 x1
(x1)' = 27.806 x0 + -0.962 x1 + -0.995 x0 x2
(x2)' = -2.659 x2 + 0.997 x0 x1
```

[115]:
```
plt.figure(figsize=(6, 4))
plt.plot(x_train[:, 0], x_train[:, 2], label='Ground truth')
plt.plot(x_sim[:, 0], x_sim[:, 2], '--', label='SINDy estimate')
plt.plot(x_train[0, 0], x_train[0, 2], "ko", label="Initial condition", markersize=8)
plt.legend()
plt.draw()
plt.show()
```



[116]:
```
def plot_dimension(dim, name):
    fig = plt.figure(figsize=(9,2))
    ax = fig.gca()
    ax.plot(time_steps, x_train[:, dim])
    ax.plot(time_steps, x_sim[:, dim], "--")
    plt.xlabel("time")
    plt.ylabel(name)

plot_dimension(0, 'x')
plot_dimension(1, 'y')
plot_dimension(2, 'z')
```





We can see that the prediction tracks the ground truth data very faithfully, until it diverges (which is inevitable by the chaotic nature of the system).

4.51.6 Challenges

The previous examples have been very basic with a lot of implicit assumptions. Applying SINDy to real-world data is more challenging on multiple fronts. The challenges arise from: 1. **Data**. How much and what quality of data is needed? Per default, SINDy relies on clean data, rapidly sampled in time, with little noise. Needs to be clean enough to compute derivatives. But these requirements can be traded off against each other: e.g., if the data is clean, little is fine. Conversely, for ample but noisy data, one can average out the noise by integration. 2. **Coordinates**. Which variables to measure? Use expert domain knowledge if possible. Alternatively, apply singular value decomposition to find most relevant variables. Or train a deep autoencoder in combination with SINDy: >Champion, Kathleen, Bethany Lusch, J. Nathan Kutz, and Steven L. Brunton. 2019. "Data-Driven Discovery of Coordinates and Governing Equations." Proceedings of the National Academy of Sciences of the United States of America 116 (45): 22445–51. https://doi.org/10.1073/pnas.1906995116.

3. **Library**. What library terms capture the dynamics best? Practically, start simple, e.g. with linear terms, then quadratic etc.. One may also use domain knowledge. Be careful, to not expand the library too big, to avoid linear dependence of columns resulting in an ill-conditioned matrix $\Theta(X)$. Prior knowledge on physics can yield symmetry constraints that cross out symmetry-incompatible terms in library.

4. **Optimization**. Which algorithm to use? How do I actually find sparse terms? Simplest is LASSO, in practice Sequential Threshold Least Squares (iteratively hard-thresholding coefficients) works better. Here, one may also incorporate *physics-informed* constraints: for example one can enforce energy conservation or global stability directly in the optimization.

In the past years, a lot has been achieved in this regard and SINDy has been successful in a variety of real-world applications, including discovering equations for plasma fluid dynamics that previously had not been analytically formulated due to the complexity of the problem.

Sources

- https://pysindy.readthedocs.io/en/latest/#how-it-works
- https://pysindy.readthedocs.io/en/latest/examples/2_introduction_to_sindy.html
- Part 1: https://www.youtube.com/watch?v=NxAn0oglMVw
- Part 2: https://www.youtube.com/watch?v=8-hoWTJwmrE
- Part 3: https://www.youtube.com/watch?v=1vrsBg92Xzo
- Part 4: https://www.youtube.com/watch?v=MmMNQe_EtCw
- Part 5: https://www.youtube.com/watch?v=pY2iJnngk4g

4.51.7 Reservoir Computing

Reservoir computing is a simple method for training recurrent neural networks without backpropagation through time and the associated notorious vanishing and exploding gradient problems. The basic steps are:

1. Randomly initialize recurrent neural network weights.
2. Fix hidden connection weights.
3. Train linear output layer with linear regression.

More formally, the state of the recurrent neural network of M neurons is given by its hidden activations $\mathbf{h} \in \mathbb{R}^M$, which are connected by randomly initialized and fixed matrix $\mathbf{W}_\mathrm{h}$. An input sequence $\mathbf{X}_{1:\tau}$ is embedded by a linear map $\mathbf{W}_\mathrm{i}$ to the state $\mathbf{h}_\tau$:

$$\begin{aligned}\mathbf{h}_1 &= \sigma(\mathbf{W}_\mathrm{h}\mathbf{h}_0 + \mathbf{W}_\mathrm{i}\mathbf{x}_1)\\ \vdots \qquad &\qquad \vdots\\ \mathbf{h}_\tau &= \sigma(\mathbf{W}_\mathrm{h}\mathbf{h}_{\tau-1} + \mathbf{W}_\mathrm{i}\mathbf{x}_\tau).\end{aligned}$$

Then, the reservoir can linearly predict the next input $\mathbf{x}_{\tau+1}$, based on the hidden state $\mathbf{h}_\tau$:

:nbsphinx-math:`begin{equation} mathbf{hat {x}}_{tau +1} = mathbf{W}_{mathrm{o}} mathbf{h}_tau,

end{equation}`

with $\mathbf{W}_\mathrm{o}$ mapping from hidden activation to output. Only the parameters of this output matrix $\mathbf{W}_\mathrm{o}$ are trained. Hence, the optimal values can be obtained analytically via ridge regression (with regularization parameter λ) as:

$$\mathbf{W}_\mathrm{o} = (\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{H}^T\mathbf{X},$$

where $\mathbf{H}$ are the hidden states, $\mathbf{I}$ the identity matrix, and $\mathbf{X}$ the targets of the regression.

4.51.8 Example: Lorenz Attractor

[117]:
```
from scipy import sparse

radius = 0.6
sparsity = 0.01
input_dim = 3
reservoir_size = 1000
n_steps_prerun = 10
regularization = 1e-2
sequence = x_train
```

Randomly initialize the network weights:

[118]:
```
weights_hidden = sparse.random(reservoir_size, reservoir_size, density=sparsity)
eigenvalues, _ = sparse.linalg.eigs(weights_hidden)
weights_hidden = weights_hidden / np.max(np.abs(eigenvalues)) * radius

weights_input = np.zeros((reservoir_size, input_dim))
q = int(reservoir_size / input_dim)
for i in range(0, input_dim):
    weights_input[i * q:(i + 1) * q, i] = 2 * np.random.rand(q) - 1

weights_output = np.zeros((input_dim, reservoir_size))
```

Embed the sequence into the hidden state of the network:

[119]:
```
def initialize_hidden(reservoir_size, n_steps_prerun, sequence):
    hidden = np.zeros((reservoir_size, 1))
    for t in range(n_steps_prerun):
        input = sequence[t].reshape(-1, 1)
        hidden = np.tanh(weights_hidden @ hidden + weights_input @ input)
    return hidden

def augment_hidden(hidden):
    h_aug = hidden.copy()
    h_aug[::2] = pow(h_aug[::2], 2.0)
    return h_aug

hidden = initialize_hidden(reservoir_size, n_steps_prerun, sequence)
hidden_states = []
targets = []

for t in range(n_steps_prerun, len(sequence) - 1):
    input = np.reshape(sequence[t], (-1, 1))
    target = np.reshape(sequence[t + 1], (-1, 1))
    hidden = np.tanh(weights_hidden @ hidden + weights_input @ input)
    hidden = augment_hidden(hidden)
    hidden_states.append(hidden)
    targets.append(target)

targets = np.squeeze(np.array(targets))
hidden_states = np.squeeze(np.array(hidden_states))
```

Ridge regression to obtain the linear output layer weights:

[120]:
```
weights_output = (np.linalg.inv(hidden_states.T@hidden_states + regularization * np.
↪eye(reservoir_size)) @ hidden_states.T@targets).T
```

[121]:
```
def predict(sequence, n_steps_predict):
    hidden = initialize_hidden(reservoir_size, n_steps_prerun, sequence)
    input = sequence[n_steps_prerun].reshape((-1, 1))
    outputs = []

    for t in range(n_steps_prerun, n_steps_prerun + n_steps_predict):
        hidden = np.tanh(weights_hidden @ hidden + weights_input @ input)
```

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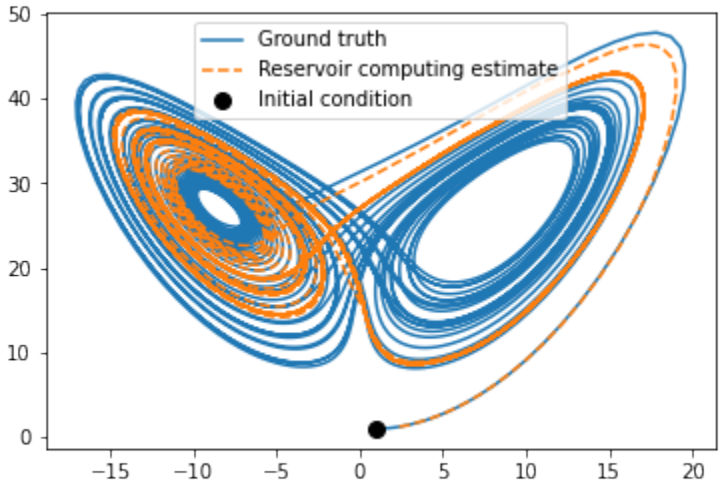
```
        hidden = augment_hidden(hidden)
        output = weights_output @ hidden
        input = output
        outputs.append(output)
    return np.array(outputs)
```

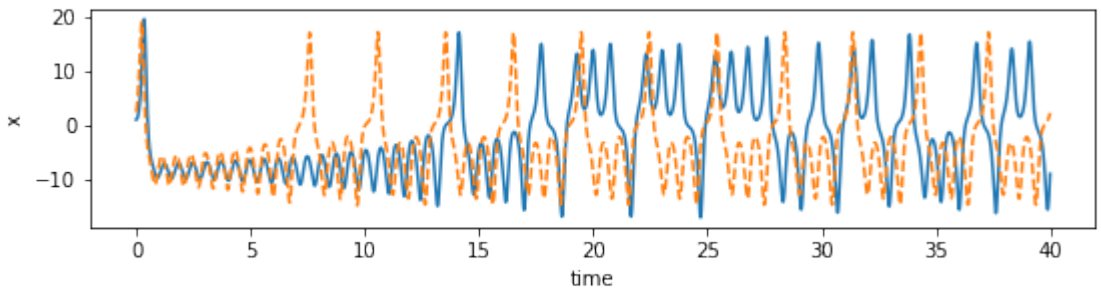
[122]:
```
x_sim = predict(sequence, 4000)
```

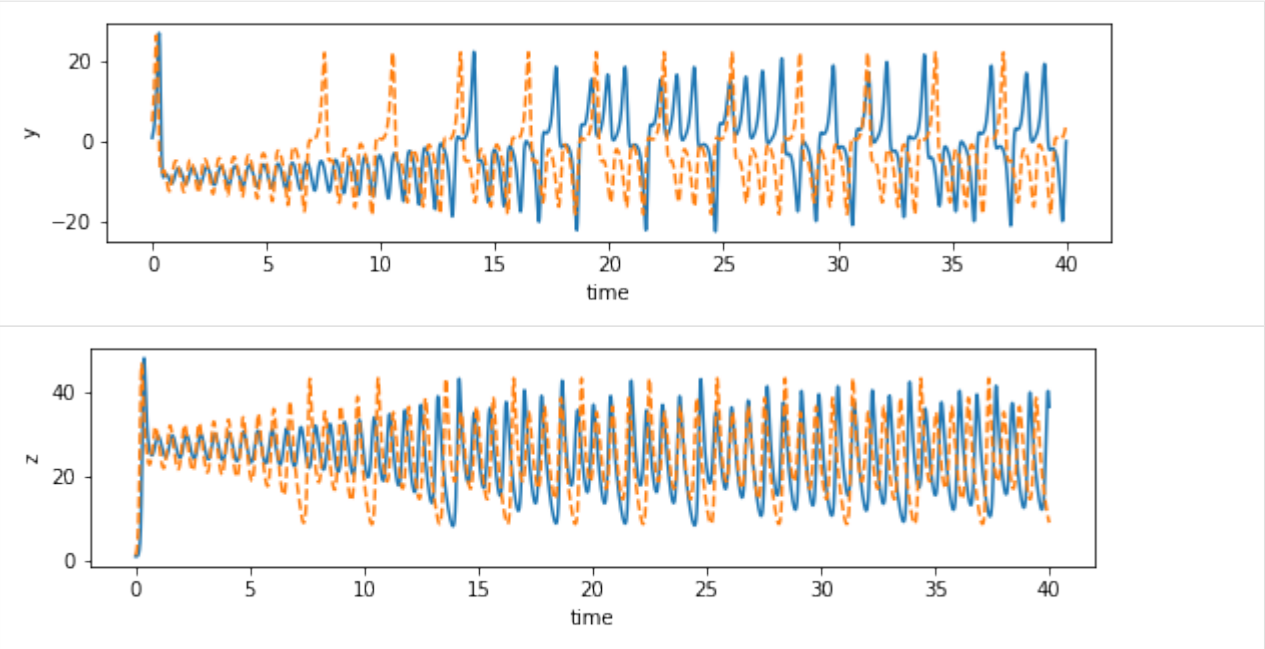
[123]:
```
plt.figure(figsize=(6, 4))
plt.plot(x_train[:4000, 0], x_train[:4000, 2], label="Ground truth")
plt.plot(x_sim[:, 0], x_sim[:, 2],'--', label="Reservoir computing estimate")
plt.plot(x_train[0, 0], x_train[0, 2], "ko", label="Initial condition", markersize=8)

plt.legend()
plt.show()
```



[124]:
```
plot_dimension(0, 'x')
plot_dimension(1, 'y')
plot_dimension(2, 'z')
```





A successful application of reservoir computing to data-driven estimation of nonlinear dynamical systems is for example:

> Jaideep Pathak et al., "Model-Free Prediction of Large Spatiotemporally Chaotic Systems from Data: A Reservoir Computing Approach," Physical Review Letters 120, no. 2 (January 12, 2018): 024102, https://doi.org/10.1103/PhysRevLett.120.024102.

4.52 DNN - Tutorial 2 Part II: Physics inspired Machine Learning

Partial Differential Equation (PDE) Solvers

Filled notebook:
Authors: Ilze Amanda Auzina

Before we start one practical thing:

> Later in this tutorial we will use datasets to train our own Neural PDE Solver. It takes a little bit of time for the datasets to be uploaded, so let's do that first! (So by the time you get to the coding part the data is already in your environment)

- Go to: drive
- Download the 3 datasets on your local machine (click on 'Download anyway' when prompted second time)
- Upload them here: click on 'Files' –> right click 'Upload' (click 'ok' on the prompt)

4.52.1 PDE vs ODE: What are PDEs?

A **partial derivative** of a function (with several variables) is a derivative with respect to one of its variables while the other variables are held constant.

For example take the Heat equation (1 dimension):

$$\frac{\delta T}{\delta t}(x,t) = \frac{\delta^2 T}{\delta x^2}(x,t)$$

Here we have one partial derivative w.r.t time (left hand side, LHS), and another partial derivative w.r.t to space (right hand side, RHS), as our function T(x,t) has 2 variables. On the LHS variable x is held constant, while on the RHS variable t is held constant.

In particular, the above PDE describes how the temperature T(x,t) changes in time for a 1 dimensional object, such as a metal rod. If we look at the PDE equation above it says that the *rate of change of temperature in time* is the same as the *the second order derivate of the spatial domain*.

This makes sense as the second order derivate gives you a measure of how a value compares to the average of its neighbours. For example, if the neighbors of a given point x_i are very cold compared to the point itself then the rate of change in temperature in time for this point will be *faster*.

In the image below we have visualized the partial derivatives of the 1d Heat equation. We can investigate the rate of change of the temperature in two domains: spatial (*see Fig 1*) and time (*see Fig 2*). (credits: 3Blue1Brwon series source)

[2]:
```
import matplotlib.pyplot as plt
import matplotlib.image as mpimg

img_space = mpimg.imread('images/SpaceDerivative.png')
img_time= mpimg.imread('images/TimeDerivative.png')
f, axarr = plt.subplots(1,2, figsize=(30,30))
axarr[0].set_axis_off()
axarr[0].set_title('Fig 1: Space Derivative', fontsize=25)
axarr[1].set_axis_off()
axarr[1].set_title('Fig 2: Time Derivative', fontsize=25)
axarr[0].imshow(img_space)
axarr[1].imshow(img_time);
```

Fig 1: Space Derivative

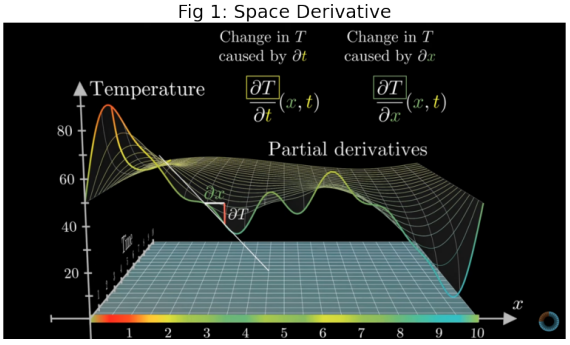
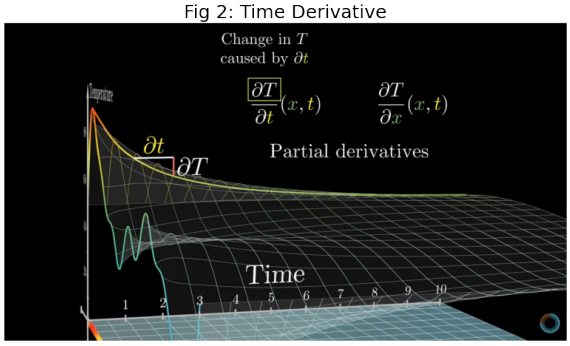


Fig 2: Time Derivative



As you can see above each of the derivatives tells only a part of the story on how the function changes, therefore we call them partial derivates. In principle, PDEs could be seen as a system of ordinary differential equations.

In **dynamical systems** compared to traditional ML we are most interested in how our function T(x,t) changes over time.

The above 1D Heat equation can be also extended to more spatial directions by extending the right hand side:

$$\frac{\delta T}{\delta t}(x, y, z, t) = \alpha * (\frac{\delta^2 T}{\delta x^2}(x, y, z, t) + \frac{\delta^2 T}{\delta y^2}(x, y, z, t) + \frac{\delta^2 T}{\delta z^2}(x, y, z, t))$$

Why do we care about PDEs?

Thay allow us to model (predict) real life systems that influence our life: - economics: Black-Scholes equation that governs price evolution - climate: Wheather prediction, think about how your google weather app knows what's the weather going to be like tomorrow - in general, the entire physical world around us

To conclude:

PDEs tells us how a function with several variables changes over time. Most of the physical world is governed by PDEs.

4.52.2 How to solve PDEs?

Let's now shift our focus on a specfic PDE, for example, the **Korteweg-de Vries** (KdV) equation.

The KdV euqation (1985) is a model of shallow water waves:

In the above x again represents a spatial location, U(x) is the value of x given a function U, and we can see the evolution of the system in time.

The PDE equation governing the above simulation is:

$$\frac{\delta U}{\delta t}(x, t) = -U(x, t) * \frac{\delta U}{\delta x}(x, t) - \frac{\delta^3 U}{\delta x^3}(x, t)$$

Similar to the heat equation in the introduction our function U has two dimentions, x and t, where x is the spatial domain and t is the time domain. The $\frac{\delta^3 U}{\delta x^3}(x, t)$ is a dispersive term and $U(x, t) * \frac{\delta U}{\delta x}(x, t)$ is a non-linear convection term.

When we are taking about solving a PDE what we want to do is to find a function U(x,t) that would: - satisfy the above given PDE - meet the boundary conditions - meet the initial conditions

These additional constraints, boundary and inital conditions, restrict the function U(x,t) that is valid for the given PDE equation

Boundary Conditions

The boundary conditions express the behaviour of a function on the boundary (border) of its area of definitions. For example, you constrain that at both ends of the spatial domain x_0 and x_L (where L is the end of your spatial domain) the function remains constant for all time:

$$\frac{\delta U}{\delta x}(x_0, t) = \frac{\delta U}{\delta x}(x_L, t) = 0$$

$$\forall t$$

Initial Conditions

An initial condition is similar to boundary conditions, but now in the time direction. For example, now you constrain what value your function U(x,t) must return at timepoint t=0. For the KdV simulation above the initial condition was:

$U(x, 0) = cos(\pi x)\ \forall x$

Solving PDE

Similary to ODEs the traditional way of solving a given PDE equation is via *numerical solvers*.

In the below cells we will implement a simple numerical solver in order to solve the above KdV equation

Numerical Solvers

[3]:
```
#Import relevant packages
%matplotlib inline
import matplotlib
from matplotlib.pyplot import cm
import numpy as np
from typing import Optional
from scipy.integrate import solve_ivp
from scipy.fftpack import diff as psdiff

from matplotlib import animation
import seaborn as sns
from IPython.display import HTML
```

Generate Initial Conditions

Initial conditions are sampled from a distribution over truncated Fourier series with random coefficients $\{A_k, \ell_k, \phi_k\}_k$ as

$$U(x,0) = \sum_{k=1}^{N} A_k \sin(2\pi\ell_k x/L + \phi_k) \, .$$

[4]:
```
def generate_params() -> (int, np.ndarray, np.ndarray, np.ndarray):
    """
    Returns parameters for initial conditions.
    Args:
        None
    Returns:
        int: number of Fourier series terms
        np.ndarray: amplitude of different sine waves
        np.ndarray: phase shift of different sine waves
        np.ndarray: frequency of different sine waves
    """
    N = 10 #Number of different waves
    lmin, lmax = 1, 3 #sine frequencies for intial conditions
    A = (np.random.rand(1, N) - 0.5)
    phi = 2.0*np.pi*np.random.rand(1, N)
    l = np.random.randint(lmin, lmax, (1, N))
    return (N, A, phi, l)

def initial_conditions(x: np.ndarray, L: int, params: Optional[list]=None) -> np.ndarray:
    """
    Return initial conditions based on initial parameters.
    Args:
        x (np.ndarray): input array of spatial grid
        L (float): length of the spatial domain
        params (Optinal[list]): input parameters for generating initial conditions
    Returns:
        np.ndarray: initial condition
```

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```
    """
    if params is None:
        params = generate_params()
    N, A, phi, l = params
    u = np.sum(A * np.sin((2 * np.pi * l * x[:, None] / L ) + phi), -1)
    return u
```

Solve via Method of Lines (MOL)

In MOL all but the temporal dimension are discretized. Having the spatial derivatives numerically implemented results in a set of coupled ODEs for the time domain, which can be solved by using integration schemes of ODE solving.

Concretely, for getting numerical spatial derivatives, we use pseudospectral methods, where the derivatives are computed in the frequency domain by first applying a fast fourier transform (FFT) to the data, then multiplying by the appropriate values and converting back to the spatial domain with the inverse FFT.

Mathematically this works since the Fourier transform of the nth derivative is given by:

$$\widehat{f^{(n)}}(\xi) = \mathcal{F}\left(\frac{d^n}{dx^n} f(x)\right) = (2\pi i \xi)^n \widehat{f}(\xi) \,,$$

where $\widehat{f^{(n)}}$ is the mathematical denotation of fourier transform of a function f, the transform variable ξ represents frequency, $f(x)$ is an absolutely continuous differentiable function, and both f and its derivative f are integrable (for more information see wikipedia section Functional relations). This method of differentiation in the Fourier space is implemented by the `diff` function in the module `scipy.fftpack`. For integration in time we use an **implicit Runge-Kutta method** of Radau IIA family, order 5.

[5]:
```
# Spatial Derivatives
def kdv_pseudospectral(t: float, u: np.ndarray, L: float) -> np.ndarray:
    """
    Compute spatial derivatives for the KdV equation, using a pseudospectral method,␣
↪descretization in x.
    Args:
        t (float): time point
        u (np.ndarray): 1D input field
        L (float): length of the spatial domain
    Returns:
        np.ndarray: reconstructed pseudospectral time derivative
    """
    # Compute the x derivatives using the pseudo-spectral method.
    ux = psdiff(u, order=1, period=L)
    uxxx = psdiff(u, order=3, period=L)
    # Compute du/dt.
    dudt = -u*ux - uxxx
    return dudt
```

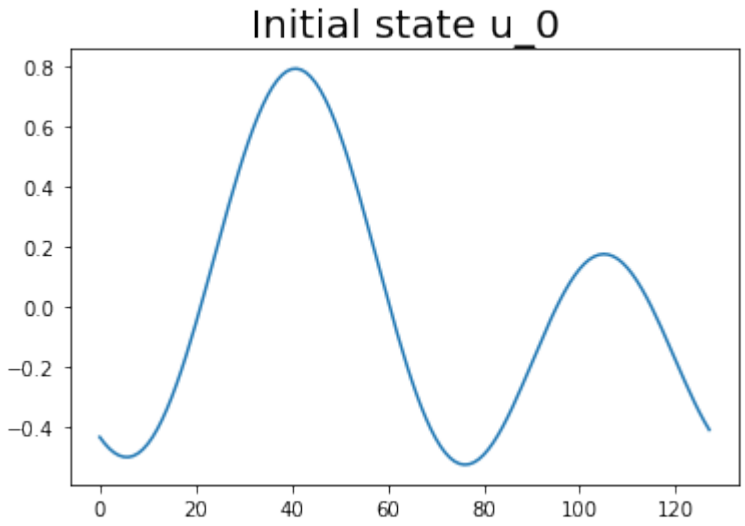
Solve for KdV trajectory

[6]:
```
# Set the size of the domain, and create the discretized grid.
np.random.seed(1)
L = 128
N = 2**7
x = np.linspace(0, (1-1.0/N)*L, N)

# Set the tolerance of the solver
tol = 1e-6

# Set the initial conditions.
u0 = initial_conditions(x, L)

# Set the time sample grid.
T = 100.
t = np.linspace(0, T, 200)

# Compute the solution using kdv_pseudospectral as spatial solver
sol_ps = solve_ivp(fun=kdv_pseudospectral,
                                t_span=[t[0], t[-1]],
                                y0=u0,
                                method='Radau',
                                t_eval=t,
                                args=(L,),
                                atol=tol,
                                rtol=tol)
```

Visualize the solved KdV

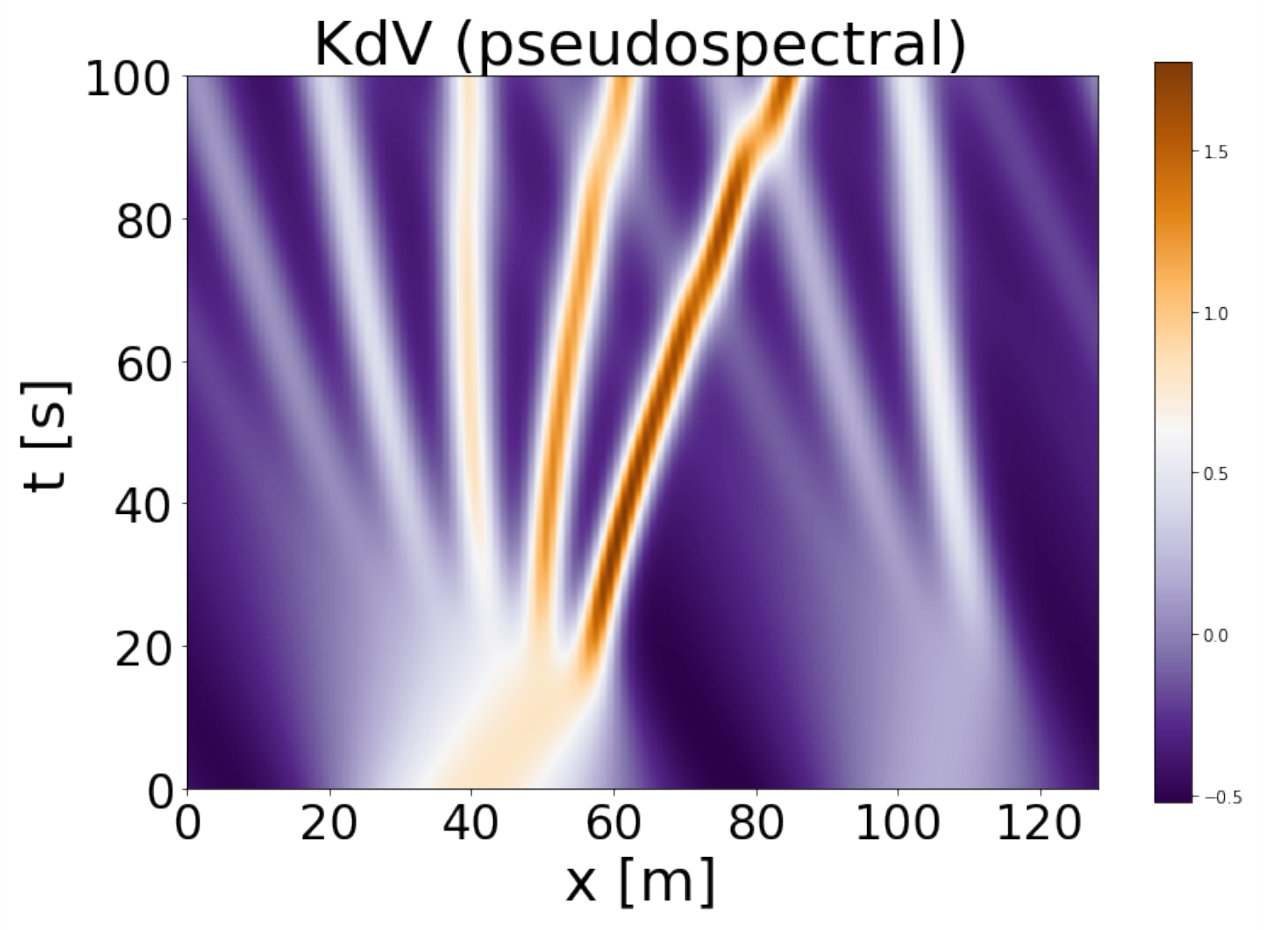
Let's first plot our initial state:

[7]:
```
plt.plot(u0)
plt.title('Initial state u_0', fontsize=20)
plt.show();
```



Now let's plot the entire time evolution, where time is as the y axis, spatial domain as the x axis, and the function value U(x,t) is the colorbar

[8]:
```
# Let's look at the trajectory obtained by using the pseudospectral spatial solver
if sol_ps.success:
    t_ps = sol_ps.y.T[::-1]
    plt.figure(figsize=(12,8))
    plt.imshow(t_ps, extent=[0,L,0,T], cmap='PuOr_r')
    plt.colorbar()
    plt.title('KdV (pseudospectral)', fontsize=36)
    plt.xlabel('x [m]', fontsize=34)
    plt.ylabel('t [s]', fontsize=34)
    plt.yticks(fontsize=28)
    plt.xticks(fontsize=28)
    plt.show()
```



In the figure above we can see the time evolution of our initial state $U(x, t_0)$. As we only have one spatial domain, each x point is a coordinate in our spatial domain, for example, the bottom left point would be the value of $U(x_0, t_0)$. The color indicates the value of our function $U(.)$, and the more brown the color the *higher* the wave. Interpret the *stripes* you see as waves and as time progresses the waves get sharper.

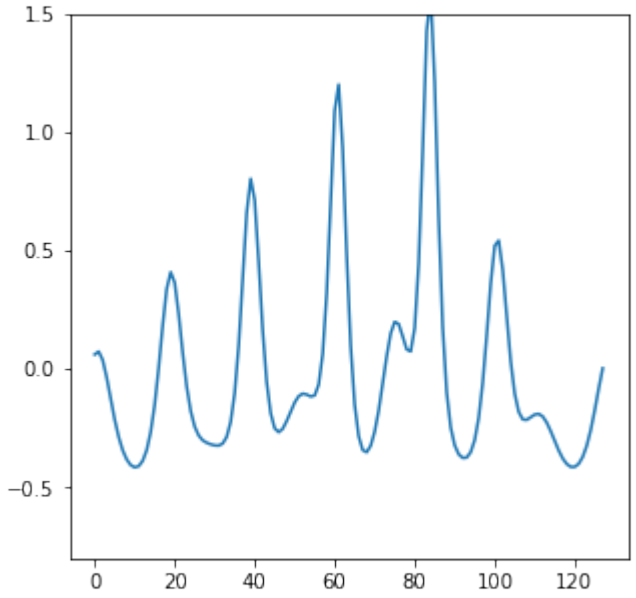
Feel free to play around with the settings under *generate_params()* and see how the simulation changes!

Let's create our own animation!

[9]:
```
plt.rcParams["animation.html"] = "jshtml"
```

[10]:
```
fig, ax = plt.subplots(figsize=(5,5))
t_ps_anim = np.flipud(t_ps)

def animate(t):
    plt.cla()
    plt.ylim([-0.8, 1.5])
    plt.plot(t_ps_anim[t,:])

matplotlib.animation.FuncAnimation(fig, animate, frames=200, interval=20)
```

[10]:
```
<matplotlib.animation.FuncAnimation at 0x167e35ee0>
```



In the animation, on the y-axis we have the output of the function, $U(x, t)$. As the animcation plays we can see the waves of our initial state to become more peaked.

Why do we care about Numerical Solvers?

This story is two-fold: - We need numerical solvers to generate data to train our ML models - Numerical solvers have higher accuracy than NN, hence, they provide a baseline for expected acuraccy for a given Neural PDE Solver

And in general the field of numerical solvers is about 100 years old, definitely there are things that we can learn from them!

4.52.3 Neural Networks as PDE Solvers

The initial interest of why we would want to replace traditional numerical solvers with deep learning is because traditional PDE solvers, such as finite element methods and finite difference methods, rely on discretizing the space into a very fine mesh. As a result traditional solvers have the following drawbacks: - The error scales steeply with the resolution. We need a high resolution to get good approximations. - The computation and storage steeply scale with the resolution (i.e. the size of the grid). - When the equation is solved on one discretization, we cannot change the discretization anymore.

So the question is: *can we use neural networks to improve upon the drawbakcs of numerical solvers?*

> In short, the answer is **yes** and in the upcoming section we will explore on how to construct such a network.

What is our network's aim?

What we would like our deep neural network to do is that given our initial and/or boundary conditions to directly output the solution, similar to image-to-image mapping. See below, we have an initial state *Initial Vorticity* and we want to predict the *'image'* at t_{15}.

[11]:
```
img_pde = mpimg.imread('images/PDEimg-img.png')
caption = "Credits: https://zongyi-li.github.io/blog/2020/fourier-pde/"
plt.figure(figsize=(10, 7))
```

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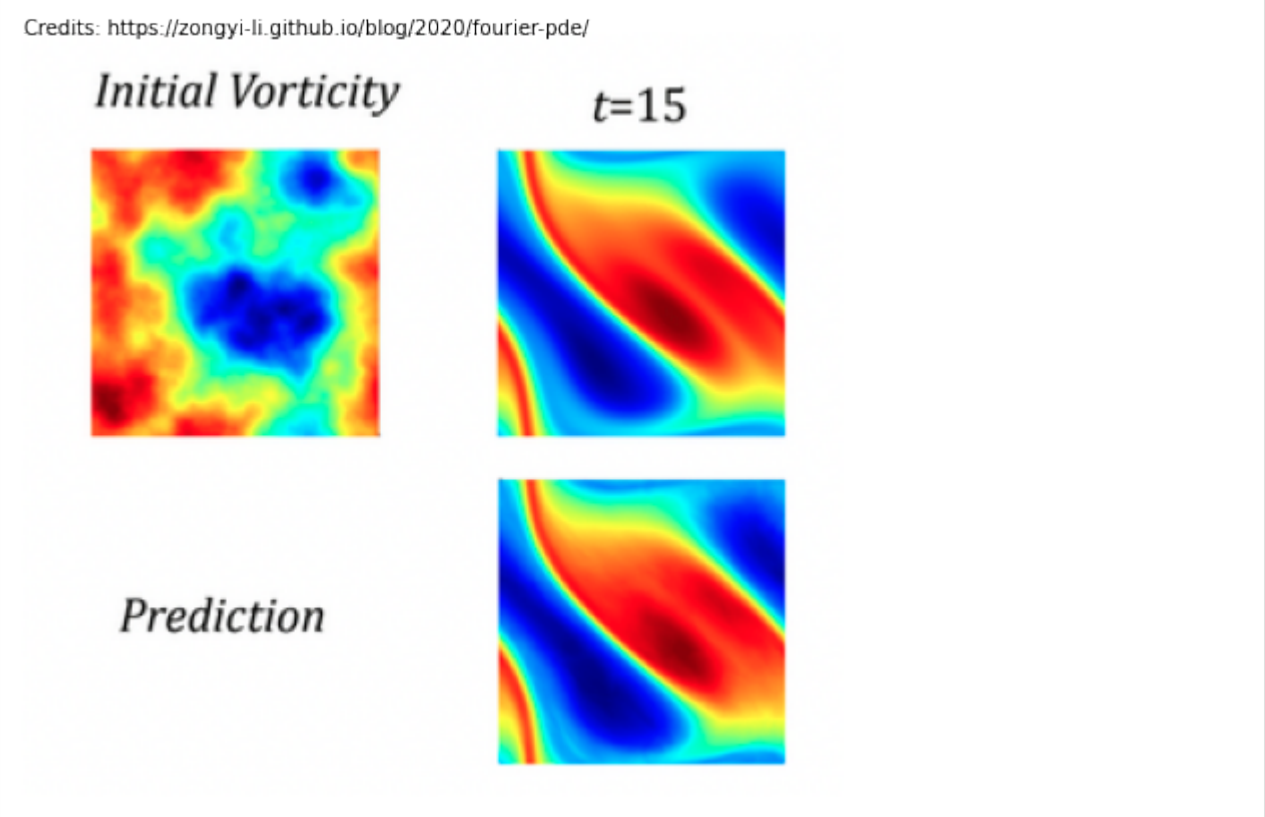
```
plt.imshow(img_pde)
plt.text(0, 0, caption, ha='left', fontsize=10)
plt.axis('off');
```



However, when we talk about PDEs we consider our input and output space to be **functions**. What we mean by this is that we have some initial function U that takes as input x, y and t, $U(x, y, t_0)$ respectively. In the above image that would be the *Initial Vorticity* state. We want our model to output perhaps the resulting function 15 time steps later $A(x, y, t_{15})$, so the state to the right. As such, **images could be considered as functions**. In the context of standard ML an image is a function of light defined on a continous region, instead of 32x32 pixel vectors.

Hence, we want our neural network, G (parameterised by θ) to map between function spaces:

$$G_\theta : UA$$

In order to do so let me introduce to you the concept of **neural operators**.

Neural Operators

Let's break down this term "**Neural Operators (NO)**" in 2 parts: (i) neural and (ii) operator. With the first one you probably already are familiar, so let's start with the second one.

Operator

The term operator comes from mathematics:

> *an operator is generally a mapping or function that acts on elements of a space to produce elements of another space*

Indeed, that is exactly what he have defined as the goal of our NN.

So what is the benefit of rephrasing the img-to-img problem to func-to-func? **Generalizability**.

> The neural operator is **mesh-independent**, this is different from standard ML methods such as CNNs. The func-to-func mapping perspective allow us to: (i) first use a numerical solver to generate some low-resolution data, (ii) then train a neural operator on this data, (iii) but now the learned NO is able to give also high-resolution predictions, despite being trained on low-resolution data. This makes both, the training and the evaluation, easier.

In short: the benefit of operator persepctive is that now we are parameterizing the model in function space - **it learns the continuous functions instead of discretized vectors**

Neural

The neural part is that just like NN: our neural operator will also consist of linear transformations, K, and non-linear activations, σ.

A standard deep neural network can be written as:

$$y = (K_{ll}\sigma_1 K_0)x$$

where defines function composition, y is the output vector, x is the input vector, K are linear or convolutional layers, and σ are the activation functions such as ReLU.

As we dicussed for operators our inputs and outputs are functions, hence we need to adjust the above to neural operator framework:

$$a(x) = (K_{ll}\sigma_1 K_0)u(x)$$

now our output vector y is replaced by a function a, and our input vector x is replaced by a function u. Both functions, u and a are able to take inputs at different discretizations (28x28, or 256x256), hence allowing the neural operator to be discretization independent.

In order for the above to be true we need to adjust the formulation of our linear layers, K, as it has to be able to take functions as input. We reformulate K as a kernel integral operator, changing the layer architecture to:

$$u_{t+1}(x) = \sigma(Wu_t(x) + (Ku_t)(x))$$

$$(Ku_t)(x) := k(x, y)u(y)dy$$

where k is a kernel function and W is the bias term. The only question remaining is how to define the kernel itself, $k(x, y)$. Recent research has investigated multiple alternatives, however the kernel that has brought the most promising results is the **Fourier Neural Operator**.

Fourier Neural Operator

What Li et al. (2020) proposed is to set the above kernel integral operator, $(Ku_t)(x)$, as a convolution operator defined in Fourier space. Why is this desirable? - it's fast: convolution in one domain (spatial domain) equals **point-wise multiplication** in the frequency domain (convolution theorem) - it's efficient: the inputs and outputs of PDEs are continous functions, so it's more efficient to represent them in Fourier space.

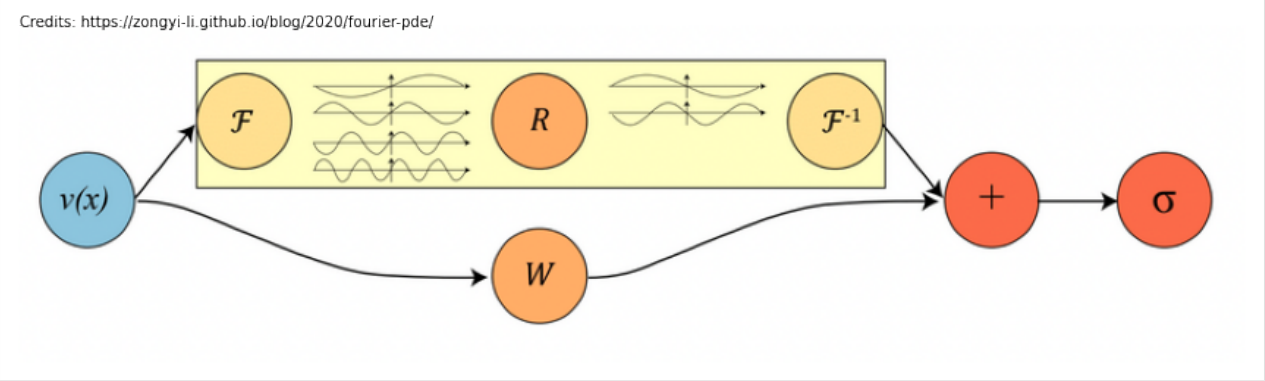
Hence, the **Fourier Integral Operator** is:

$$(Ku_t)(x) =^{-1} (R_\phi(u_t))(x)$$

where R_ϕ is the linear tranform of the lower Fourier modes. Let's break down what is happening in the above function: - first we do a Fourier transform: $(Fu_t)(x)$ - then a linear transform: $R \cdot ()$ - and lastly we perform an inverse fourier transform: $F^{-1}(\cdot)$

In the image below we have depicted a complete **Fourier layer** ($v(x)$ is $u(x)$ in our notation):

[12]:
```
img_fourier = mpimg.imread('images/fourierlayer.png')
caption = "Credits: https://zongyi-li.github.io/blog/2020/fourier-pde/"
plt.figure(figsize=(15, 10))
plt.imshow(img_fourier)
plt.text(0, 0, caption, ha='left', fontsize=10)
plt.axis('off');
```



As you can see in the above figure R_ϕ acts as a linear transformation on the lower frequency modes and sets the higher modes to zeros. Nonetheless, despite the fact that Fourier Integral Operator on it's own loses the higher frequency modes and works only with periodic boundary conditions, the operator as a whole does not suffer from this: > The bias term helps to recover the non-periodic boundaries, and the non-linear activations help to recover the higher frequency modes. The activations act on the spatial domain, which is also the reason why we need the inverse fourier transform

Resolution Invariance

The Fourier layers are discretization-invariant, because they can learn from and evaluate functions which are discretized in an arbitrary way. Since parameters are learned directly in Fourier space, resolving the functions in physical space simply amounts to projecting on the basis of wave functions which are well-defined everywhere on the space. This allows us to transfer among discretization.

4.52.4 Time to code a Neural PDE Solver

We will train our Neural PDE Solver on the KdV PDE that was introduced earlier in this notebook.

The Data

the data is located in your runtime environment. If you click on 'Files' on the left side, you will see the downloaded files: - KdV_train_512_easy.h5 - KdV_valid_easy.h5 - KdV_test_easy.h5

> Each dataset containts 512 trajectories. The length, L, of the spatial domain is 128, while the spatial resolution of the dataset is 256. We stimulate each trajectory for 100 time steps, with a temporal resolution of 140.
>
> KdV equation initial conditions are generated by the same principle as in the earlier example in the notebook

Fourier Integral Operator

Let's first implement the euqation of the **Fourier Integral Operator** that we discussed in the previous section.

[13]:
```
import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.nn.parameter import Parameter
```

[14]:
```
################################################################
#  1d Fourier Integral Operator
################################################################
class SpectralConv1d(nn.Module):
    def __init__(self, in_channels: int, out_channels: int, modes: int):
        super(SpectralConv1d, self).__init__()
        """
        Initializes the 1D Fourier layer. It does FFT, linear transform, and Inverse FFT.
        Args:
            in_channels (int): input channels to the FNO layer
            out_channels (int): output channels of the FNO layer
            modes (int): number of Fourier modes to multiply, at most floor(N/2) + 1
        """
        self.in_channels = in_channels
        self.out_channels = out_channels
        self.modes = modes
        self.scale = (1 / (in_channels*out_channels))
        self.weights = nn.Parameter(self.scale * torch.rand(in_channels, out_channels,␣
↪self.modes, dtype=torch.cfloat))

    # Complex multiplication
    def compl_mul1d(self, input, weights):
        """
        Complex multiplication of the Fourier modes.
        [batch, in_channels, x], [in_channel, out_channels, x] -> [batch, out_channels,␣
↪x]
            Args:
                input (torch.Tensor): input tensor of size [batch, in_channels, x]
                weights (torch.Tensor): weight tensor of size [in_channels, out_channels,
↪ x]
```

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```
            Returns:
                torch.Tensor: output tensor with shape [batch, out_channels, x]
        """
        return torch.einsum("bix,iox->box", input, weights)

    def forward(self, x: torch.Tensor) -> torch.Tensor:
        """
        Fourier transformation, multiplication of relevant Fourier modes,␣
↪backtransformation
        Args:
            x (torch.Tensor): input to forward pass os shape [batch, in_channels, x]
        Returns:
            torch.Tensor: output of size [batch, out_channels, x]
        """
        batchsize = x.shape[0]
        # Fourier transformation
        x_ft = torch.fft.rfft(x)

        # Multiply relevant Fourier modes
        out_ft = torch.zeros(batchsize, self.out_channels, x.size(-1)//2 + 1,  device=x.
↪device, dtype=torch.cfloat)
        out_ft[:, :, :self.modes] = self.compl_mul1d(x_ft[:, :, :self.modes], self.
↪weights)

        #Return to physical space
        x = torch.fft.irfft(out_ft, n=x.size(-1))
        return x
```

Now once we have our integral kernel, we are ready to build our neural network.

Overall Network Architecture

We will follow the original architecture as desribed by the FNO paper: the network is constructed by stacking four Fourier layers with ReLU activations.

In addition, we will add some minor improvements as described by LPSDA paper: we will predict in 'batches' (mutliple time points)

[41]:
```
################################################################
#  1d Fourier Network
################################################################
class FNO1d(nn.Module):
    def __init__(self, modes, width, time_future, time_history):
        super(FNO1d, self).__init__()

        """
        The overall network. It contains 4 layers of the Fourier layer.
        1. Lift the input to the desire channel dimension by self.fc0 .
        2. 4 layers of the integral operators u' = (W + K)(u).
            W defined by self.w; K defined by self.conv .
        3. Project from the channel space to the output space by self.fc1 and self.fc2 .

        input: a driving function observed at T timesteps + 1 locations (u(1, x), ...,␣
↪u(T, x),  x).
```

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```
        input shape: (batchsize, x=s, c=2)
        output: the solution of a later timestep
        output shape: (batchsize, x=s, c=1)
        """
        self.modes = modes
        self.width = width
        self.time_future = time_future
        self.time_history = time_history
        self.fc0 = nn.Linear(self.time_history+1, self.width)

        self.conv0 = SpectralConv1d(self.width, self.width, self.modes)
        self.conv1 = SpectralConv1d(self.width, self.width, self.modes)
        self.conv2 = SpectralConv1d(self.width, self.width, self.modes)
        self.conv3 = SpectralConv1d(self.width, self.width, self.modes)
        self.w0 = nn.Conv1d(self.width, self.width, 1)
        self.w1 = nn.Conv1d(self.width, self.width, 1)
        self.w2 = nn.Conv1d(self.width, self.width, 1)
        self.w3 = nn.Conv1d(self.width, self.width, 1)

        self.fc1 = nn.Linear(self.width, 128)
        self.fc2 = nn.Linear(128, self.time_future)

    def forward(self, u):
        grid = self.get_grid(u.shape, u.device)
        x = torch.cat((u, grid), dim=-1)
        x = self.fc0(x)
        x = x.permute(0, 2, 1)

        x1 = self.conv0(x)
        x2 = self.w0(x)
        x = x1 + x2
        x = F.gelu(x)

        x1 = self.conv1(x)
        x2 = self.w1(x)
        x = x1 + x2
        x = F.gelu(x)

        x1 = self.conv2(x)
        x2 = self.w2(x)
        x = x1 + x2
        x = F.gelu(x)

        x1 = self.conv3(x)
        x2 = self.w3(x)
        x = x1 + x2

        x = x.permute(0, 2, 1)
        x = self.fc1(x)
        x = F.gelu(x)
        x = self.fc2(x)
        return x
```

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```
    def get_grid(self, shape, device):
        batchsize, size_x = shape[0], shape[1]
        gridx = torch.tensor(np.linspace(0, 1, size_x), dtype=torch.float)
        gridx = gridx.reshape(1, size_x, 1).repeat([batchsize, 1, 1])
        return gridx.to(device)
```

Helper functions

[42]:
```
import h5py
import torch
from typing import Tuple
from torch.utils.data import Dataset
from torch.utils.data import DataLoader
from torch import nn

#function to torch dataloader from the dataset
def create_dataloader(data_string: str, mode: str, nt: int, nx: int, batch_size:int, num_
↪workers:int):
    try:
        dataset = HDF5Dataset(data_string,mode,nt=nt,nx=nx)
        loader = DataLoader(dataset,batch_size=batch_size,shuffle=True,num_workers=num_
↪workers)
    except:
        raise Exception("Datasets could not be loaded properly")

    return loader


#Function to format the data in the correct format
def to_coords(x: torch.Tensor, t: torch.Tensor) -> torch.Tensor:
    """
    Transforms the coordinates to a tensor X of shape [time, space, 2].
    Args:
        x: spatial coordinates
        t: temporal coordinates
    Returns:
        torch.Tensor: X[..., 0] is the space coordinate (in 2D)
                      X[..., 1] is the time coordinate (in 2D)
    """
    x_, t_ = torch.meshgrid(x, t)
    x_, t_ = x_.T, t_.T
    return torch.stack((x_, t_), -1)

#Helper class to open the .h5 formated file
class HDF5Dataset(Dataset):
    """
    Load samples of an PDE Dataset, get items according to PDE.
    """
    def __init__(self, path: str,
                 mode: str,
                 nt: int,
```

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```
                nx: int,
                dtype=torch.float64,
                load_all: bool=False):
        """Initialize the dataset object.
        Args:
            path: path to dataset
            mode: [train, valid, test]
            nt: temporal resolution
            nx: spatial resolution
            shift: [fourier, linear]
            pde: PDE at hand
            dtype: floating precision of data
            load_all: load all the data into memory
        """
        super().__init__()
        f = h5py.File(path, 'r')
        self.mode = mode
        self.dtype = dtype
        self.data = f[self.mode]
        self.dataset = f'pde_{nt}-{nx}'


        if load_all:
            data = {self.dataset: self.data[self.dataset][:]}
            f.close()
            self.data = data

    def __len__(self):
        return self.data[self.dataset].shape[0]

    def __getitem__(self, idx: int) -> Tuple[torch.Tensor, torch.Tensor, torch.Tensor]:
        """
        Returns data items for batched training/validation/testing.
        Args:
            idx: data index
        Returns:
            torch.Tensor: data trajectory used for training/validation/testing
            torch.Tensor: dx
            torch.Tensor: dt
        """
        u = self.data[self.dataset][idx]
        x = self.data['x'][idx]
        t = self.data['t'][idx]
        dx = self.data['dx'][idx]
        dt = self.data['dt'][idx]


        if self.mode == "train":
            X = to_coords(torch.tensor(x), torch.tensor(t))
            sol = (torch.tensor(u), X)

            u = sol[0]
```

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```
            X = sol[1]
            dx = X[0, 1, 0] - X[0, 0, 0]
            dt = X[1, 0, 1] - X[0, 0, 1]
        else:
            u = torch.from_numpy(u)
            dx = torch.tensor([dx])
            dt = torch.tensor([dt])
        return u.float(), dx.float(), dt.float()

#function to create x - y data pairs: 20 past timepoints as x, 20 future timepoints as y
def create_data(datapoints: torch.Tensor, start_time: list, time_future: int, time_
↪history: int) -> Tuple[torch.Tensor, torch.Tensor]:
    """
    Getting data of PDEs for training, validation and testing.
    Args:
        datapoints (torch.Tensor): trajectory input
        start_time (int list): list of different starting times for different␣
↪trajectories in one batch
        pf_steps (int): push forward steps
    Returns:
        torch.Tensor: neural network input data
        torch.Tensor: neural network labels
    """
    data = torch.Tensor()
    labels = torch.Tensor()
    # Loop over batch and different starting points
    # For every starting point, we take the number of time_history points as training␣
↪data
    # and the number of time future data as labels
    for (dp, start) in zip(datapoints, start_time):
        end_time = start+time_history
        d = dp[start:end_time]
        target_start_time = end_time
        target_end_time = target_start_time + time_future
        l = dp[target_start_time:target_end_time]

        data = torch.cat((data, d[None, :]), 0)
        labels = torch.cat((labels, l[None, :]), 0)

    return data, labels
```

Train the Neural PDE Solver

First we will define the configurations of our experiment and create the data loader for training, validation and test data

[43]:
```
######################################################################
#  configurations
######################################################################

#Experiment Settings
ntrain = 512 #train samples
```

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```
nt = 140 #temporal resolution
nx = 256 #spatial resoltuion
time_history = 20 #time steps to be considered as input to the solver
time_future = 20 #time steps to be considered as output of the solver
device = 'cpu'  #change to cpu of no cuda available
print_interval = 20

#model parameters
modes = 16 # number of Fourier modes to multiply
width = 64 # input and output channels to the FNO layer
batch_size = 16
num_epochs = 1 #set to one so faster computation, in principle 20 is best
learning_rate = 0.0001
lr_decay = 0.4
num_workers = 0
```

[35]:
```
######################################################################
# read data
######################################################################
train_loader = create_dataloader("KdV_train_10_1_3_512_easy.h5", mode="train", nt=nt,␣
↪nx=nx, batch_size=batch_size, num_workers=num_workers)
valid_loader = create_dataloader("KdV_valid_10_1_3_easy.h5", mode="valid", nt=nt, nx=nx,␣
↪batch_size=batch_size, num_workers=num_workers)
test_loader = create_dataloader("KdV_test_10_1_3_easy.h5", mode = "test", nt=nt, nx=nx,␣
↪batch_size=batch_size, num_workers=num_workers)
```

Initialize the model

[44]:
```
import operator
from functools import reduce
# print the number of parameters
def count_params(model):
    c = 0
    for p in list(model.parameters()):
        c += reduce(operator.mul,
                    list(p.size()+(2,) if p.is_complex() else p.size()))
    return c

# model
model = FNO1d(modes, width, time_future, time_history).to(device)
print('Number of paramters: {}'.format(count_params(model)))
```

```
Number of paramters: 553236
```

Select an optimizer

*we also implement a scheduler 'MultiStepLR' that decays the learning rate, to lear more read*info

[45]:
```
# Optimizer
from torch import optim
optimizer = optim.AdamW(model.parameters(), lr=learning_rate)
scheduler = optim.lr_scheduler.MultiStepLR(optimizer, milestones=[0, 5, 10, 15],␣
↪gamma=lr_decay)
```

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Select a training objective

[46]:
```
criterion = torch.nn.MSELoss(reduction="none")
```

Below are functions for the training and test loop

[47]:
```
import random

def bootstrap(x: torch.Tensor, Nboot: int=64, binsize: int=1) -> Tuple[torch.Tensor,␣
↪torch.Tensor]:
    """
    Bootstrapping mean or median to obtain standard deviation.
    Args:
        x (torch.Tensor): input tensor, which contains all the results on the different␣
↪trajectories of the set at hand
        Nboot (int): number of bootstrapping steps, 64 is quite common default value
        binsize (int):
    Returns:
        torch.Tensor: bootstrapped mean/median of input
        torch.Tensor: bootstrapped variance of input
    """
    boots = []
    x = x.reshape(-1, binsize, *x.shape[1:])
    for i in range(Nboot):
        boots.append(torch.mean(x[torch.randint(len(x), (len(x),))], axis=(0, 1)))
    return torch.tensor(boots).mean(), torch.tensor(boots).std()

def training_loop(loader,model, optimizer, criterion, device, batch_size):
  """
  Training loop.
  Loop is over the mini-batches and for every batch we pick a random timestep.
  This is done iteratively for the number of timesteps in one training sample.
  One average, we therefore start at every starting point in every trajectory during one␣
↪episode.
  Args:
      model (torch.nn.Module): neural network model
      optimizer (torch.optim): chosen optimizer
      loader (DataLoader): train/valid/test dataloader
      criterion (torch.nn.modules.loss): loss criterion
      device: device (cpu/gpu)
  """
  losses = []
  max_start_time = (nt - time_history) - time_future
  for (u, _, _) in loader:
      optimizer.zero_grad()
      start_time = random.choices([t for t in range(time_history, max_start_time + 1,␣
↪time_history)], k=batch_size)

      data, labels = create_data(u, start_time, time_history, time_future)
      data, labels = data.to(device), labels.to(device)
```

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```
      # Change [batch, time, space] -> [batch, space, time]
      data = data.permute(0, 2, 1)

      #forward pass
      pred = model(data)

      loss = criterion(pred.permute(0, 2, 1), labels)
      loss = loss.sum()
      loss.backward()
      losses.append(loss.detach() / batch_size)
      optimizer.step()

  losses = torch.stack(losses)
  return losses

def test(loader,model,criterion, device, batch_size):
    """
    Test routine.
    Both step wise losses and enrolled forward losses are computed.
    Args:
        model (torch.nn.Module): neural network model
        loader (DataLoader): train/valid/test dataloader
        criterion (torch.nn.modules.loss): loss criterion
        device: device (cpu/gpu)
    Returns:
        (torch.Tensor, torch.Tensor, torch.Tensor, torch. Tensor): mean and normalized␣
↪mean errors
        of full trajectory unrolling
    """
    losses, nlosses = [], []
    max_start_time = (nt - time_history) - time_future
    for (u, _, _) in loader:
        losses_tmp, nlosses_tmp = [], []
        with torch.no_grad():
            # the first time steps are used for data augmentation according to time␣
↪translate
            # we ignore these timesteps in the testing
            for start in range(time_history, max_start_time+1, time_future):

                end_time = start + time_history
                target_end_time = end_time + time_future
                if start == time_history:
                    data = u[:, start:end_time].to(device)
                    data = data.permute(0, 2, 1)
                else:
                    data = torch.cat([data, pred], -1)
                    data = data[..., -time_history:]

                labels = u[:, end_time: target_end_time].to(device)
                pred = model(data)
```

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```
                loss = criterion(pred.permute(0, 2, 1), labels)
                nlabels = torch.mean(labels ** 2, dim=-1, keepdim=True)
                nloss = loss / nlabels
                loss, nloss = loss.sum(), nloss.sum()
                loss, nloss = loss / nx / batch_size, nloss / nx / batch_size
                losses_tmp.append(loss)
                nlosses_tmp.append(nloss)

        losses.append(torch.sum(torch.stack(losses_tmp)))
        nlosses.append(torch.sum(torch.stack(nlosses_tmp)))

    losses = torch.stack(losses)
    nlosses = torch.stack(nlosses)

    mean, std = bootstrap(losses, 64, 1)
    nmean, nstd = bootstrap(nlosses, 64, 1)
    print(f'Unrolled forward losses: {mean:.4f} +- {std:.4f}')
    print(f'Unrolled forward losses (normalized): {nmean:.4f} +- {nstd:.4f}')

    return mean, std, nmean, nstd
```

Train the PDE solver

[48]:
```
from datetime import datetime
min_val_loss = 10e30
test_loss, ntest_loss = 10e30, 10e30
test_loss_std, ntest_loss_std = 0., 0.

# Log file and save path for model
dateTimeObj = datetime.now()
timestring = f'{dateTimeObj.date().month}{dateTimeObj.date().day}{dateTimeObj.time().
↪hour}{dateTimeObj.time().minute}'


save_path = f'FNO1d_KdV_future{time_future}_time{timestring}.pt'

for epoch in range(num_epochs):
    print(f"Epoch {epoch}")
    ################################################################
    # train model
    ################################################################
    model.train()
    #run every epoch (twice) as often as we have number of time steps in one trajectory
    for i in range(nt*2):
      losses = training_loop(train_loader, model, optimizer, criterion, device, batch_
↪size)
      if(i % print_interval == 0):
          print(f'Training Loss (progress: {i / (nt * 2):.2f}): {torch.mean(losses)}')

    ################################################################
    # evaluate model on validation data
```

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```
    ################################################################
    print("Evaluation on validation dataset:")
    model.eval()
    # Test the losses (full trajectory)
    val_loss, _, _, _ = test(valid_loader,model,criterion, device, batch_size)

    ################################################################
    # evaluate model on test
    ################################################################
    if(val_loss < min_val_loss):
        print("Evaluation on test dataset:")
        test_loss, test_loss_std, ntest_loss, ntest_loss_std = test(test_loader,model,
↪criterion, device, batch_size)
        # Save model
        torch.save(model.state_dict(), save_path)
        print(f"Saved model at {save_path}\n")
        min_val_loss = val_loss

    scheduler.step()
```

```
Epoch 0
Training Loss (progress: 0.00): 2225.366943359375
Training Loss (progress: 0.07): 317.81427001953125
Training Loss (progress: 0.14): 203.3621826171875
Training Loss (progress: 0.21): 130.92327880859375
Training Loss (progress: 0.29): 93.80006408691406
Training Loss (progress: 0.36): 68.2781982421875
Training Loss (progress: 0.43): 54.970794677734375
Training Loss (progress: 0.50): 47.671485900878906
Training Loss (progress: 0.57): 40.30413055419922
Training Loss (progress: 0.64): 31.2979793548584
Training Loss (progress: 0.71): 30.720670700073242
Training Loss (progress: 0.79): 27.46445083618164
Training Loss (progress: 0.86): 22.985952377319336
Training Loss (progress: 0.93): 20.814678192138672
Evaluation on validation dataset:
Unrolled forward losses: 4.6350 +- 0.5282
Unrolled forward losses (normalized): 5.8777 +- 0.4042
Evaluation on test dataset:
Unrolled forward losses: 3.5452 +- 0.3387
Unrolled forward losses (normalized): 5.2532 +- 0.2734
Saved model at FNO1d_KdV_future20_time4241851.pt
```

Predict Future time Step

Let's see how well our model performs compared to the underlying ground truth!

at the moment we are loading a model trained on 20 epochs, pulled from the github repo, if you want you can change the file path to the model you just trained in your notebook

[59]:
```
# load model
modelpath = 'models/FNO1d_KdV_samples512_future20_time424184.pt' #if you want, replace␣
↪with the model you just have trained!
model = FNO1d(modes=16, width=64, time_future=20, time_history=20).to(device)
model.load_state_dict(torch.load(modelpath,map_location = torch.device(device))) #if you␣
↪want replace with the model you trained!
model.eval()
```

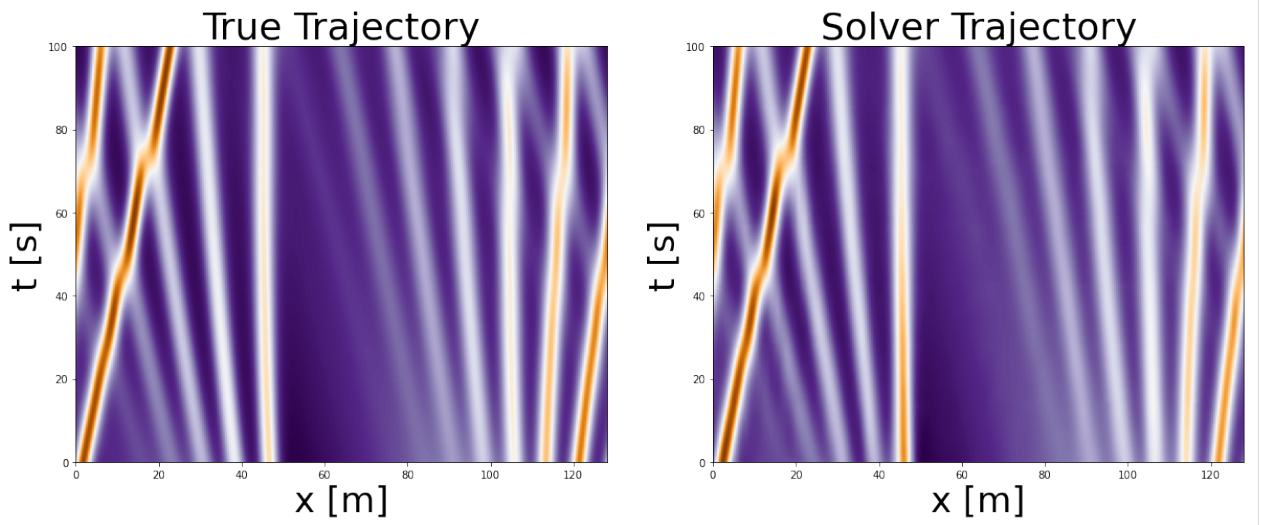
[59]:
```
FNO1d(
  (fc0): Linear(in_features=21, out_features=64, bias=True)
  (conv0): SpectralConv1d()
  (conv1): SpectralConv1d()
  (conv2): SpectralConv1d()
  (conv3): SpectralConv1d()
  (w0): Conv1d(64, 64, kernel_size=(1,), stride=(1,))
  (w1): Conv1d(64, 64, kernel_size=(1,), stride=(1,))
  (w2): Conv1d(64, 64, kernel_size=(1,), stride=(1,))
  (w3): Conv1d(64, 64, kernel_size=(1,), stride=(1,))
  (fc1): Linear(in_features=64, out_features=128, bias=True)
  (fc2): Linear(in_features=128, out_features=20, bias=True)
)
```

We will pass to our solver only the first 20 timesteps, after that the solver will predict autoregressively

[60]:
```
start = 0
end_time = 20
trajectory = np.zeros(shape=(140,256))


#sample from test and generate
with torch.no_grad():
  u, _, _ = next(iter(test_loader))
  true_trajectory = u[0]
  data = u[:1, start:end_time].to(device)
  trajectory[start:end_time,:] = torch.squeeze(data).cpu().detach().numpy()
  start += end_time
  end_time += time_future
  data = data.permute(0,2,1)
  while end_time <= 140:
    pred = model(data)
    data = pred
    trajectory[start:end_time,:] = torch.squeeze(data.permute(0,2,1)).cpu().detach().
↪numpy()
    start = end_time
    end_time += time_future
```

[61]:
```
#Plot True trajectory: produced by a numerical solver
# and Solver trajectory: produced by our NN
L=128
T=100
f, axarr = plt.subplots(1,2, figsize=(20,20))
axarr[0].set_title('True Trajectory', fontsize=36)
axarr[1].set_title('Solver Trajectory', fontsize=36)
axarr[0].imshow(true_trajectory, extent=[0,L,0,T], cmap='PuOr_r')
axarr[1].imshow(trajectory, extent=[0,L,0,T], cmap='PuOr_r')
axarr[0].set_xlabel('x [m]', fontsize=34)
axarr[0].set_ylabel('t [s]', fontsize=34)
axarr[1].set_xlabel('x [m]', fontsize=34)
axarr[1].set_ylabel('t [s]', fontsize=34);
```



Execute the above 2 cells multiple times: the trajectory will change as we are using next function on the test dataset. You can see how well the model performs on different initial conditions (different wave formations).

As you can see after visual inspection our trained NN performs quite well on multiple initial conditions of the given PDE. Often in the literature this is highlighted as the benefit of Neural PDE Solvers –> improved generalizability accross multiple initial conditions. However, I would take this with a bit of a grain of salt as in order to train this network we first actually had to use a numerical solver that generated all the trajectories for these different initial conditions.

Zero-Shot Resolution

We trained our network on 256 resolution of the spatial domain:

[62]:
```
u, _, _ = next(iter(train_loader))
print('Spatial resolution of training data: {}'.format(u[0].shape[1]))
print('Time resoltuion of training data: {}'.format(u[0].shape[0]))
```

```
Spatial resolution of training data: 256
Time resoltuion of training data: 140
```

Now let's see what happens if we input to our network a higher resolution, let's say **512**. We are going to keep the temporal resolution unchanged, 140

First let's generate such initial data and true trajectory by a numerical solver

We changed the parameter N –> it defines the resolution of our 128 length rod

[76]:
```
# Set the size of the domain, and create the discretized grid.
np.random.seed(3)
L = 128
N = 2**9
x = np.linspace(0, (1-1.0/N)*L, N)

# Set the tolerance of the solver
tol = 1e-6

# Set the initial conditions.
u0 = initial_conditions(x, L)

# Set the time sample grid.
T = 100.
t = np.linspace(0, T, 140)

# Compute the solution using kdv_pseudospectral as spatial solver
sol_ps_higher = solve_ivp(fun=kdv_pseudospectral,
                                t_span=[t[0], t[-1]],
                                y0=u0,
                                method='Radau',
                                t_eval=t,
                                args=(L,),
                                atol=tol,
                                rtol=tol)

true_trajectory_h = sol_ps_higher.y.T[::-1]
print('The spatial resolution {} and the temporal {}'.format(true_trajectory_h.shape[1],
↪true_trajectory_h.shape[0]))
```

```
The spatial resolution 512 and the temporal 140
```

Now let's use the first 20 timepoints as input to our network, and allow the network to predict the latter.

[89]:
```
start = 0
end_time = 20
trajectory_h = np.zeros(shape=(140,512))
correct_dir = np.flipud(true_trajectory_h)
trajectory_h[start:end_time,:] = correct_dir[start:end_time,:]

#take initial datapoints and generate the whole trajectory
with torch.no_grad():
  while start < 120:
    data = torch.from_numpy(correct_dir[start:end_time,:]).to(device)
    data = torch.unsqueeze(data, 0)
    data = data.permute(0,2,1)
    pred = model(data.float())
    start += 20
    end_time += 20
    trajectory_h[start:end_time,:] = torch.squeeze(pred.permute(0,2,1)).cpu().detach().
↪numpy()
```

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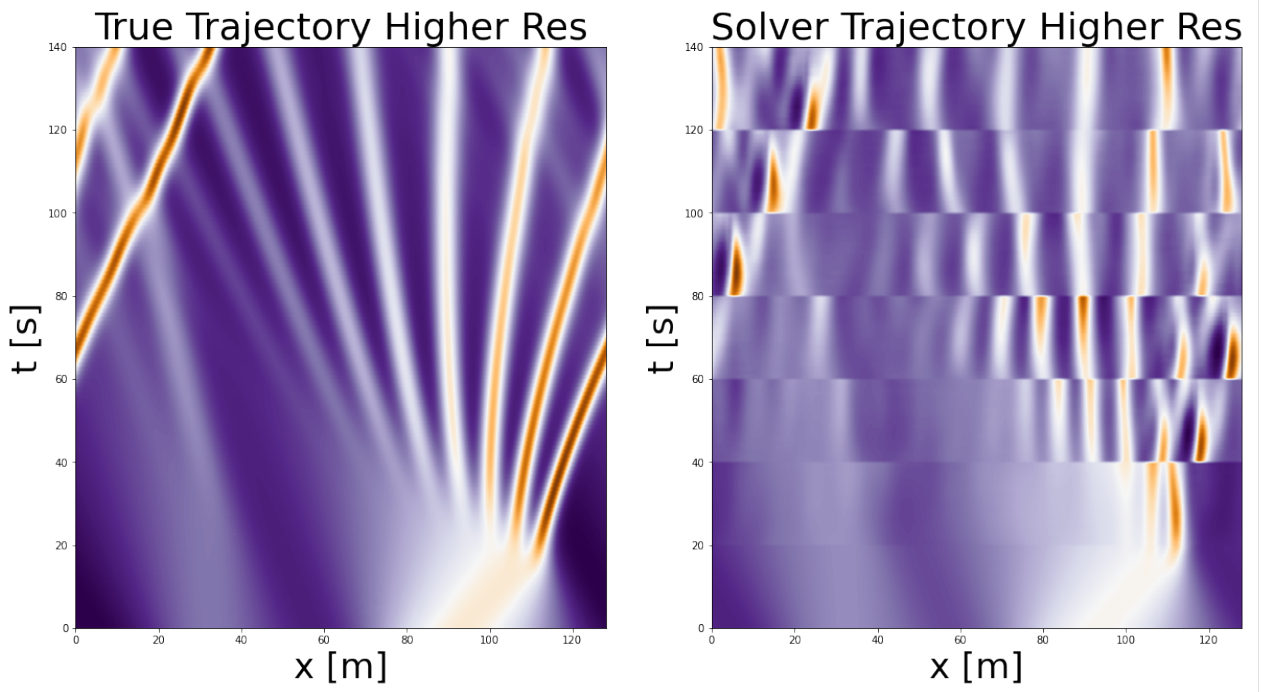
```
trajectory_h = np.flipud(trajectory_h)
```

[90]:
```
#Let's plot the true and predicted trajectory
L=128
T=140
f, axarr = plt.subplots(1,2, figsize=(20,20))
axarr[0].set_title('True Trajectory Higher Res', fontsize=36)
axarr[1].set_title('Solver Trajectory Higher Res', fontsize=36)
axarr[0].imshow(true_trajectory_h, extent=[0,L,0,T], cmap='PuOr_r')
axarr[1].imshow(trajectory_h, extent=[0,L,0,T], cmap='PuOr_r')
axarr[0].set_xlabel('x [m]', fontsize=34)
axarr[0].set_ylabel('t [s]', fontsize=34)
axarr[1].set_xlabel('x [m]', fontsize=34)
axarr[1].set_ylabel('t [s]', fontsize=34);
```



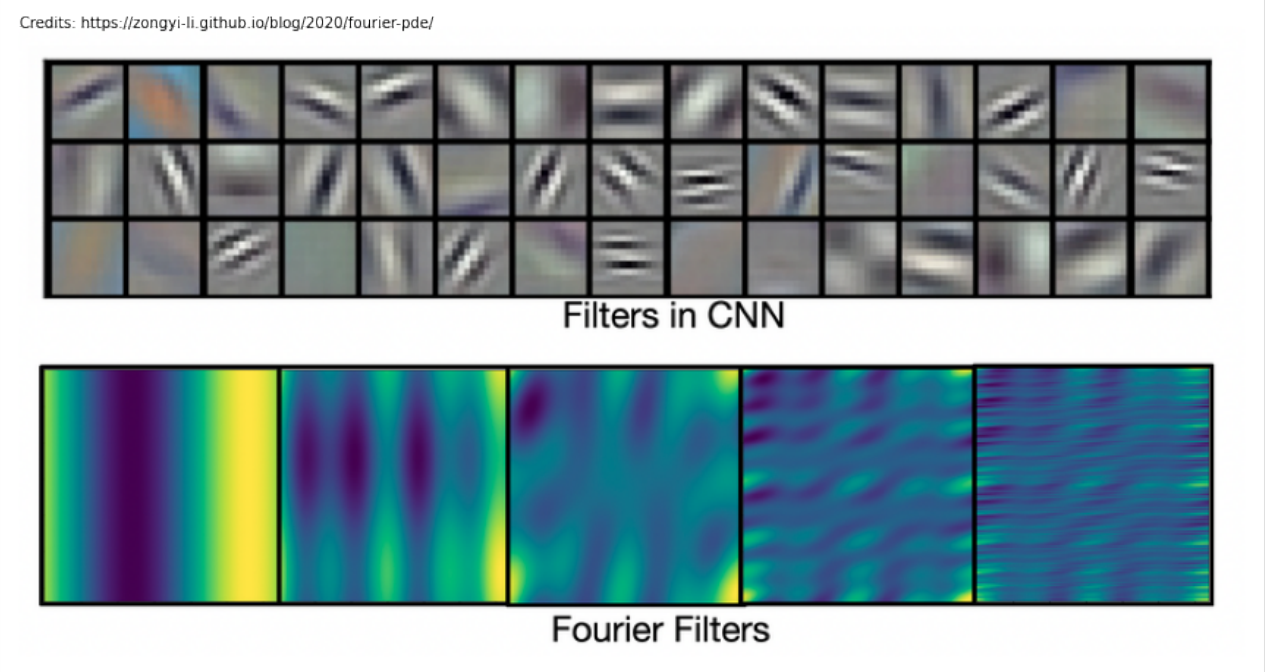
As we can see our PDE Solver is able to take as input higher resolution and also output higher resolution. As such, it has the quality of being **resolution-invariant**.

In the same time we see that the output of our predictions isn't too accurate. One way how we can improve this is by adding two additional channels as input, the spatial and temporal resolutions (dx and dt). For further details see the LPSDA paper

4.52.5 Fourier Filters compared to CNNs

One of the reasons proposed by Li et al. why fourier filters are more suited for dynamical problems than CNNs is because filters in convolution neural networks are usually local, while fourier filters are global sinusoidal functions. As such, CNNs are better in capturing local patterns such as edges and shapes, while fourier filters are better for representing continous functions (see image below).

[92]:
```
img_fourier = mpimg.imread('images/filters.png')
caption = "Credits: https://zongyi-li.github.io/blog/2020/fourier-pde/"
plt.figure(figsize=(15, 10))
plt.imshow(img_fourier)
plt.text(0, 0, caption, ha='left', fontsize=10)
plt.axis('off');
```



4.52.6 Related Work

Now, after reading all of this you might be wondering: *how did they think of fourier filter in the first place?*

Truth be told, the authors actually first tried multiple different neural operators: graph NO, multipole graph NO, low-rank NO, and from all of these the fourier NO turned out to be the most promising. However, it is quite interesting to think why so. Actually in math Fourier transform is often used to solve differential equations as it can reformulate them as problems that are easier to solve. Hence, intuitively it makes sense that also for neural networks –> operating on a problem in fourier space might be easier.

The paper, based on which this tutorial was created, was published in ICLR 2020. Since then more researchers have built upon this topic. Here I would like to highlight some of them:

- Message Passing: uses a different underlying architecture but has nice tricks for longer/more stable rollouts
- LEADS: Model generalization across environements
- Factorized FNO: this paper implements well known tricks from deep learning in order to create deeper FNO architectures

- Lie Point Symmetry: this paper uses pre-existing knowledge of PDE symmetries to improve generalizability and rollouts

4.52.7 Investigate Yourself

I hope that after this tutorial you have gotten more curious about modelling dynamical systems, as well as we have broaden your perspective on deep learning possibilities!

Below are a few things that you can try to change in the code to play around with it:

- Simply play around with the parameters: number of modes to keep, hidden layer size, the depth of your network etc. How does that affect your output?
- Implement a CNN, how does it perform in comparison?
- What happens for very long rollouts?
- How does the model trained on KdV perform on a different PDE? Is it able to generlize?
- We were working on a 1d problem, can you adjust it to 2d?

4.52.8 Acknowledgements

This tutorial was inspired/based upon on the following great resources:

- Z.Li Blogpost
- J.Brandsetter github

4.53 DS - Dynamical Systems & Neural ODEs

Filled notebook:
Empty notebook:
Authors: Riccardo Valperga (Part 1) & Miltos Kofinas (Part 2)

4.53.1 0. Introduction

This is a tutorial on dynamical systems, Ordinary Differential Equations (ODEs) and numerical solvers, and Neural Ordinary Differential Equations (Neural ODEs).

Below, we import our standard libraries. In this tutorial, we will use PyTorch Lightning. Additionally, we will use the ODE solvers from Torchdiffeq. You don't need to use GPUs for this tutorial, you can run the entire codebase in a CPU.

[ ]:
```
%matplotlib inline
import time
import logging
import statistics
from typing import Optional, List

import numpy as np
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
from mpl_toolkits.mplot3d import Axes3D
```

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```
from matplotlib.animation import FuncAnimation
from IPython.display import HTML

import torch
import torch.nn as nn
import torch.utils.data as data
import torch.nn.functional as F
from torch.utils.data import Dataset

try:
    import torchdiffeq
except ModuleNotFoundError:
    !pip install --quiet torchdiffeq
    import torchdiffeq

try:
    import rich
except ModuleNotFoundError:
    !pip install --quiet rich
    import rich

try:
    import pytorch_lightning as pl
except ModuleNotFoundError:
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl
from torchmetrics.classification import Accuracy

pl.seed_everything(42)

torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(f"Device: {device}")
```

```
     || 229 kB 4.4 MB/s
     || 51 kB 5.0 MB/s


Global seed set to 42
```

```
Device: cpu
```

Dynamical Systems Primer

The most accurate definition of dynamical system is the following:

A dynamical system is a triple

$$(\mathcal{S}, \mathcal{T}, \Phi)$$

where - $\mathcal{S}$ is the *state space* - $\mathcal{T}$ is the *parameter space*, and - $\Phi : (\mathcal{T} \times \mathcal{S}) \longrightarrow \mathcal{S}$ is the evolution.

Some notes: - This is a very general definition that includes all sort of dynamical systems that you might encounter. - In this tutorial we deal with ODEs where Φ plays the role of the *general solution*: indeed a 1-parameter family of transformations of the state space. $\mathcal{T} = \mathbb{R}_+$ is the time, and usually, $\mathcal{S} = \mathbb{R}^n$ is the state space. The evolution takes a point in space (initial value), a point in time, and returns the a point in space. This is the concept of a *flow*.

4.53.2 1. Differential Equations

We will deal with *initial value problems* (IVP) defined by a first-order ODE, and an initial value:

$$\dot{y} = f(y, t), \quad y(t_0) = y_0,$$

where we use the shorthand notation $\dot{y} := \frac{\mathrm{d}y}{\mathrm{d}t}$ common in physics.

A general solution to an ODE is a function $y : I \times \mathbb{R}^n\mathbb{R}^n$: a 1-parameter (usually time is the parameter) family of transformations of the state space. A 1-parameter family of transformations is often called a *flow*. The existence and uniqueness of solutions to an IVP is ensured by the Picard-Lindelöf theorem, provided the RHS of the ODE is *Lipschitz continuous*. Lipschitz continuity is a property that pops up quite often in ODE-related results in ML so we provide a definition here:

A function $f : X \subset \mathbb{R}^n\mathbb{R}^n$ is called *Lipschitz continuous* (with constant λ) if

$$||f(x_1) - f(x_2)|| \leq \lambda ||x_1 - x_2|| \quad \forall x_1, x_2 \in X.$$

Note that this is a stronger condition than just continuity.

The rest of the tutorial is dedicated to numerical integration methods for finding solutions to IVPs.

Euler method

Solving differential equations analytically is not an option for complicated fs, given, for example, by neural networks. We need numerical solvers. Runge-Kutta methods are a family of iterative methods that find approximate solutions to IVPs. We will start with the simplest and most intuitive Runge-Kutta method, the **Euler** method.

Consider the IVP

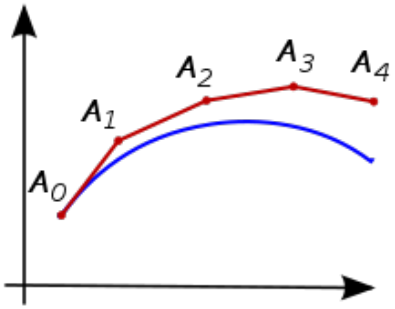
$$\dot{y} = f(y, t), \quad y(t_0) = y_0.$$

where $y(t_0)$, and f are given.

Pick a step-size $h > 0$, a number of steps N, and define

$$y_{n+1} = y_n + hf(y_n, t_n)$$
$$t_{n+1} = t_n + h.$$

This is the most basic numerical integrator. One intuition behind the Euler method is that we are evolving the trajectories by iteratively taking small steps in the direction of the slope.



(Figure credit: Wikipedia)

Derivation

The mathematical explanation behind that intuition can be derived by taking the forward finite difference formula for the derivative:

$$\dot{y}(t_0) = \lim_{h \to 0} \frac{y(t_0 + h) - y(t_0)}{h} \approx \frac{y(t_0 + h) - y(t_0)}{h}.$$

By rearranging the terms, we can derive the forward Euler method.

We can also explain how this method works by considering the Taylor expansion of the solution $y(t)$ around t_{n+1}

$$y(t_{n+1}) = y(t_n) + h \frac{\mathrm{d}y}{\mathrm{d}t}\Big|_{t_n} + O\big(h^2\big),$$

and using the fact that $\frac{\mathrm{d}y}{\mathrm{d}t}\big|_{t_n} = \dot{y}_{t_n} = f(y_n, t_n)$. We are left with

$$y(t_{n+1}) = y(t_n) + hf(y_n, t_n) + O\big(h^2\big),$$

which is precisely the Euler method step above.

Runge-Kutta Methods

Euler method is the simplest numerical integrator in a family of methods known as Runge-Kutta methods. Here we describe the RK4 method.

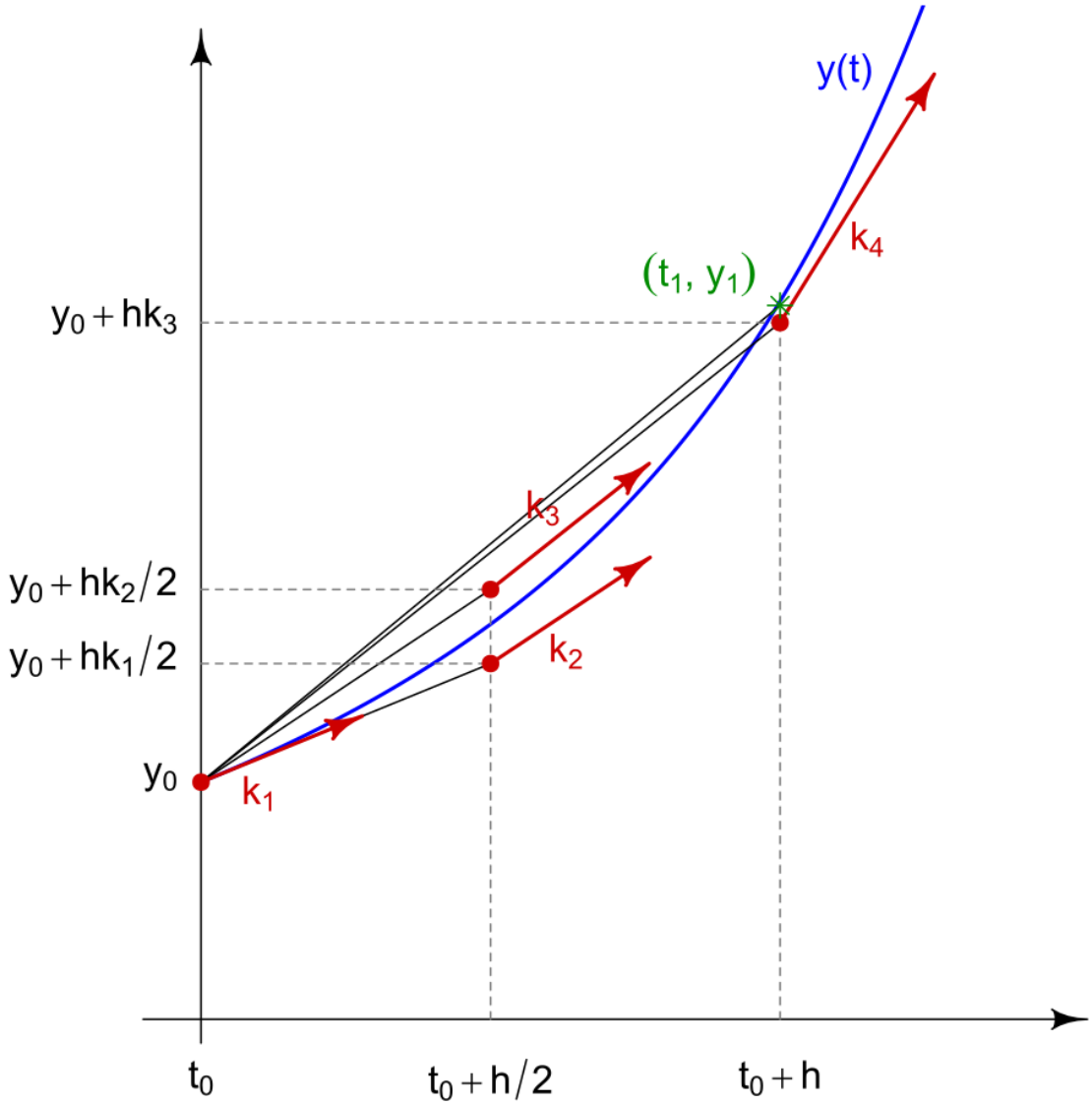
Consider the same IVP as above. Again, pick a step-size $h > 0$, a number of steps N, and define

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{6} h(k_1 + 2k_2 + 2k_3 + k_4) \\ t_{n+1} &= t_n + h \end{aligned}$$

for $n = 0, 1, 2, 3, \ldots, N$ with

$$\begin{aligned} k_1 &= f\left(y_n, t_n\right) \\ k_2 &= f\left(y_n + h\frac{k_1}{2}, t_n + \frac{h}{2}\right) \\ k_3 &= f\left(y_n + h\frac{k_2}{2}, t_n + \frac{h}{2}\right) \\ k_4 &= f\left(y_n + hk_3, t_n + h\right). \end{aligned}$$

NB: As you probably noticed, Euler method is just RK4 but considering only k_1.



(Figure credit: Wikipedia)

Intuition

Here we give an intuitive explanation of why this method approximates solutions to IVPs. As with the Euler method, we will use the Taylor expansion of the solution.

Let $y(t)$ be the solution. Let us wite the Taylor expansion of $y(t)$ in the neighborhood of t_n to the h^2 term:

$$y(t_{n+1}) = y(t_n) + h\frac{dy}{dt}\Big|_{t_n} + \frac{h^2}{2}\frac{d^2y}{dt^2}\Big|_{t_n} + O(h^3).$$

we know that $\frac{dy}{dt}\big|_{t_n} = f(y_n, t_n)$ and therefore

$$\frac{d^2y}{dt^2}\Big|_{t_n} = \frac{df(y,t)}{dt}\Big|_{t_n} = \frac{\partial f}{\partial t}\Big|_{t_n} + f\frac{\partial f}{\partial y}\Big|_{t_n},$$

where we used the chain rule. The Taylor expansion becomes

$$y(t_{n+1}) = y(t_n) + hf(y_n, t_n) + \frac{h^2}{2}\left[\frac{\partial f}{\partial t}\Big|_{t_n} + f\frac{\partial f}{\partial y}\Big|_{t_n}\right] + O\big(h^3\big).$$

If we look at k_2 we can Taylor expand it correctly to $O\big(h^3\big)$ as

$$k_2 = f(y_n + \beta k_1, t_n + \alpha h) = h\left(f(y_n, t_n) + \alpha h\frac{\partial f}{\partial t}\Big|_{t_n} + \beta f\frac{\partial f}{\partial y}\Big|_{t_n}\right) + O\big(h^3\big),$$

which is precisely the third term in the Taylor expansion of $y(t_n)$. Comparing with the previous equation we find conditions on α and β. Note that the value of these coefficients depends on the order to which we decide to stop. Higher order coefficients can be computed in the same way.

Approximation errors

This method is called *classic Runge-Kutta* or *RK4*. This is a fourth-order method meaning that the *local truncation error* is of order $O\big(h^5\big)$, and the *total truncation error* is of order $O\big(h^4\big)$. Local truncation and total accumulation errors are defined as follows:

For a one-step integration method, such as RK4, of form

$$y_{n+1} = y_n + hA(y_n, t_n, h, f),$$

the *local truncation error* at time t_{n+1}, τ_{n+1} is

$$\tau_{n+1} = y(t_{n+1}) - y(t_n) - hA(y_n, t_n, h, f).$$

The *total truncation error* at time t_{n+1}, e_{n+1} is

$$e_{n+1} = y(t_{n+1}) - (y_0 + hA(y_0, t_0, h, f) + \cdots + hA(y_n, t_n, h, f)).$$

Example: Lotka-Volterra equations

Consider the IVP

$$\dot{x} = x - xy$$
$$\dot{y} = xy - y,$$

with initial value $(x_0, y_0) = (1, 2)$. There is no closed form solution to this system of ODEs. We compare performances of RK4 and simple Euler for different values of step-size h.

[ ]:
```
def LV(x, y):
  return np.array([x - x*y, x*y - y])

def rk4(f, x0, y0, h, n):

    v = [0]*(n+1)
    v[0] = np.array([x0, y0])
```

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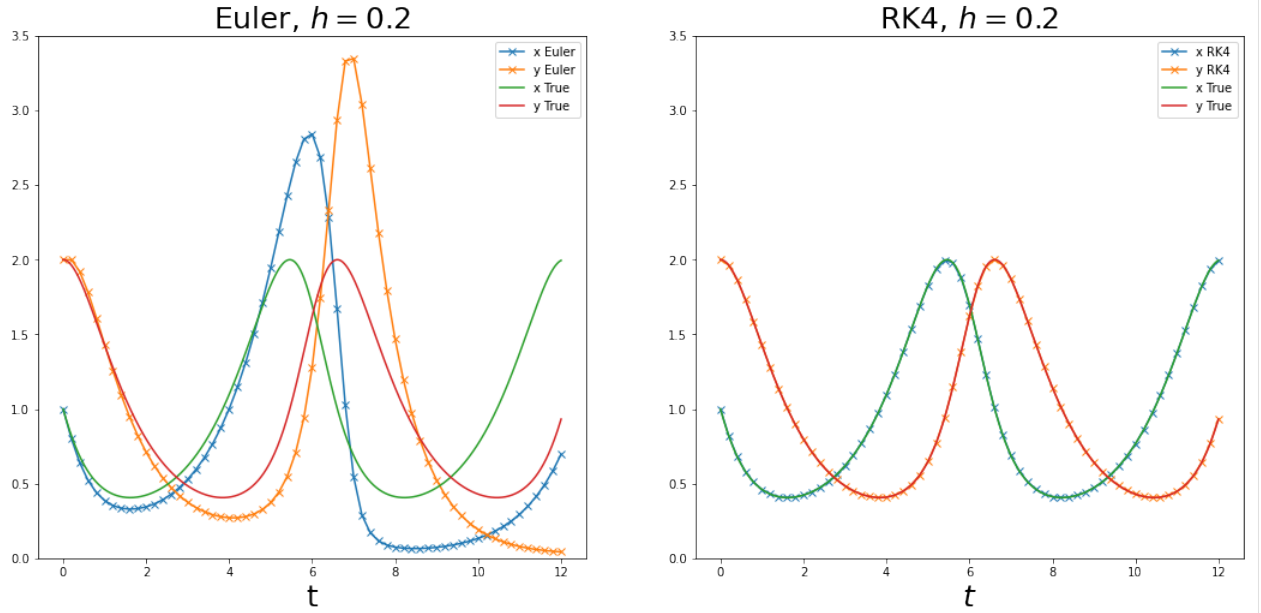
```
    x = x0
    y = y0
    for i in range(1, n + 1):
        k1 = h*f(x, y)
        k2 = h*f(x + 0.5*k1[0], y + 0.5*k1[1])
        k3 = h*f(x + 0.5*k2[0], y + 0.5*k2[1])
        k4 = h*f(x + k3[0], y + k3[1])
        v[i] =  v[i-1] + (k1 + k2 + k2 + k3 + k3 + k4)/6
        x = v[i][0]
        y = v[i][1]

    t = np.array([i*h for i in range(0, n+1)])
    return t, np.array(v)

def euler(f, x0, y0, h, n):

    v = [0]*(n+1)
    v[0] = np.array([x0, y0])
    x = x0
    y = y0

    for i in range(1, n + 1):
        v[i] =  v[i-1] + h*f(x, y)
        x = v[i][0]
        y = v[i][1]

    t = np.array([i*h for i in range(0, n+1)])
    return t, np.array(v)

def plot_integrator(v_euler, v_rk4, t_euler, t_rk4, v_true, t_true, h):

    fig = plt.figure(figsize=(18,8))
    ax0 = fig.add_subplot(121)
    ax1 = fig.add_subplot(122)

    ax0.plot(t_euler, v_euler, marker = 'x')
    ax1.plot(t_rk4, v_rk4, marker = 'x')

    ax0.plot(t_true, v_true)
    ax1.plot(t_true, v_true)

    ax0.set_ylim(0, 3.5)
    ax1.set_ylim(0, 3.5)

    ax0.set_xlabel(r"t", fontsize=25)
    ax0.set_title("Euler, $h=$"+h, fontsize=25)
    ax0.legend(["x Euler", "y Euler", "x True", "y True"])
    ax1.set_xlabel(r"$t$", fontsize=25)
    ax1.set_title("RK4, $h=$"+h, fontsize=25)
    ax1.legend(["x RK4", "y RK4", "x True", "y True"])
```

[ ]:
```
h = 0.2

t_euler, v_euler = euler(LV, 1., 2., h, 60)
t_rk4, v_rk4 = rk4(LV, 1., 2., h, 60)
t_true, v_true = rk4(LV, 1., 2., 0.003, 4000)

plot_integrator(v_euler, v_rk4, t_euler, t_rk4, v_true, t_true, str(h))
```



Phase space and phase portrait

It is useful to introduce the concept of phase space and phase portrait. Let us consider the differential equation of the simple pendulum of mass 1, length 1, and g set to 1 for convenience:

$$\ddot{\theta} + \sin\theta = 0.$$

This is a second-order ODE, but it can be transformed in the following equivalent system of first-order ODEs by introducing the auxiliary variable $p_\theta = \dot{\theta}$:

$$\begin{aligned} \dot{\theta} &= p_\theta \\ \dot{p_\theta} &= -\sin(\theta) \end{aligned} \tag{4.99}$$

$S^1 \times \mathbb{R}$ is called the *phase space*, and $(\theta, p_\theta) \in S^1 \times \mathbb{R}$ are called *phase space variables* (θ is periodic and therefore lives in $S^1 = \{x \mod 2\pi | x \in \mathbb{R}\}$).

Given a solution $(\theta(t), p_\theta(t))$ we can represent it as a path in the phase space $S^1 \times \mathbb{R}$:

[ ]:
```
def pendulum(x, y):
  return np.array([y, -np.sin(x)])

def plot_phase_space(v):

    fig = plt.figure(figsize=(10,6))
```

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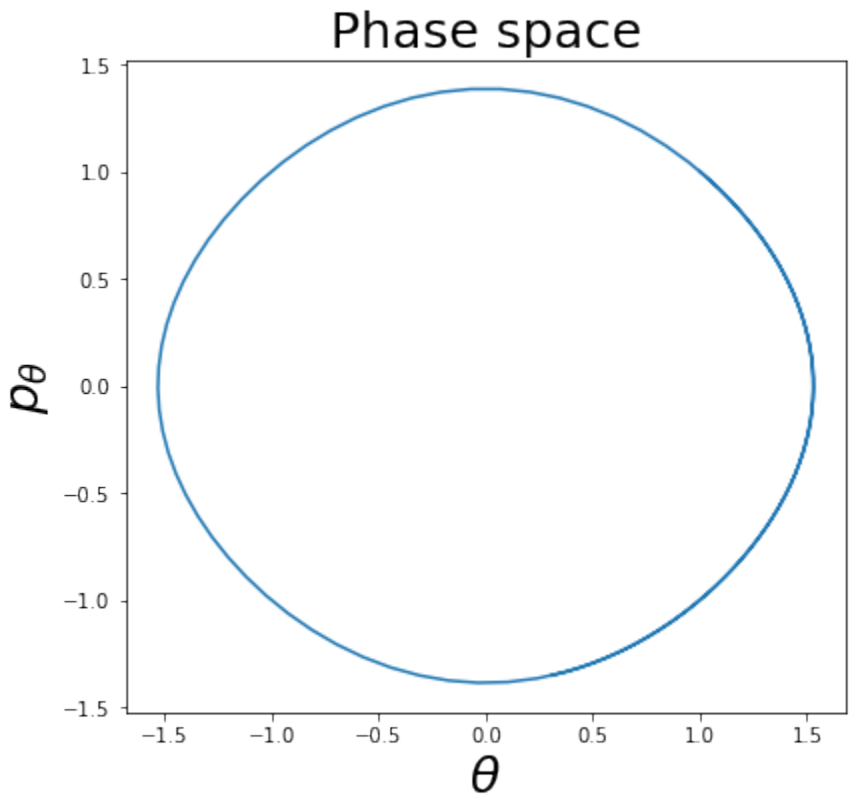
```
    ax0 = fig.add_subplot(111)

    ax0.plot([p[0] for p in v], [p[1] for p in v])

    ax0.set_xlabel(r"$\theta$", fontsize=25)
    ax0.set_ylabel(r"$p_{\theta}$", fontsize=25)
    ax0.set_title("Phase space", fontsize=25)
    ax0.set_aspect('equal')
```

[ ]:
```
t_pendulum, v_pendulum = rk4(pendulum, 1., 1., 0.1, 100)
plot_phase_space(v_pendulum)
```



A collection of paths in the phase space is called *phase space portrait* (or phase space diagram, or sometimes state space diagram), which can be thought as a geometric representation of the trajectories (here solutions of a system of ODEs) of a dynamical system in the phase plane. In a phase space portrait each initial conditions is represented by a different curve, or in the case of trivial solution (such as $(0, 0)$ in our example) a point.

[ ]:
```
def plot_phase_space_pendulum(V):

    fig = plt.figure(figsize=(18,8))
    ax0 = fig.add_subplot(121)
    for v in V:
      ax0.plot([p[0] for p in v], [p[1] for p in v], color='b')

    ax0.set_xlabel(r"$\theta$", fontsize=25)
    ax0.set_ylabel(r"$p_{\theta}$", fontsize=25)
```

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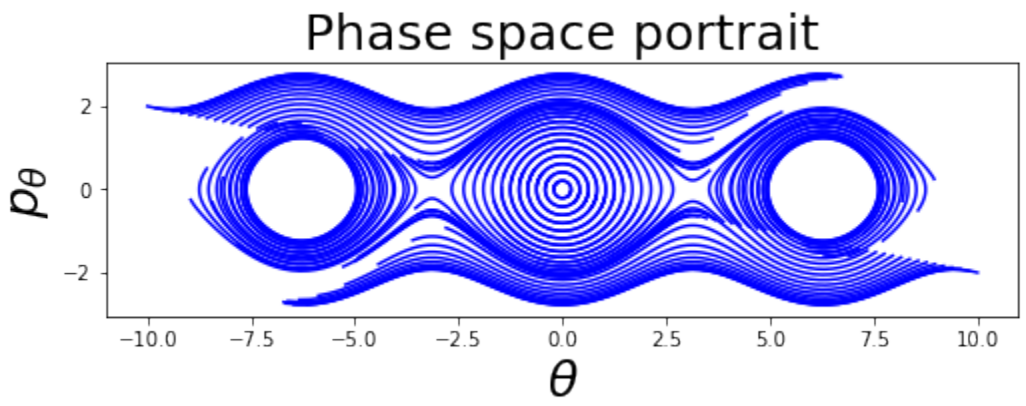
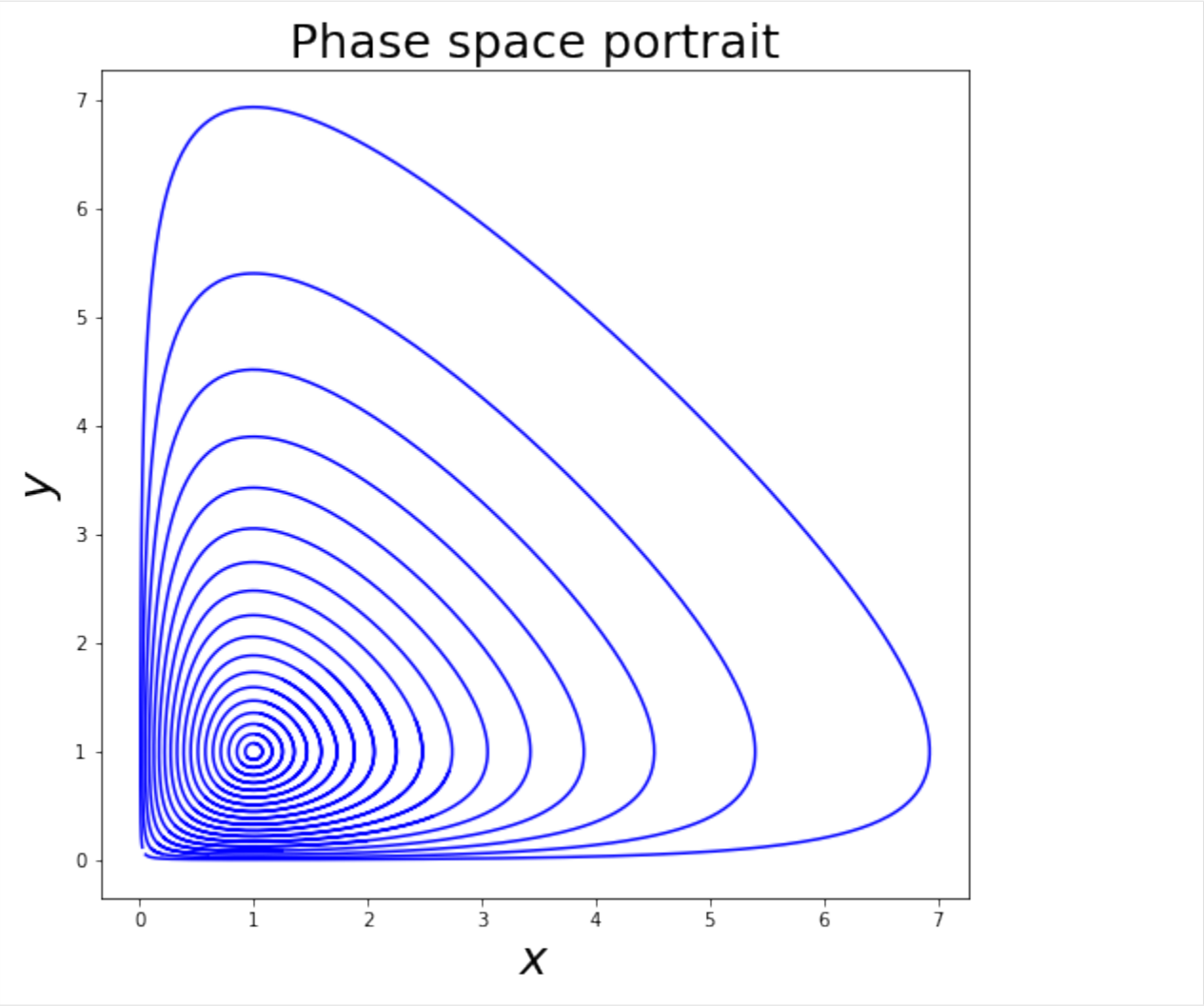
```
    ax0.set_title("Phase space portrait", fontsize=25)
    ax0.set_aspect('equal')

def plot_phase_space_LV(V):

    fig = plt.figure(figsize=(18,8))
    ax0 = fig.add_subplot(121)
    for v in V:
      ax0.plot([p[0] for p in v], [p[1] for p in v], color='b')

    ax0.set_xlabel(r"$x$", fontsize=25)
    ax0.set_ylabel(r"$y$", fontsize=25)
    ax0.set_title("Phase space portrait", fontsize=25)
```

[ ]:
```
IV = [[5*i, -i] for i in np.linspace(-2, 2, 99)] # initial values
paths = []
for iv in IV:
  t, v = rk4(pendulum, iv[0], iv[1], 0.1, 70)
  paths.append(v)

plot_phase_space_pendulum(paths)
```



We can plot the phase space of the Lotka-Volterra system.

[ ]:
```
IV = [[i, i] for i in np.linspace(0, 1, 20)] # initial values
paths = []
for iv in IV:
  t, v = rk4(LV, iv[0], iv[1], 0.01, 1000)
  paths.append(v)

plot_phase_space_LV(paths)
```



4.53.3 2. Neural ODEs

Introduction

Given the intriguing properties of ODEs/solvers and the centuries-long literature on the topic, it seems intriguing to combine them with neural networks, i.e. try to model the transition function with a neural network. This combination could yield a powerful modelling tool, since neural networks are universal function approximators —they can in theory approximate any differentiable function to an arbitrary precision.

Remembering our earlier definitions, we have a first-order ODE:

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t), \theta), \quad \mathbf{y}(t_0) = y_0, \quad f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$$

Our goal is to solve initial value problems (IVP), i.e. predict $\mathbf{y}(t_1)$ given $\mathbf{y}(t_0)$.

$$\mathbf{y}(t_1) = \mathbf{y}(t_0) + \int_{t_0}^{t_1} f(\mathbf{y}(t), t, \theta) \mathrm{d}t = \text{ODESolve}(\mathbf{y}(t_0), f, t_0, t_1, \theta)$$

We can use a numerical solver to perform the forward pass and solve the IVP. If we use, for example, Euler's method,

we have the following update rule:

$$\mathbf{y}(t+h) = \mathbf{y}(t) + hf(\mathbf{y}(t), t)$$

This formula looks almost identical to a ResNet block, and this was one of the main motivations for Neural ODEs.

Comparison to Resnets

Many popular deep learning architectures like ResNets[2] update hidden states by employing residual connections:

$$\mathbf{y}_{l+1} = \mathbf{y}_l + f(\mathbf{y}_l, \theta_l)$$

where f is a neural network with parameters θ_l, and $\mathbf{y}_l$ and $\mathbf{y}_{l+1}$ are the hidden states at subsequent layers, $l \in \{0, \ldots, L\}$.

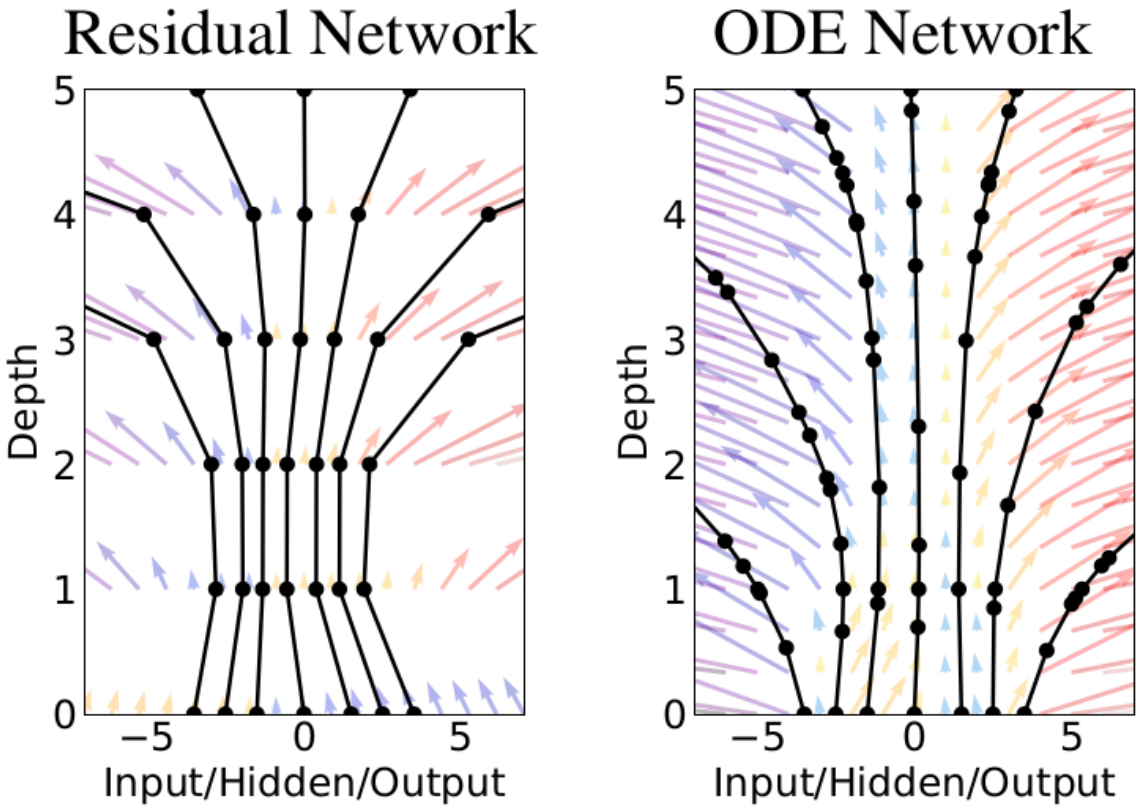
These updates can be seen as Euler discretizations of continuous transformations.

$$\dot{\mathbf{y}} = f(\mathbf{y}, t, \theta) \tag{4.101}$$

$$\downarrow \text{ Euler Discretization} \tag{4.102}$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + hf(\mathbf{y}_n, t_n, \theta) \tag{4.103}$$

Circling back to the continuous realm again, what happens in a residual network (with step sizes h) if we consider the continuous limit of each discrete layer in the network? In other words, what happens as we add more layers and take smaller steps? The answer seems rather astounding: instead of having a discrete number of layers between the input and output domains, we allow the evolution of the hidden states to become continuous!



(Figure credit: https://arxiv.org/abs/1806.07366)

[2] He, Kaiming, et al. "**Deep residual learning for image recognition**". CVPR 2016. https://arxiv.org/abs/1512.03385

Backpropagation

We now have a way to perform the forward pass for our model. How do we backpropagate and train the network, though?

One very straightforward way to perform backprop is to to back-propagate through the solver. This would work since the forward pass operations are continuous and differentiable. The problem, however, is that this incurs a high-memory cost and we would need to save all intermediate activations of the solver.

More importantly, though, our goal should be to try to approximate the exact derivative, rather than differentiating the approximation.

We want to optimize our scalar-valued loss function L with respect to the model parameters θ.

$$L(\mathbf{x}(t_1)) = L\left(\mathbf{x}(t_0) + \int_{t_0}^{t_1} f(\mathbf{x}(t), t, \theta)\mathrm{d}t\right) = L\left(\text{ODESolve}(\mathbf{x}(t_0), f, t_0, t_1, \theta)\right)$$

To optimize L we require gradients with respect to θ. The problem is to efficiently calculate $\frac{\mathrm{d}L(\mathbf{x}(t_1))}{\mathrm{d}\theta}$ without storing all the function activations from the forward pass. **Adjoint method to the rescue**! The adjoint sensitivity method was developed in 1962 by Pontryagin et al.[1] It leverages the fact that the forward pass is the solution to an ODE, and computes gradients by solving a second, augmented ODE backwards in time.

Similar to standard neural networks, we start with determining how the gradient of the loss depends on the hidden state. This quantity is called the *adjoint* $\mathbf{a}(t) = \frac{\partial L}{\partial \mathbf{x}(t)}$. It satisfies the following IVP:

$$\dot{\mathbf{a}}(t) = -\mathbf{a}(t)^\top \frac{\partial f(\mathbf{x}(t), t, \theta)}{\partial \mathbf{x}}, \quad \mathbf{a}(t_1) = \frac{\partial L}{\partial \mathbf{x}(t_1)}.$$

Thus, starting from the initial (remember we are running backwards) value $\mathbf{a}(t_1) = \frac{\partial L}{\partial \mathbf{x}(t_1)}$, we can compute $\mathbf{a}(t_0) = \frac{\partial L}{\partial \mathbf{x}(t_0)}$ by another call to an ODE solver.

Finally, computing the gradients with respect to the parameters θ requires evaluating a third integral, which depends on both $\mathbf{x}(t)$ and $\mathbf{a}(t)$:

$$\frac{\mathrm{d}L}{\mathrm{d}\theta} = -\int_{t_1}^{t_0} \mathbf{a}(t)^\top \frac{\partial f}{\partial \theta}\mathrm{d}t,$$

So this method trades off computation for memory – in fact the memory requirement for this gradient calculation is $\mathcal{O}(1)$ with respect to the number of layers!

Here you can find a very good explanation of the following result based on Lagrange multipliers:

[1] Pontryagin, L.S. et al. "**The mathematical theory of optimal processes**". 1962

The full algorithm for *reverse mode auto-differentiation* is as follows:

Algorithm 1 Reverse-mode derivative of an ODE initial value problem

Input: dynamics parameters θ, start time t_0, stop time t_1, final state $\mathbf{z}(t_1)$, loss gradient $\partial L / \partial \mathbf{z}(t_1)$

$s_0 = [\mathbf{z}(t_1), \frac{\partial L}{\partial \mathbf{z}(t_1)}, \mathbf{0}_{|\theta|}]$ ▷ Define initial augmented state

def aug_dynamics($[\mathbf{z}(t), \mathbf{a}(t), \cdot], t, \theta$): ▷ Define dynamics on augmented state

  return $[f(\mathbf{z}(t), t, \theta), -\mathbf{a}(t)^\intercal \frac{\partial f}{\partial \mathbf{z}}, -\mathbf{a}(t)^\intercal \frac{\partial f}{\partial \theta}]$ ▷ Compute vector-Jacobian products

$[\mathbf{z}(t_0), \frac{\partial L}{\partial \mathbf{z}(t_0)}, \frac{\partial L}{\partial \theta}] = \text{ODESolve}(s_0, \text{aug\_dynamics}, t_1, t_0, \theta)$ ▷ Solve reverse-time ODE

return $\frac{\partial L}{\partial \mathbf{z}(t_0)}, \frac{\partial L}{\partial \theta}$ ▷ Return gradients

(Figure credit: https://arxiv.org/abs/1806.07366)

Time to program some Neural ODEs

In this tutorial we will be working will Half Moons Dataset, a non-linearly separable, binary classification dataset.

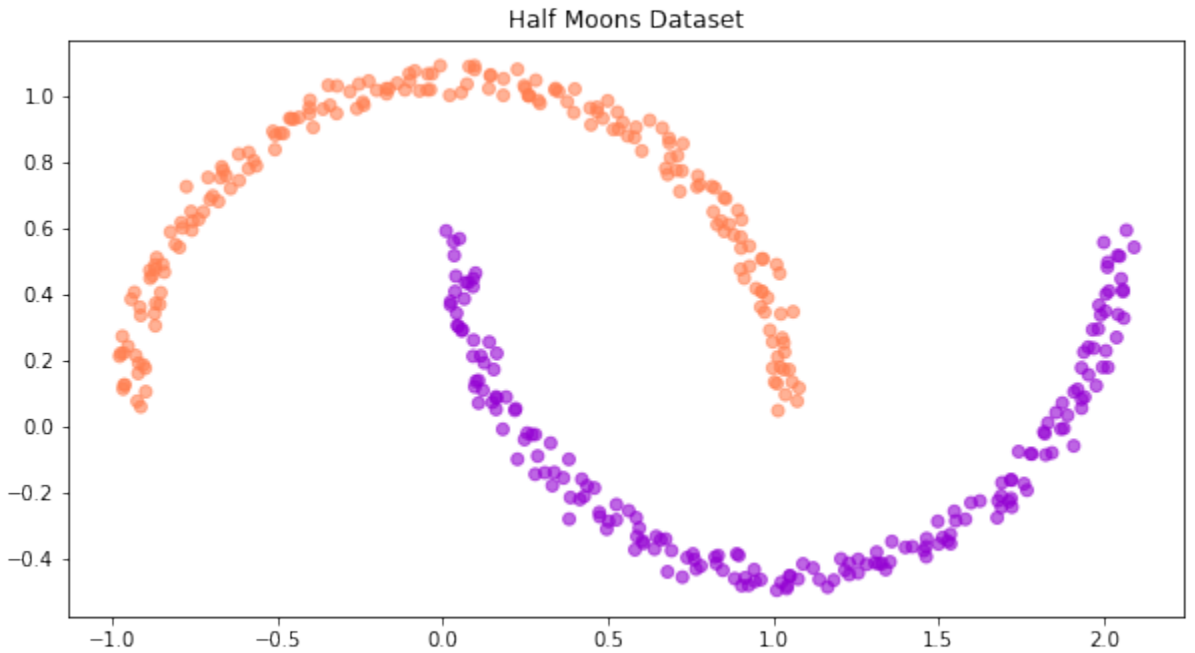
This tutorial has been based on the excellent TorchDyn tutorials (https://github.com/DiffEqML/torchdyn), as well as the original TorchDiffEq examples (https://github.com/rtqichen/torchdiffeq).

[ ]:
```
class MoonsDataset(Dataset):
    """Half Moons Classification Dataset

    Adapted from https://github.com/DiffEqML/torchdyn
    """
    def __init__(self, num_samples=100, noise_std=1e-4):
        self.num_samples = num_samples
        self.noise_std = noise_std
        self.X, self.y = self.generate_moons(num_samples, noise_std)

    @staticmethod
    def generate_moons(num_samples=100, noise_std=1e-4):
        """Creates a *moons* dataset of `num_samples` data points.
        :param num_samples: number of data points in the generated dataset
        :type num_samples: int
        :param noise_std: standard deviation of noise magnitude added to each data point
        :type noise_std: float
        """
        num_samples_out = num_samples // 2
        num_samples_in = num_samples - num_samples_out
        theta_out = np.linspace(0, np.pi, num_samples_out)
        theta_in = np.linspace(0, np.pi, num_samples_in)
        outer_circ_x = np.cos(theta_out)
        outer_circ_y = np.sin(theta_out)
        inner_circ_x = 1 - np.cos(theta_in)
        inner_circ_y = 1 - np.sin(theta_in) - 0.5

        X = np.vstack([np.append(outer_circ_x, inner_circ_x),
                       np.append(outer_circ_y, inner_circ_y)]).T
        y = np.hstack([np.zeros(num_samples_out), np.ones(num_samples_in)])

        if noise_std is not None:
            X += noise_std * np.random.rand(num_samples, 2)

        X = torch.Tensor(X)
        y = torch.LongTensor(y)
        return X, y

    def __len__(self):
        return self.num_samples

    def __getitem__(self, idx):
        return self.X[idx], self.y[idx]
```

[ ]:
```
def plot_binary_classification_dataset(X, y, title=None):
    CLASS_COLORS = ['coral', 'darkviolet']
    fig, ax = plt.subplots(figsize=(10, 10))
    ax.scatter(X[:, 0], X[:, 1], color=[CLASS_COLORS[yi.int()] for yi in y], alpha=0.6)
    ax.set_aspect('equal')
    if title is not None:
        ax.set_title(title)

    return fig, ax
```

Let's create a sample dataset and visualize it.

[ ]:
```
sample_dataset = MoonsDataset(num_samples=400, noise_std=1e-1)
fig, ax = plot_binary_classification_dataset(sample_dataset.X, sample_dataset.y, title=
↪'Half Moons Dataset')
```



Let's now create the train, validation, and test sets, with their corresponding data loaders. We will create a single big dataset and randomly split it in train, val, and test sets.

[ ]:
```
def split_dataset(dataset_size:int, split_percentages:List[float]) -> List[int]:
    split_sizes = [int(pi * dataset_size) for pi in split_percentages]
    split_sizes[0] += dataset_size - sum(split_sizes)
    return split_sizes


class ToyDataModule(pl.LightningDataModule):
    def __init__(self, dataset_size:int, split_percentages:Optional[float]=None):
        super().__init__()
        self.dataset_size = dataset_size
        if split_percentages is None:
            split_percentages = [0.8, 0.1, 0.1]
```

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```
        self.split_sizes = split_dataset(self.dataset_size, split_percentages)

    def prepare_data(self):
        pass

    def setup(self, stage: Optional[str] = None):
        pass

    def train_dataloader(self):
        train_loader = torch.utils.data.DataLoader(self.train_set, batch_size=len(self.
↪train_set), shuffle=True)
        return train_loader

    def val_dataloader(self):
        val_loader = torch.utils.data.DataLoader(self.val_set, batch_size=len(self.val_
↪set), shuffle=False)
        return val_loader

    def test_dataloader(self):
        test_loader = torch.utils.data.DataLoader(self.test_set, batch_size=len(self.
↪test_set), shuffle=False)
        return test_loader


class HalfMoonsDataModule(ToyDataModule):
    def __init__(self, dataset_size:int, split_percentages:Optional[float]=None):
        super().__init__(dataset_size, split_percentages=split_percentages)

    def setup(self, stage: Optional[str] = None):
        dataset = MoonsDataset(num_samples=self.dataset_size, noise_std=1e-1)
        self.train_set, self.val_set, self.test_set = torch.utils.data.random_
↪split(dataset, self.split_sizes)
```

Now we define the core of our Neural ODE model.

[ ]:
```
class _ODEFunc(nn.Module):
    def __init__(self, module, autonomous=True):
        super().__init__()
        self.module = module
        self.autonomous = autonomous

    def forward(self, t, x):
        if not self.autonomous:
            x = torch.cat([torch.ones_like(x[:, [0]]) * t, x], 1)
        return self.module(x)


class ODEBlock(nn.Module):
    def __init__(self, odefunc: nn.Module, solver: str = 'dopri5',
                 rtol: float = 1e-4, atol: float = 1e-4, adjoint: bool = True,
                 autonomous: bool = True):
        super().__init__()
```

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```
        self.odefunc = _ODEFunc(odefunc, autonomous=autonomous)
        self.rtol = rtol
        self.atol = atol
        self.solver = solver
        self.use_adjoint = adjoint
        self.integration_time = torch.tensor([0, 1], dtype=torch.float32)

    @property
    def ode_method(self):
        return torchdiffeq.odeint_adjoint if self.use_adjoint else torchdiffeq.odeint

    def forward(self, x: torch.Tensor, adjoint: bool = True, integration_time=None):
        integration_time = self.integration_time if integration_time is None else␣
↪integration_time
        integration_time = integration_time.to(x.device)
        ode_method =  torchdiffeq.odeint_adjoint if adjoint else torchdiffeq.odeint
        out = ode_method(
            self.odefunc, x, integration_time, rtol=self.rtol,
            atol=self.atol, method=self.solver)
        return out
```

We will wrap everything together in a **LightningModule**.

[ ]:
```
class Learner(pl.LightningModule):
    def __init__(self, model:nn.Module, t_span:torch.Tensor, learning_rate:float=5e-3):
        super().__init__()
        self.model = model
        self.t_span = t_span
        self.learning_rate = learning_rate
        self.accuracy = Accuracy(num_classes=2)

    def forward(self, x):
        return self.model(x)

    def inference(self, x, time_span):
        return self.model(x, adjoint=False, integration_time=time_span)

    def inference_no_projection(self, x, time_span):
        return self.model.forward_no_projection(x, adjoint=False, integration_time=time_
↪span)

    def training_step(self, batch, batch_idx):
        x, y = batch
        y_pred = self(x)
        y_pred = y_pred[-1]  # select last point of solution trajectory
        loss = nn.CrossEntropyLoss()(y_pred, y)
        self.log('train_loss', loss, prog_bar=True, logger=True)
        return loss

    def validation_step(self, batch, batch_idx):
        x, y = batch
        y_pred = self(x)
```

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```
        y_pred = y_pred[-1]  # select last point of solution trajectory
        loss = nn.CrossEntropyLoss()(y_pred, y)
        self.log('val_loss', loss, prog_bar=True, logger=True)
        acc = self.accuracy(y_pred.softmax(dim=-1), y)
        self.log('val_accuracy', acc, prog_bar=True, logger=True)
        return loss

    def test_step(self, batch, batch_idx):
        x, y = batch
        y_pred = self(x)
        y_pred = y_pred[-1]  # select last point of solution trajectory
        loss = nn.CrossEntropyLoss()(y_pred, y)
        self.log('test_loss', loss, prog_bar=True, logger=True)
        acc = self.accuracy(y_pred.softmax(dim=-1), y)
        self.log('test_accuracy', acc, prog_bar=True, logger=True)
        return loss

    def configure_optimizers(self):
        optimizer = torch.optim.Adam(self.model.parameters(), lr=self.learning_rate)
        return optimizer
```

Finally, it is time to actually define a Neural ODE and train it. We will use a simple 2-layer MLP with a *tanh* activation and 64 hidden dimensions. We will train the model using the adjoint method for backpropagation.

A quick note on the architectural choices for our model. As mentioned in the first part of this tutorial, the **Picard-Lindelöf theorem** (Coddington and Levinson, 1955) states that the solution to an initial value problem **exists and is unique** if the differential equation is *uniformly Lipschitz continuous* in $\mathbf{z}$ and *continuous* in t. It turns out that this theorem holds for our model if the neural network has finite weights and uses Lipshitz nonlinearities, such as tanh or relu. However, not all tools are our deep learning arsenal is Lipshitz. For example, as shown in The Lipschitz Constant of Self-Attention by Hyunjik Kim et al., standard self-attention is **not** Lipshitz. The authors propose alternative forms of self-attention that are Lipshitz.

[ ]:
```
adjoint = True
data_module = HalfMoonsDataModule(1000)
t_span = torch.linspace(0, 1, 2)
f = nn.Sequential(
    nn.Linear(2, 64),
    nn.Tanh(),
    nn.Linear(64, 2))
model = ODEBlock(f, adjoint=adjoint)
learner = Learner(model, t_span)

trainer = pl.Trainer(
    max_epochs=200,
    accelerator="gpu" if torch.cuda.is_available() else "cpu",
    devices=1,
    callbacks=[
        pl.callbacks.ModelCheckpoint(mode="max", monitor="val_accuracy"),
        pl.callbacks.RichProgressBar(),
    ],
    log_every_n_steps=1,
)
trainer.fit(learner, datamodule=data_module)
```

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```
val_result = trainer.validate(learner, datamodule=data_module, verbose=True)
test_result = trainer.test(learner, datamodule=data_module, verbose=True)
```

```
GPU available: False, used: False
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
Missing logger folder: /content/lightning_logs
```

```
  Name      Type      Params
0 | model    | ODEBlock | 322
1 | accuracy | Accuracy |   0
-----------------------------
```

```
Trainable params: 322
Non-trainable params: 0
Total params: 322
Total estimated model params size (MB): 0
```

```
Output()
```

```
Output()
```

```
     Validate metric            DataLoader 0
┌──────────────────────────┬──────────────────────────┐
│       val_accuracy       │           1.0            │
│         val_loss         │ 0.0021277053747326136    │
└──────────────────────────┴──────────────────────────┘
```

```
Output()
```

```
      Test metric            DataLoader 0
┌──────────────────────────┬──────────────────────────┐
│       test_accuracy      │           1.0            │
│         test_loss        │ 0.0018281997181475163    │
└──────────────────────────┴──────────────────────────┘
```

Excellent! It seems that in less that 200 epochs we have achieved perfect validation accuracy. Let's now use the trained model to run inference and visualize the trajectories using a dense time span of 100 timesteps.

[ ]:
```
@torch.no_grad()
def run_inference(learner, data_loader, time_span):
    learner.to(device)
    trajectories = []
    classes = []
    time_span = torch.from_numpy(time_span).to(device)
    for data, target in data_loader:
        data = data.to(device)
        traj = learner.inference(data, time_span).cpu().numpy()
        trajectories.append(traj)
        classes.extend(target.numpy())
    trajectories = np.concatenate(trajectories, 1)
    return trajectories, classes

time_span = np.linspace(0.0, 1.0, 100)
trajectories, classes = run_inference(learner, data_module.train_dataloader(), time_span)

colors = ['coral', 'darkviolet']
class_colors = [colors[ci] for ci in classes]
```

We will now define a few functions to visualize the learned trajectories, the state-space, and the learned vector field.

[1]:
```
#@title You can omit reading this piece of code.

def plot_trajectories(time_span, trajectories, class_colors):
    fig = plt.figure(figsize=(12,6))
    ax0 = fig.add_subplot(121)
    ax1 = fig.add_subplot(122)
    for i in range(trajectories.shape[1]):
        ax0.plot(time_span, trajectories[:, i, 0], color=class_colors[i], alpha=0.1)
        ax1.plot(time_span, trajectories[:, i, 1], color=class_colors[i], alpha=0.1)

    ax0.set_xlabel(r"$t$ [Depth]")
    ax0.set_ylabel(r"$\mathbf{z}_0(t)$")
    ax0.set_title("Dimension 0")
    ax1.set_xlabel(r"$t$ [Depth]")
    ax1.set_ylabel(r"$\mathbf{z}_1(t)$")
    ax1.set_title("Dimension 1")


def plot_trajectories_3d(time_span, trajectories, class_colors):
    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(111, projection='3d')
    for i in range(trajectories.shape[1]):
        ax.plot(trajectories[:, i, 0], trajectories[:, i, 1], time_span,
                color=class_colors[i], alpha=0.1)

    ax.set_title('3D Trajectories')
    ax.set_xlabel(r"$\mathbf{z}_0(t)$")
    ax.set_ylabel(r"$\mathbf{z}_1(t)$")
    ax.set_zlabel(r"$t$")
```

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```
def plot_trajectories_animation(time_span, trajectories, colors, classes, lim=10.0):
    def animate_frame(t):
        ax.cla()
        ax.set_xlim(-lim, lim)
        ax.set_ylim(-lim, lim)
        ax.set_title('Trajectories')
        ax.set_xlabel(r"$\mathbf{z}_0(t)$")
        ax.set_ylabel(r"$\mathbf{z}_1(t)$")

        zero_classes = np.array(classes) == 0
        one_classes = np.array(classes) == 1

        scatter_zero = ax.plot(
            trajectories[t, zero_classes, 0], trajectories[t, zero_classes, 1],
            'o', color=colors[0], alpha=0.2+0.8*t/len(time_span))
        scatter_one = ax.plot(
            trajectories[t, one_classes, 0], trajectories[t, one_classes, 1],
            'o', color=colors[1], alpha=0.2+0.8*t/len(time_span))
        return scatter_zero, scatter_one

    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(111)
    anim = FuncAnimation(fig, animate_frame, frames=len(time_span))
    plt.close(fig)
    return anim


def plot_augmented_trajectories_animation(time_span, trajectories, colors, classes,␣
↪lim=10.0):
    def animate_frame(t):
        ax.cla()
        ax.set_xlim(-lim, lim)
        ax.set_ylim(-lim, lim)
        ax.set_zlim(-lim, lim)
        ax.set_title('Trajectories')
        ax.set_xlabel(r"$\mathbf{z}_0(t)$")
        ax.set_ylabel(r"$\mathbf{z}_1(t)$")
        ax.set_zlabel(r"$\mathbf{z}_2(t)$")

        zero_classes = np.array(classes) == 0
        one_classes = np.array(classes) == 1

        scatter_zero = ax.plot(
            trajectories[t, zero_classes, 0], trajectories[t, zero_classes, 1],␣
↪trajectories[t, zero_classes, 2],
            'o', color=colors[0], alpha=0.2+0.8*t/len(time_span))
        scatter_one = ax.plot(
            trajectories[t, one_classes, 0], trajectories[t, one_classes, 1],␣
↪trajectories[t, one_classes, 2],
            'o', color=colors[1], alpha=0.2+0.8*t/len(time_span))
```

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```
        return scatter_zero, scatter_one

    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(111, projection='3d')
    anim = FuncAnimation(fig, animate_frame, frames=len(time_span))
    plt.close(fig)
    return anim


def plot_state_space(trajectories, class_colors, ax=None):
    if ax is None:
        fig = plt.figure(figsize=(8, 8))
        ax = fig.add_subplot(111)

    for i in range(trajectories.shape[1]):
        ax.plot(trajectories[:, i, 0], trajectories[:, i, 1],
                color=class_colors[i], alpha=0.1)

    ax.set_title('State-Space Diagram')
    ax.set_xlabel(r"$x$")
    ax.set_ylabel(r"$y$")


def plot_augmented_state_space(trajectories, class_colors, ax=None):
    if ax is None:
        fig = plt.figure(figsize=(8, 8))
        ax = fig.add_subplot(111, projection='3d')

    for i in range(trajectories.shape[1]):
        ax.plot(trajectories[:, i, 0], trajectories[:, i, 1], trajectories[:, i, 2],
                color=class_colors[i], alpha=0.1)

    ax.set_title('State-Space Diagram')
    ax.set_xlabel(r"$x$")
    ax.set_ylabel(r"$y$")
    ax.set_zlabel(r"$z$")


def plot_static_vector_field(model, trajectory, N=50, device='cpu', ax=None):
    X, Y = np.mgrid[trajectory[..., 0].min():trajectory[..., 0].max():N*1j,
                    trajectory[..., 1].min():trajectory[..., 1].max():N*1j]
    X = X.T
    Y = Y.T
    P = np.vstack([X.ravel(), Y.ravel()]).T
    P = torch.Tensor(P).to(device)

    with torch.no_grad():
        vector_field = model.odefunc(0.0, P).cpu()
    vector_norm = vector_field.norm(dim=1).view(N, N).numpy()

    vector_field = vector_field.view(N, N, 2).numpy()
```

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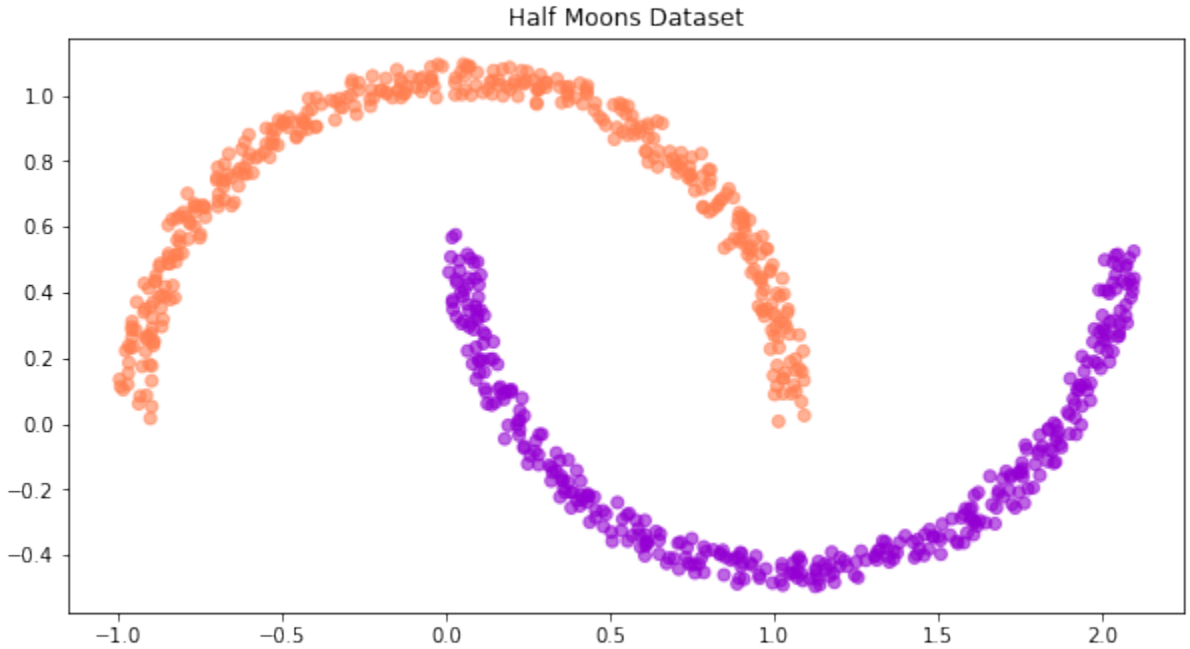
```
    if ax is None:
        fig = plt.figure(figsize=(8, 8))
        ax = fig.add_subplot(111)
    ax.contourf(X, Y, vector_norm, cmap='RdYlBu')
    ax.streamplot(X, Y, vector_field[:, :, 0], vector_field[:, :, 1], color='k')

    ax.set_xlim([X.min(), X.max()])
    ax.set_ylim([Y.min(), Y.max()])
    ax.set_xlabel(r"$x$")
    ax.set_ylabel(r"$y$")
    ax.set_title("Learned Vector Field")
```

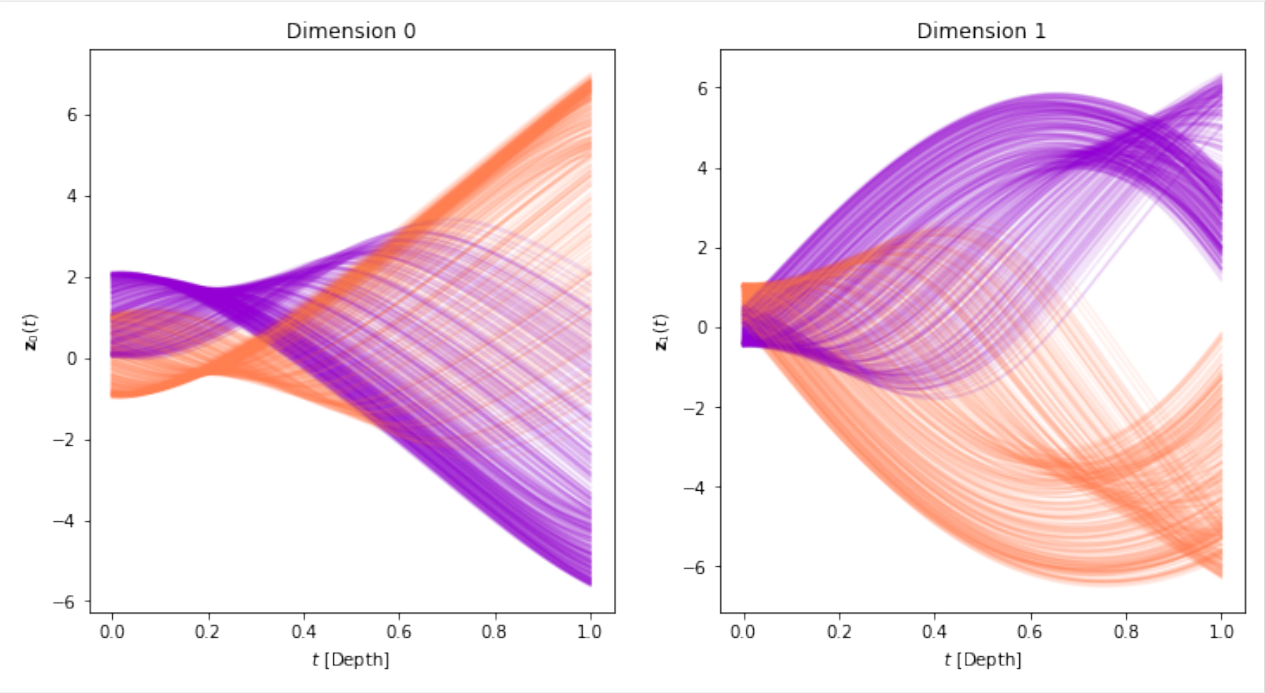
Before we visualize the trajectories, let's plot the (training) data once again:

[ ]:
```
fig, ax = plot_binary_classification_dataset(*data_module.train_set[:], title='Half␣
↪Moons Dataset')
```



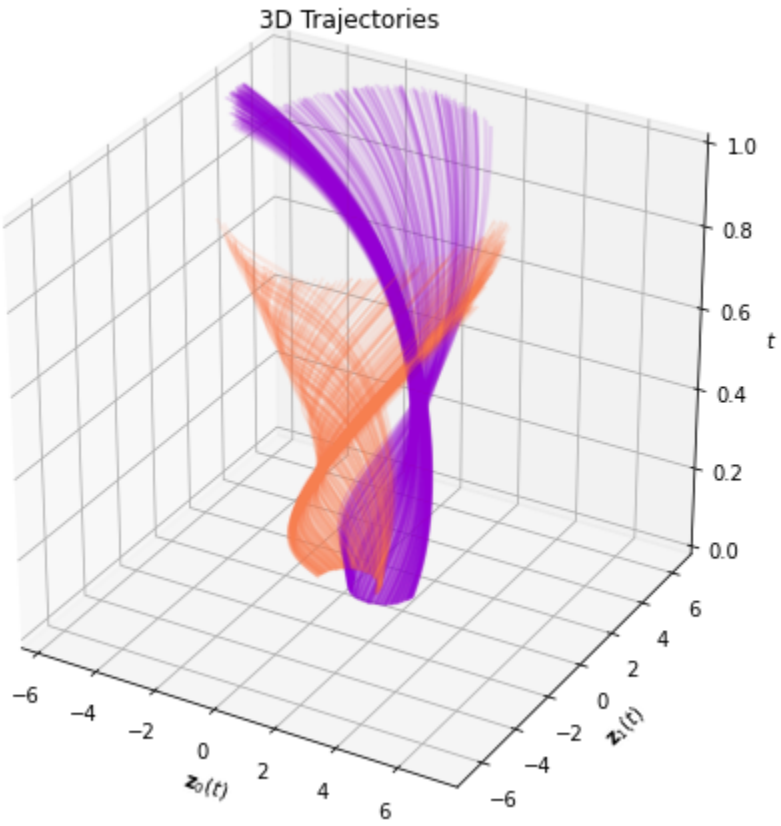
Below we visualize the evolution for each of the 2 inputs dimensions as a function of time (depth):

[ ]:
```
plot_trajectories(time_span, trajectories, class_colors)
```



And the same evolution combined in a single plot:

[ ]:
```
plot_trajectories_3d(time_span, trajectories, class_colors)
```



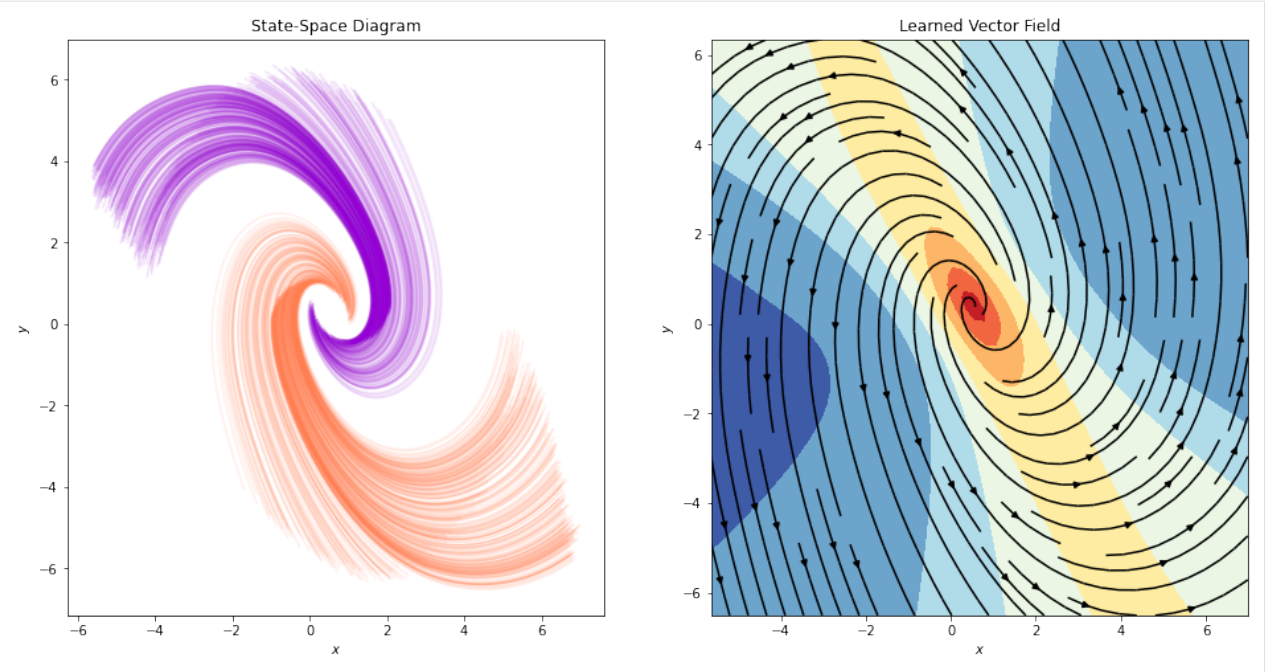
The 3D plot can be somewhat complicated to decipher. Thus, we also plot an animated version of the evolution. Each timestep of the animation is a slice on the temporal axis of the figure above.

[ ]:
```
anim = plot_trajectories_animation(time_span, trajectories, colors, classes, lim=8.0)
HTML(anim.to_html5_video())
```

```
<IPython.core.display.HTML object>
```

Finally, let's visualize the state-space diagram and the learned vector field:

[ ]:
```
fig, ax = plt.subplots(1, 2, figsize=(16, 8))
plot_state_space(trajectories, class_colors, ax=ax[0])
plot_static_vector_field(model, trajectories, ax=ax[1], device=device)
```



Neural ODEs can only describe homeomorphisms

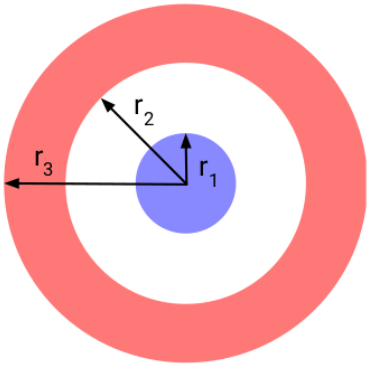
It seems that the network can indeed do a very good job at separating data from these 2 classes. We will now move to different setting, which appears similar at first in terms of difficulty, but will turn out to be very hard, even impossible theoretically for Neural ODEs to solve in their basic form.

Neural ODEs describe homeomorphisms (flows). Inputs/hidden states/outputs have the same dimensionality. They form non-intersecting trajectories.

Since Neural ODEs cannot model non-homeomorphisms, they cannot, for example, separate a 2d concentric annuli/circles dataset.

$$0 < r_1 < r_2 < r_3, \quad g : \mathbb{R}^2 \to \mathbb{R}$$

$$\begin{cases} g(\mathbf{x}) = 0, & \|\mathbf{x}\| \leq r_1, \\ g(\mathbf{x}) = 1, & r_2 \leq \|\mathbf{x}\| \leq r_3 \end{cases}$$



(Figure credit: Emilien Dupont et al.)

Neural ODEs cannot represent that function, the features of NODEs preserve the topology of the input space. NODEs can only continuously deform the input space, and cannot, for example, tear a connected region apart.

In practice, however, Neural ODEs are not trained on continuous regions of space, they are rather trained on a finite number of data points. This means that NODEs can "cheat" and stretch space, squeezing through the gaps between data points. This can lead to ill-posed ODE problems that are numerically expensive to solve.

Let's see this effect in practice. First, we will define a similar dataset that comprises 2 2D concentric circles.

[ ]:
```
def rand_sphere(num_samples:int, dim:int, radius:float) -> torch.Tensor:
    """Uniform sample from a `dim`-dimensional sphere of radius `radius`
    :param num_samples: number of points to sample
    :type num_samples: int
    :param dim: dimension of the hyper-sphere
    :type dim: int
    :param radius: radius of the hyper-sphere
    :type radius: float
    """
    v = torch.randn(num_samples, dim)
    points = radius * F.normalize(v, dim=-1)
    return points


class ConcentricCircles(Dataset):
    """Concentric Circles Classification Dataset

    Adapted from https://github.com/DiffEqML/torchdyn
    """
    def __init__(self, num_samples=100, noise_std=1e-4, inner_radius=0.5,
                 outer_radius=1.0):
        self.num_samples = num_samples
        self.noise_std = noise_std
        self.X, self.y = self.generate_concentric_circles(num_samples, noise_std)

    @staticmethod
    def generate_concentric_circles(num_samples:int=100, noise_std:float=1e-4,
                                    inner_radius:float=0.5, outer_radius:int=1.0):
        """Creates a *concentric circles* dataset of `num_samples` datasets points.
        :param num_samples: number of datasets points in the generated dataset
        :type num_samples: int
        :param noise_std: standard deviation of noise magnitude added to each datasets␣
↪point
        :type noise_std: float
        :param inner_radius: radius of the inner circle
        :type inner_radius: float
        :param outer_radius: radius of the outer circle
        :type outer_radius: float
        """
        y = torch.zeros(num_samples, dtype=torch.long)
        y[:num_samples // 2] = 1

        X = torch.zeros((num_samples, 2))
        X[:num_samples // 2] = rand_sphere(num_samples // 2, 2, inner_radius)
        X[num_samples // 2:] = rand_sphere(num_samples - num_samples // 2, 2, outer_
↪radius)
```

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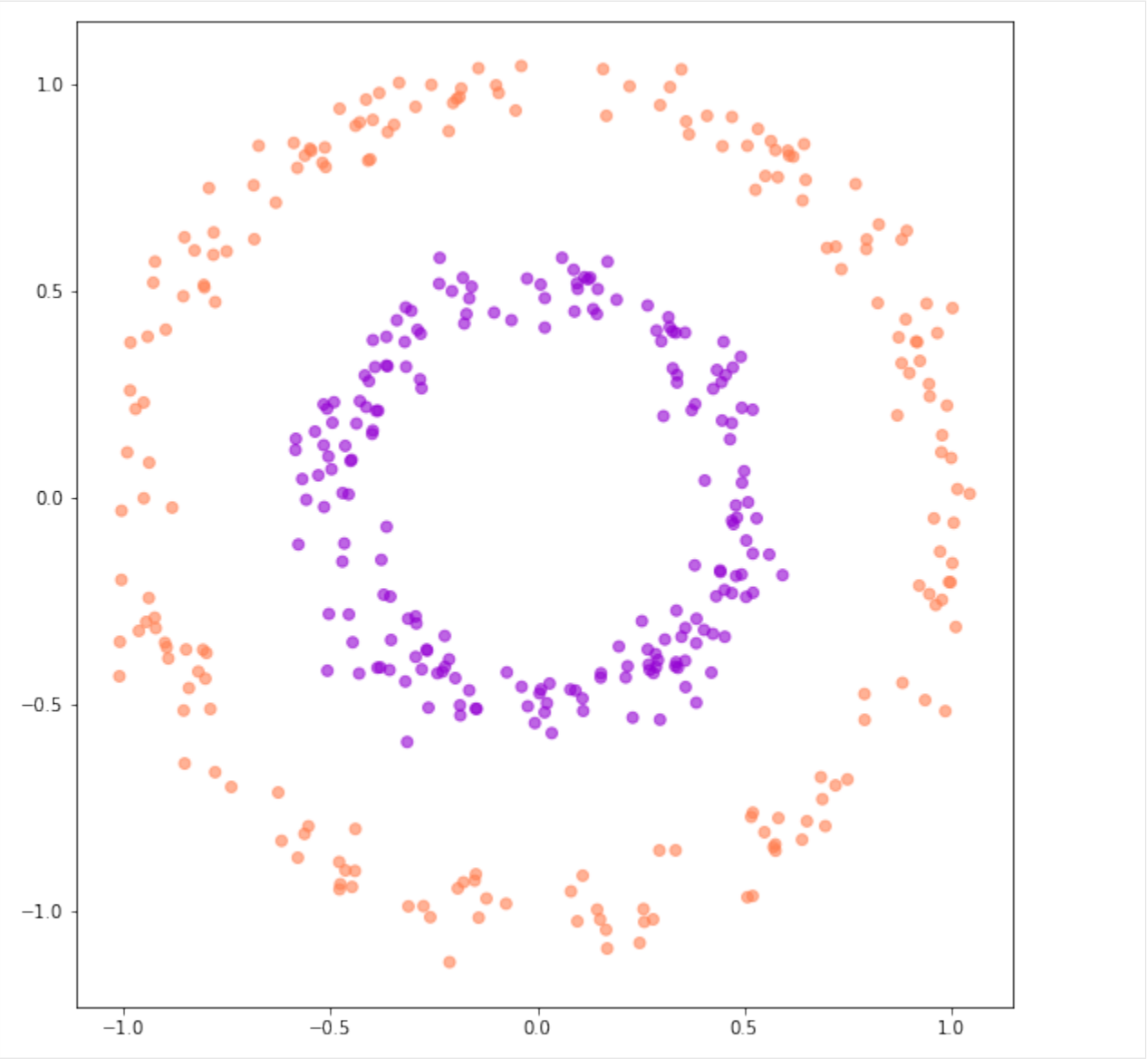
```
        X += noise_std * torch.randn((num_samples, 2))

        return X, y

    def __len__(self):
        return self.num_samples

    def __getitem__(self, idx):
        return self.X[idx], self.y[idx]

class ConcentricCirclesDataModule(ToyDataModule):
    def __init__(self, dataset_size:int, split_percentages:Optional[float]=None):
        super().__init__(dataset_size, split_percentages=split_percentages)

    def setup(self, stage: Optional[str] = None):
        dataset = ConcentricCircles(num_samples=self.dataset_size, noise_std=5e-2)
        self.train_set, self.val_set, self.test_set = torch.utils.data.random_
↪split(dataset, self.split_sizes)
```

[ ]:
```
sample_circles_set = ConcentricCircles(num_samples=401, noise_std=5e-2)
fig, ax = plot_binary_classification_dataset(*sample_circles_set[:])
```



We will now train a Neural ODE on this dataset. We will use a 3-layer MLP with ReLU activations and 64 hidden dimensions.

[ ]:
```
circles_data_module = ConcentricCirclesDataModule(1000)

adjoint = True
t_span = torch.linspace(0, 1, 2)
f = nn.Sequential(nn.Linear(2, 64), nn.Tanh(), nn.Linear(64, 64), nn.Tanh(), nn.
↪Linear(64, 2))
model = ODEBlock(f, adjoint=adjoint)
learner = Learner(model, t_span)

trainer = pl.Trainer(
    max_epochs=300,
    accelerator="gpu" if torch.cuda.is_available() else "cpu",
    devices=1,
```

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```
    callbacks=[
        pl.callbacks.ModelCheckpoint(mode="max", monitor="val_accuracy"),
        pl.callbacks.RichProgressBar(),
    ],
    log_every_n_steps=1,
)

trainer.fit(learner, datamodule=circles_data_module)
val_result = trainer.validate(learner, datamodule=circles_data_module, verbose=True)
test_result = trainer.test(learner, datamodule=circles_data_module, verbose=True)
```

```
GPU available: False, used: False
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
```

```
    Name      Type      Params

 0  model     ODEBlock    4.5 K
 1  accuracy  Accuracy        0
```

```
Trainable params: 4.5 K
Non-trainable params: 0
Total params: 4.5 K
Total estimated model params size (MB): 0
```

```
Output()
```

```
Output()
```

```
     Validate metric             DataLoader 0

       val_accuracy          0.9900000095367432
         val_loss            0.042514488101005554
```

```
Output()
```

```
       Test metric               DataLoader 0

       test_accuracy         0.9900000095367432
```

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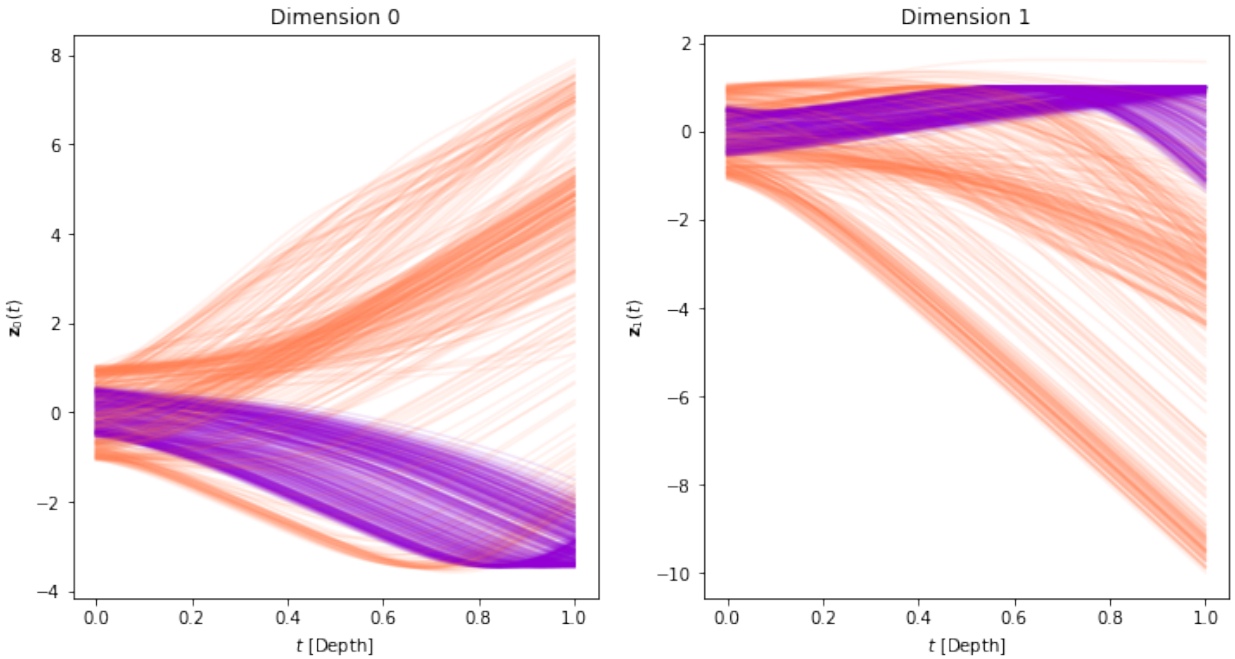
```
        test_loss           │    0.037914443761110306    │
```

Interestingly, the model can achieve perfect accuracy, even though in theory it cannot separate the 2 classes. Let's visualize the trajectories and see how this can be the case. SImilar to the previous experiment, we will first run inference and save the trajectories using a dense time span.

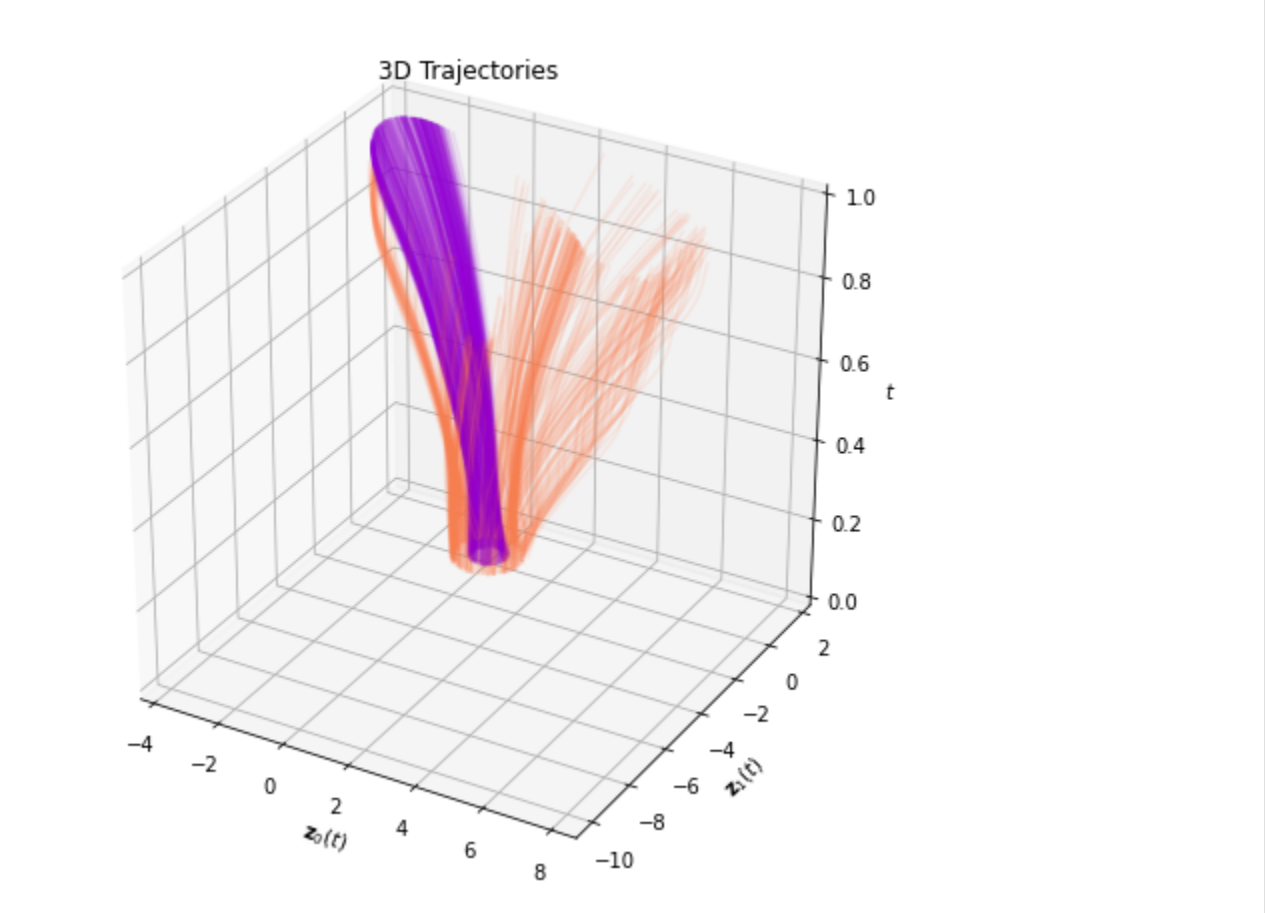
[ ]:
```
num_timesteps = 100
time_span = np.linspace(0.0, 1.0, num_timesteps)
trajectories, classes = run_inference(learner, circles_data_module.train_dataloader(),␣
↪time_span)

colors = ['coral', 'darkviolet']
class_colors = [colors[ci] for ci in classes]
```

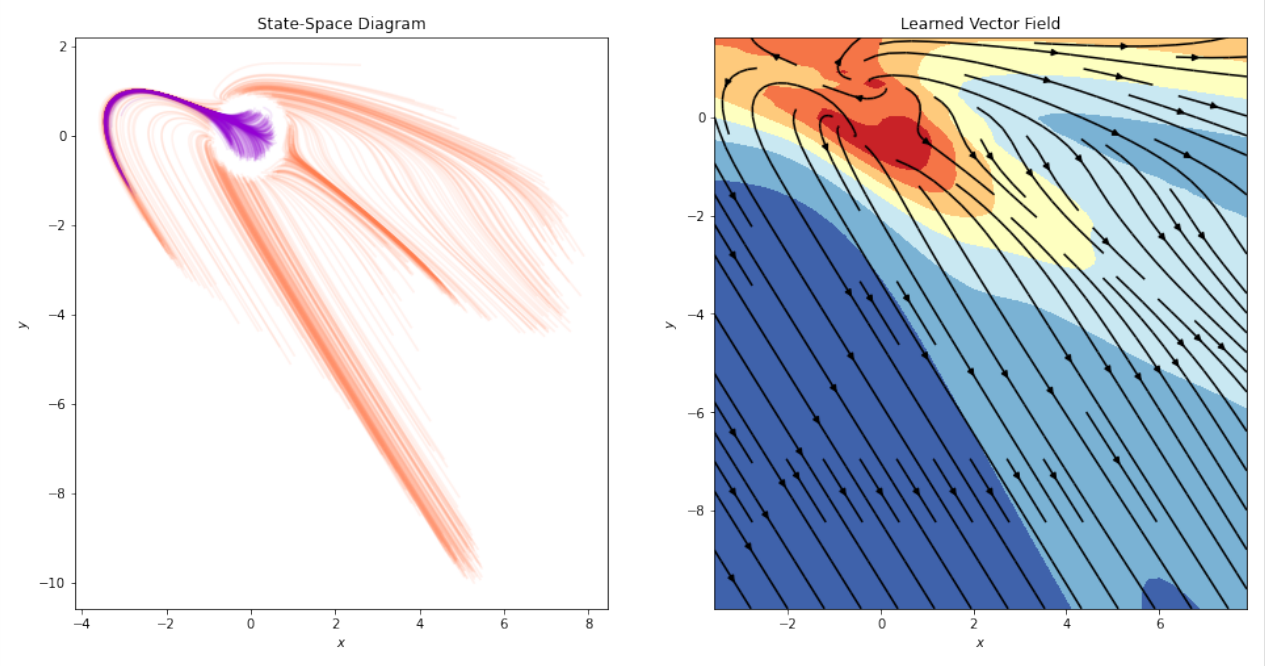
[ ]:
```
plot_trajectories(time_span, trajectories, class_colors)
```



[ ]:
```
plot_trajectories_3d(time_span, trajectories, class_colors)
```



[ ]:
```
fig, ax = plt.subplots(1, 2, figsize=(16, 8))
plot_state_space(trajectories, class_colors, ax=ax[0])
plot_static_vector_field(model, trajectories, ax=ax[1], device=device)
```



It is not clear neither from the trajectories, nor from the state-space, how the model manages to separate the data. Let's use an animated visualization of the evolution once again.

[ ]:
```
anim = plot_trajectories_animation(time_span, trajectories, colors, classes, lim=12.0)
HTML(anim.to_html5_video())
```

```
<IPython.core.display.HTML object>
```

The animation clearly shows that the model is cheating by stretching a part of space so much that data points from the inner circle can flow that region. Even though this offers perfect accuracy in this dataset, it comes at the expense of generalization capabilities, and increased train and inference time, since the network has to run many more function evaluations to achieve these results.

Augmented Neural ODEs

These issues were first observed (in the context of Neural ODEs) by Emilien Dupont et al., in their work on Augmented Neural ODEs. The authors propose a very simple yet elegant solution to the problem: they augment the space on which they learn and solve the ODE, from $\mathbb{R}^d$ to $\mathbb{R}^{d+p}$. The initial state $\mathbf{x}$ is augmented with additional dimensions $\mathbf{a}$ that are initialized with 0.

The augmented ODE problem is formulated as:

$$\begin{bmatrix}\dot{\mathbf{h}}(t)\\ \dot{\mathbf{a}}(t)\end{bmatrix} = \mathbf{f}\left(\begin{bmatrix}\mathbf{h}(t)\\ \mathbf{a}(t)\end{bmatrix}\right), \quad \begin{bmatrix}\mathbf{h}(0)\\ \mathbf{a}(0)\end{bmatrix} = \begin{bmatrix}\mathbf{x}\\ \mathbf{0}\end{bmatrix}$$

The final predictions in the original space are achieved via a final network that transforms the output augmented states:

$$\hat{\mathbf{y}} = \mathbf{g}\left(\begin{bmatrix}\mathbf{h}(T)\\ \mathbf{a}(T)\end{bmatrix}\right),$$

where $\mathbf{g}$ can be an *MLP* or even a simple *linear* layer.

We will now define a simple Augmenter module, and a Neural ODE wrapper that incorporates the Augmenter and the output network.

[ ]:
```
class ZeroAugmenter(nn.Module):
    def __init__(self, axis=1, num_dims=1):
        super().__init__()
        self.axis = axis
        self.num_dims = num_dims

    def forward(self, x):
        aug_dims = list(x.shape)
        aug_dims[self.axis] = self.num_dims
        augmentation = torch.zeros(aug_dims, device=x.device, dtype=x.dtype)
        return torch.cat([x, augmentation], dim=self.axis)


class AugmentedNODEWrapper(nn.Module):
    def __init__(self, augmenter, neural_ode, out_net):
        super().__init__()
        self.augmenter = augmenter
        self.neural_ode = neural_ode
        self.out_net = out_net

    def forward(self, x: torch.Tensor, adjoint: bool = True, integration_time=None):
        x = self.augmenter(x)
        x = self.neural_ode(x, adjoint, integration_time)
        x = self.out_net(x)
        return x

    def forward_no_projection(self, x: torch.Tensor, adjoint: bool = True, integration_
↪time=None):
        x = self.augmenter(x)
        x = self.neural_ode(x, adjoint, integration_time)
        return x
```

We will continue with the same dataset as before, namely the 2D concentric circles. We will use a single augmentation dimension and a simple linear layer $\mathbf{g} : \mathbb{R}^3 \to \mathbb{R}^2$.

[ ]:
```
circles_data_module = ConcentricCirclesDataModule(1000)

adjoint = True
t_span = torch.linspace(0, 1, 2)
augmentation_dims = 1
f = nn.Sequential(nn.Linear(2+augmentation_dims, 64), nn.Tanh(), nn.Linear(64,␣
↪2+augmentation_dims))
no_augm_model = ODEBlock(f, adjoint=adjoint)
model = AugmentedNODEWrapper(ZeroAugmenter(num_dims=augmentation_dims), no_augm_model,␣
↪nn.Linear(2+augmentation_dims, 2))
learner = Learner(model, t_span)

trainer = pl.Trainer(
    max_epochs=100,
    accelerator="gpu" if torch.cuda.is_available() else "cpu",
    devices=1,
    callbacks=[
        pl.callbacks.ModelCheckpoint(mode="max", monitor="val_accuracy"),
```

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```
        pl.callbacks.RichProgressBar(),
    ],
    log_every_n_steps=1,
)

trainer.fit(learner, datamodule=circles_data_module)
val_result = trainer.validate(learner, datamodule=circles_data_module, verbose=True)
test_result = trainer.test(learner, datamodule=circles_data_module, verbose=True)
```

```
GPU available: False, used: False
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
```

```
    Name      Type                  Params

 0  model     AugmentedNODEWrapper     459
 1  accuracy  Accuracy                   0
```

```
Trainable params: 459
Non-trainable params: 0
Total params: 459
Total estimated model params size (MB): 0
```

```
Output()
```

```
Output()
```

```
      Validate metric             DataLoader 0

        val_accuracy                       1.0
          val_loss          7.259416634042282e-06
```

```
Output()
```

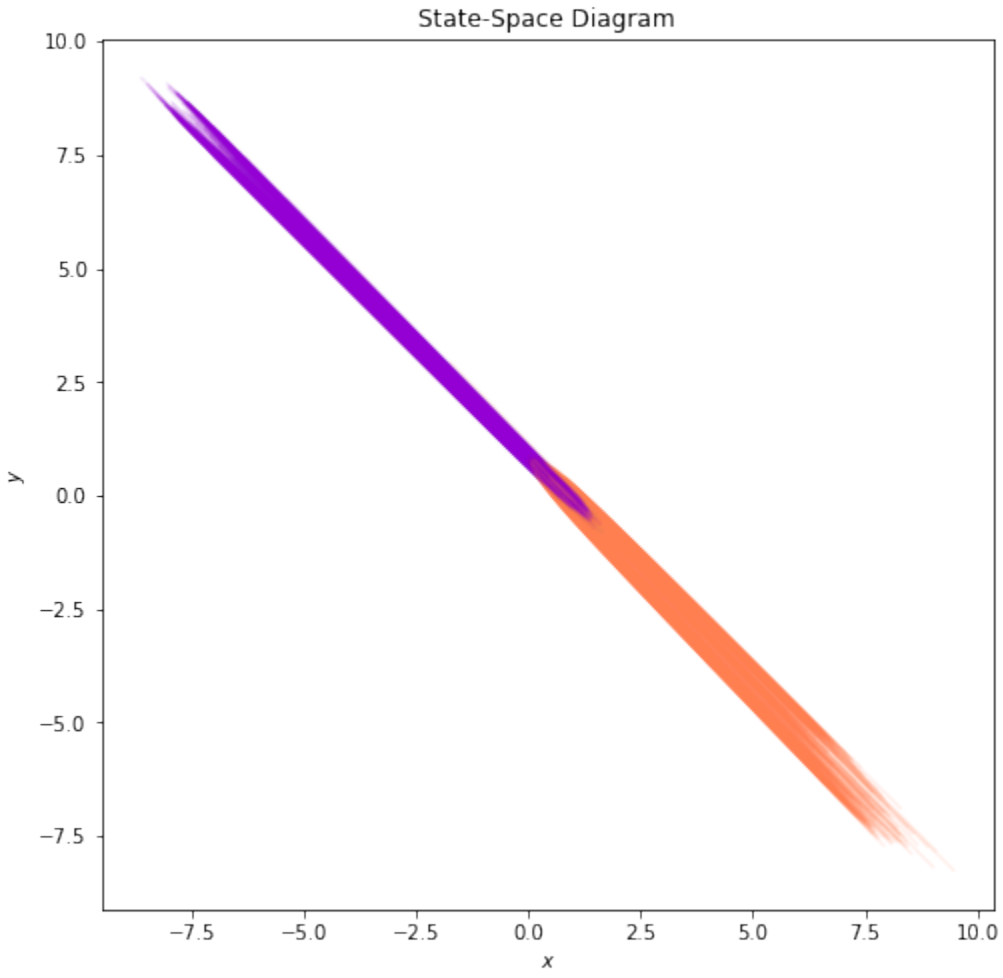
```
       Test metric              DataLoader 0

        test_accuracy                      1.0
          test_loss          5.69325675314758e-06
```

Even with a single augmentation dimension, the model can very quickly achieve perfect accuracy in the validation set. Let us now compute and visualize the trajectories, in order to gain a better understanding of what is actually going on.

[ ]:
```
num_timesteps = 100
time_span = np.linspace(0.0, 1.0, num_timesteps)
trajectories, classes = run_inference(learner, circles_data_module.train_dataloader(),␣
↪time_span)
```

[ ]:
```
plot_state_space(trajectories, class_colors)
```



[ ]:
```
anim = plot_trajectories_animation(time_span, trajectories, colors, classes, lim=8.0)
HTML(anim.to_html5_video())
```

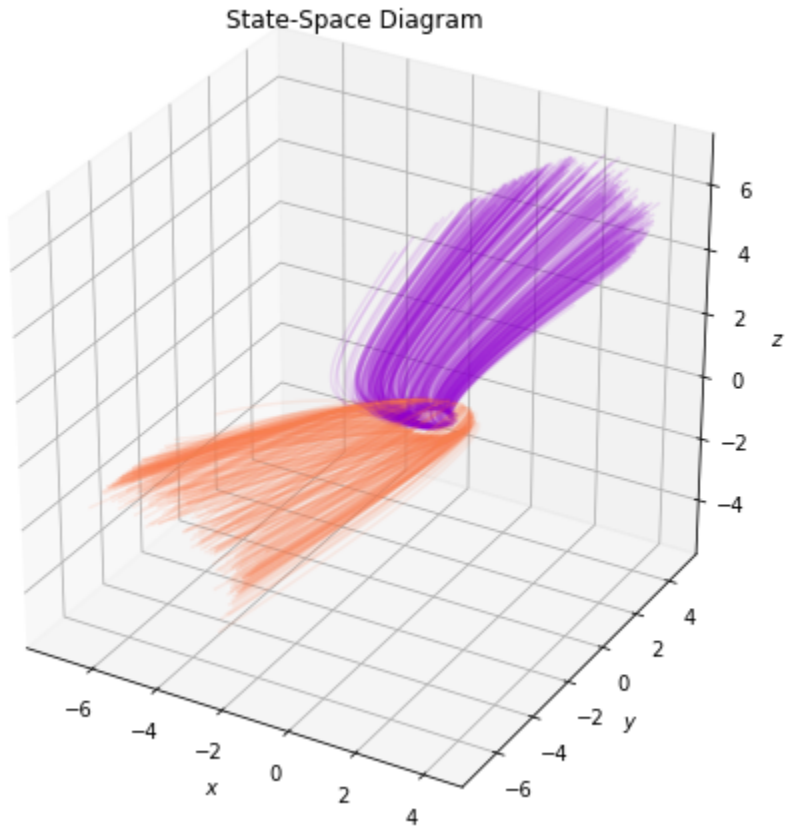
```
<IPython.core.display.HTML object>
```

From the 2D plots, it is not exactly clear how the model can achieve perfect separation. Thus, in what follows, we will visualize the trajectories and the state-space in the augmented 3D space.

[ ]:
```
@torch.no_grad()
def run_inference_no_projection(learner, data_loader, time_span):
    trajectories = []
    classes = []
    learner = learner.to(device)
    time_span = torch.from_numpy(time_span).to(device)
    for data, target in data_loader:
        data = data.to(device)
        traj = learner.inference_no_projection(data, time_span).cpu().numpy()
        trajectories.append(traj)
        classes.extend(target.numpy())
    trajectories = np.concatenate(trajectories, 1)
    return trajectories, classes

num_timesteps = 100
time_span = np.linspace(0.0, 1.0, num_timesteps)
trajectories, classes = run_inference_no_projection(learner, circles_data_module.train_
↪dataloader(), time_span)
colors = ['coral', 'darkviolet']
class_colors = [colors[ci] for ci in classes]
```

[ ]:
```
plot_augmented_state_space(trajectories, class_colors)
```



```
[ ]: anim = plot_augmented_trajectories_animation(time_span, trajectories, colors, classes,␣
     ↪lim=8.0)
     HTML(anim.to_html5_video())
```

```
<IPython.core.display.HTML object>
```

4.53.4 Further Reading

Neural ODEs is an exciting topic that has received a lot of attention in the past few years, ever since their introduction in Neurips 2018. Some of many many work in this field include:

- Neural Stochastic Differential Equations (Neural SDEs)
- Neural Controlled Differential Equations (Neural CDEs)
- Graph ODEs
- Hamiltonial Neural Networks
- Lagrangian Neural Networks

If you want to see a quick overview of different works in the field, Michael Poli maintains the excellent Awesome Neural ODE, a collection of resources regarding the interplay between neural differential equations, dynamical systems, deep learning, control, numerical methods and scientific machine learning.

Torchdyn is an excellent library for Neural Differential Equations.

Implicit Layers is a list of tutorials on implicit functions and automatic differentiation, Neural ODEs, and Deep Equilibrium Models.

Here is an excellent blogpost on ODEs and Neural ODEs.

Patrick Kidger's doctoral dissertation is an excellent textbook on Neural Differential Equations.

4.53.5 References

[1] Chen, Ricky T. Q. et al. "**Neural ordinary differential equations**". *NeurIPS* 2018. https://arxiv.org/abs/1806.07366

[2] Dupont, Emilien et al. "**Augmented Neural ODEs**". *NeurIPS* 2019. https://arxiv.org/abs/1904.01681

[3] Pontryagin, L.S. et al. "**The mathematical theory of optimal processes**". 1962

4.54 SGA - Sampling Discrete Structures

Notebook:
Author: Adeel Pervez

In these tutorials we discuss methods for sampling discrete variables from unstructured vectors to more structured objects such as subsets, permutations and graphs which can be incorporated in differentiable models.

At the foundation of these methods are continuous relaxations for discrete (binary or categorical) random variables. So the first part of the tutorial gives an introduction to sampling form discrete distributions with the Gumbel-Softmax trick. We use the method to train a variational autoencoder with categorical latent variables.

4.54.1 Categorical Sampling with Gumbel-Argmax

Suppose we are given a categorical distribution with C values as weights $w_i \in (0, \infty)$. We would like to obtain a sample from this distribution. The probability of each category c_i is given by the following softmax distribution

$$p_i = \frac{\exp(\log(w_i))}{\sum_j \exp(\log(w_j))}$$

The Gumbel-Argmax method for sampling this distribution is the following: Sample $U_k \sim Uniform(0, 1)$ iid and compute $r_k = \log \alpha_k - log(-\log U_k)$. Then choose the index i of the maximum r_k (ie take the argmax) and return the 1-hot vector with the ith index set to 1 and the rest to 0. The form of noise $-log(-\log U_k)$ added to form r_k has a Gumbel distribution whence the method gets its name. The cumulative distribution function of the Gumbel distribution (with location 0 and scale 1) is given as

$$F(z) = \exp(-\exp(-z))$$

You can take a look at a proof that this indeed samples from the softmax distribution here.

In short sampling a categorical variable with the Gumbel reparameterization proceeds as follows.

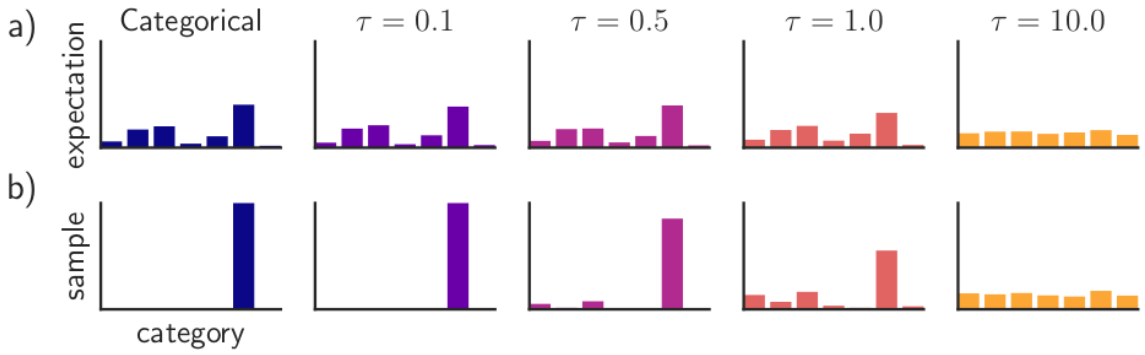
1. Given weights w_i compute $r_i = w_i + g_i$ where g_i are iid Gumbel samples
2. Argmax: Return index of largest r_i as a 1-hot vector

4.54.2 Softmax Relaxation

The above procedure still cannot be used in a differentiable model since the argmax operation has zero gradient except at points of discontinuity. So instead we use the `softmax` as a differentiable approximation to the argmax. In order to control the approximation we introduce a tunable temperature hyperparameter τ which controls how far the softmax outputs are from being 1-hot.

$$p_i = \frac{\exp(r_i/\tau)}{\sum_j \exp(r_j/\tau)}$$

The following figure (Paper Link) shows the effect of temperature on the distribution and samples.



A smaller temperature indicates a tighter approximation and the larger the temperature the looser the approximation. Of course, if the temperature is too small we wouldn't be able to train the model since the gradients would be very small. On the other hand, a large temperature would make the categorical outputs very far from being discrete, so it is important to choose an appropriate temperature for the problem at hand. One possibility is to slowly anneal the temperature from large to small so that close to the end of training the relaxed categorical outputs are closed to discrete. In practice, however, the temperature is often kept fixed during each training trial and tuned with cross-validation.

With the softmax relaxation the sampling then proceeds as follows

1. Given weights w_i compute $r_i = w_i + g_i$ where g_i are iid Gumbel samples
2. Apply softmax with temperature to obtain a relaxed categorical sample

4.54.3 Categorical VAE

As an example of the Gumbel Softmax relaxation we show a VAE with a categorical variable latent space for MNIST. The latent space has the structure of a vector of categorical variables each with the same fixed number of categories. In the following example the latent space has 30 categorical variables each of dimension 10. Since this is a VAE we also need to define a prior on the latent space which we define to be the uniform categorical distribution.

The following implementation uses code from here with minor modification.

We being with the required imports and hyperparameter definitions.

[1]:
```
import numpy as np

import torch
import torch.nn.functional as F
from torch import nn, optim
from torch.nn import functional as F
from torchvision import datasets, transforms
from torchvision.utils import save_image
from torch.distributions.one_hot_categorical import OneHotCategorical

import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline

cuda=True
```

[2]:
```
batch_size = 100
epochs = 10
latent_dim = 30
categorical_dim = 10
temp = 1.0
```

Gumbel Sampling

We now define the Gumbel-Softmax sampling routines. The `sample_gumbel` function samples scale 0 location 1 Gumbel variables by sampling uniform random variables in $U(0, 1)$ and computing $-\log(-\log(U(0, 1))$. The categorical parameters are input as unnormalized log probabilities. The `gumbel_softmax_sample` function adds the Gumbel noise to the logits, applies the temperature and the softmax function. In the `gumbel_softmax` function we also add evaluation code which simply returns a sample (unrelaxed) from the categorical distribution parameterized by `logits`.

[3]:
```
def sample_gumbel(shape, eps=1e-20):
    U = torch.rand(shape)
    if cuda:
        U = U.cuda()
    return -torch.log(-torch.log(U + eps) + eps)

def gumbel_softmax_sample(logits, temperature):
```

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```
    y = logits + sample_gumbel(logits.size())
    return F.softmax(y / temperature, dim=-1)

def gumbel_softmax(logits, temperature, evaluate=False):
    if evaluate:
        d =  OneHotCategorical(logits=logits.view(-1, latent_dim, categorical_dim))
        return d.sample().view(-1, latent_dim * categorical_dim)

    y = gumbel_softmax_sample(logits, temperature)
    return y.view(-1, latent_dim * categorical_dim)
```

VAE model

Now we define the VAE model. The encoder computes the categorical probability parameters from which relaxed categorical variables can be sampled and passed into the decoder.

[4]:
```
class VAE_gumbel(nn.Module):
    def __init__(self, temp):
        super(VAE_gumbel, self).__init__()

        self.fc1 = nn.Linear(784, 512)
        self.fc2 = nn.Linear(512, 256)
        self.fc3 = nn.Linear(256, latent_dim * categorical_dim)

        self.fc4 = nn.Linear(latent_dim * categorical_dim, 256)
        self.fc5 = nn.Linear(256, 512)
        self.fc6 = nn.Linear(512, 784)

        self.relu = nn.ReLU()
        self.sigmoid = nn.Sigmoid()

    def encode(self, x):
        h1 = self.relu(self.fc1(x))
        h2 = self.relu(self.fc2(h1))
        return self.relu(self.fc3(h2))

    def decode(self, z):
        h4 = self.relu(self.fc4(z))
        h5 = self.relu(self.fc5(h4))
        return self.sigmoid(self.fc6(h5))

    def forward(self, x, temp, evaluate=False):
        q = self.encode(x.view(-1, 784))
        q_y = q.view(q.size(0), latent_dim, categorical_dim)
        z = gumbel_softmax(q_y, temp, evaluate)
        return self.decode(z), F.softmax(q_y, dim=-1).reshape(*q.size())
```

KL Divergence

Since this is a VAE we also need to compute a KL divergence of the latent probability distribution with the uniform prior $p(x) = 1/C$ for all x where C is the total number of categories.

:nbsphinx-math:`begin{align} KLD(q||p) &= E_qleft[logfrac{q(x)}{p(x)}right]\

&= sum_{i=1}^{C} q(x_i) log (C cdot q(x_i))

end{align}`

Here $q(x)$ is the latent probability distribution

Finally we compute the reconstruction loss of the input as the binary cross entropy between the reconstruction parameters and the input image and add that to the KL divergence to get the VAE loss.

[5]:
```
def loss_function(recon_x, x, qy):
    BCE = F.binary_cross_entropy(recon_x, x.view(-1, 784), size_average=False) / x.
↪shape[0]

    log_ratio = torch.log(qy * categorical_dim + 1e-20)
    KLD = torch.sum(qy * log_ratio, dim=-1).mean()

    return BCE + KLD
```

Next we build the model and train

[6]:
```
model = VAE_gumbel(temp)
if cuda:
    model.cuda()
optimizer = optim.Adam(model.parameters(), lr=1e-3)
```

[7]:
```
kwargs = {'num_workers': 1, 'pin_memory': True} if cuda else {}
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST('./data/MNIST', train=True, download=True,
                   transform=transforms.ToTensor()),
    batch_size=batch_size, shuffle=True, **kwargs)
test_loader = torch.utils.data.DataLoader(
    datasets.MNIST('./data/MNIST', train=False, transform=transforms.ToTensor()),
    batch_size=batch_size, shuffle=True, **kwargs)
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torchvision/
↪datasets/mnist.py:498: UserWarning: The given NumPy array is not writeable, and␣
↪PyTorch does not support non-writeable tensors. This means you can write to the␣
↪underlying (supposedly non-writeable) NumPy array using the tensor. You may want to␣
↪copy the array to protect its data or make it writeable before converting it to a␣
↪tensor. This type of warning will be suppressed for the rest of this program.␣
↪(Triggered internally at  /opt/conda/conda-bld/pytorch_1623448224956/work/torch/csrc/
↪utils/tensor_numpy.cpp:180.)
  return torch.from_numpy(parsed.astype(m[2], copy=False)).view(*s)
```

For training we compute both the relaxed and the unrelaxed objective. The unrelaxed objective is not itself used for training. However, since that's the objective we want to improve, it's a good idea to also evaluate it so that we can observe how far the relaxed objective is from the actual objective. This also allows us to get an idea of how low or high to set the temperature so that the relaxed objective is not too far from the true objective while achieving reasonable training performance.

[8]:
```
def train(epoch):
    model.train()
    train_loss = 0
    train_loss_unrelaxed = 0
    #temp = args.temp
    for batch_idx, (data, _) in enumerate(train_loader):
        if cuda:
            data = data.cuda()
        optimizer.zero_grad()
        recon_batch, qy = model(data, temp)
        loss = loss_function(recon_batch, data, qy)
        loss.backward()
        train_loss += loss.item() * len(data)
        optimizer.step()

        #Unrelaxed training objective for comparison
        recon_batch_eval, qy_eval = model(data, temp, evaluate=True)
        loss_eval = loss_function(recon_batch_eval, data, qy_eval)
        train_loss_unrelaxed += loss_eval.item() * len(data)

    print('Epoch: {} Average loss relaxed: {:.4f} Unrelaxed: {:.4f}'.format(
        epoch, train_loss / len(train_loader.dataset) , train_loss_unrelaxed / len(train_
↪loader.dataset)))
```

[9]:
```
def test(epoch):
    model.eval()
    test_loss = 0
    for i, (data, _) in enumerate(test_loader):
        if cuda:
            data = data.cuda()
        recon_batch, qy = model(data, temp, evaluate=True)
        test_loss += loss_function(recon_batch, data, qy).item() * len(data)
    test_loss /= len(test_loader.dataset)
    print('Eval loss: {:.4f}'.format(test_loss))
```

Finally we can run the training. You can try training with different values of the temperature to see how that affects the relaxed objective relative to the true one.

[10]:
```
def run():
    for epoch in range(1, epochs + 1):
        train(epoch)
        test(epoch)
run()
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torch/nn/_
↪reduction.py:42: UserWarning: size_average and reduce args will be deprecated, please␣
↪use reduction='sum' instead.
  warnings.warn(warning.format(ret))
```

```
Epoch: 1 Average loss relaxed: 197.1857 Unrelaxed: 199.8391
Eval loss: 178.9625
Epoch: 2 Average loss relaxed: 154.2037 Unrelaxed: 163.6063
```

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```
Eval loss: 152.1406
Epoch: 3 Average loss relaxed: 136.7130 Unrelaxed: 148.5179
Eval loss: 144.5594
Epoch: 4 Average loss relaxed: 129.4279 Unrelaxed: 141.8772
Eval loss: 138.8380
Epoch: 5 Average loss relaxed: 124.0670 Unrelaxed: 137.2079
Eval loss: 135.5893
Epoch: 6 Average loss relaxed: 120.2097 Unrelaxed: 133.9328
Eval loss: 131.6892
Epoch: 7 Average loss relaxed: 117.3797 Unrelaxed: 131.4627
Eval loss: 130.6390
Epoch: 8 Average loss relaxed: 115.1937 Unrelaxed: 129.7081
Eval loss: 128.6939
Epoch: 9 Average loss relaxed: 113.3871 Unrelaxed: 128.1377
Eval loss: 128.0002
Epoch: 10 Average loss relaxed: 111.9536 Unrelaxed: 127.0920
Eval loss: 126.7100
```

Generating Samples

We can now generate some samples from the trained decoder. For this we sample some uniform categorical variables from the prior and pass them into the decoder.

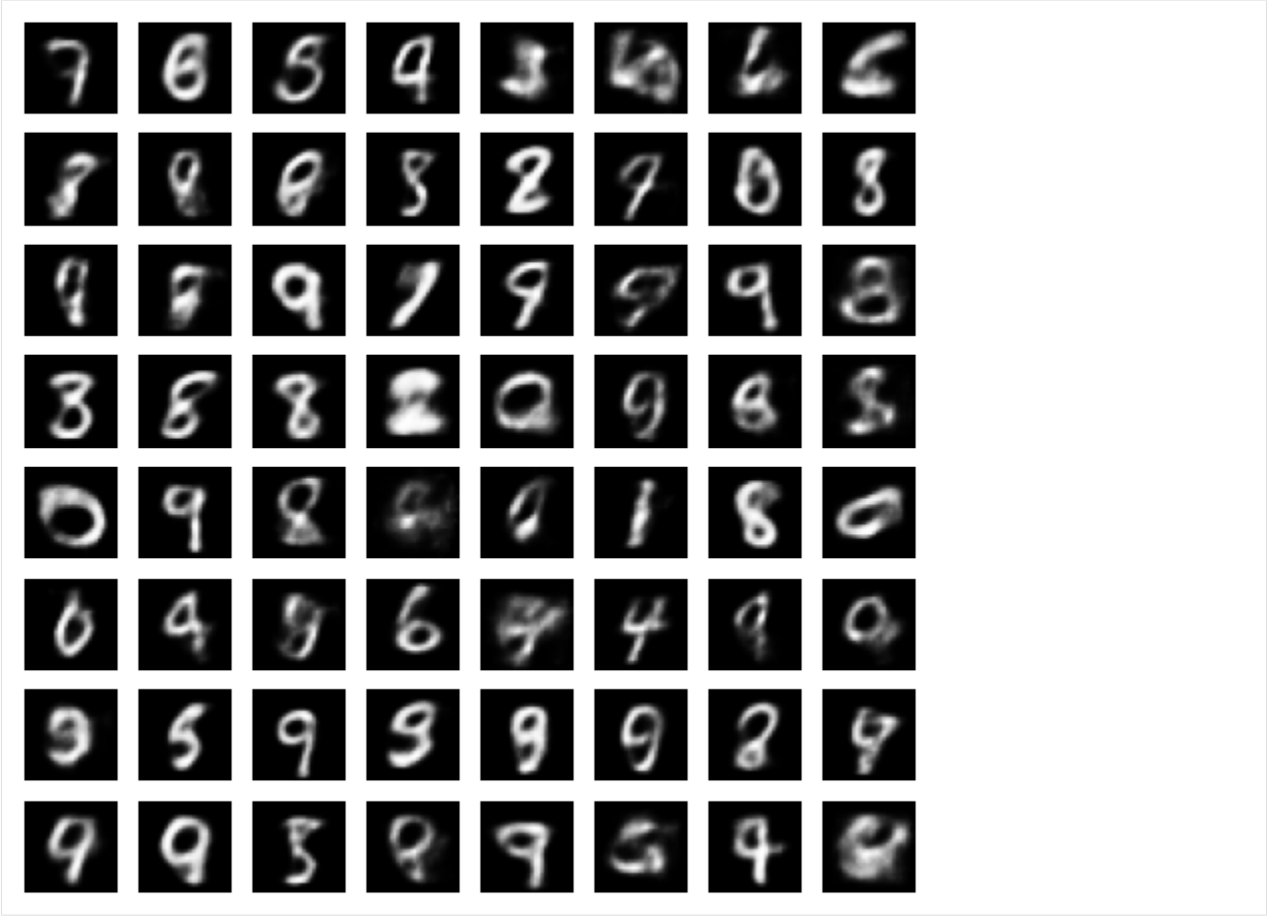
[11]:
```
def generate_samples():
    #generate uniform probability vector
    model.eval()
    probs = torch.ones([64, latent_dim, categorical_dim])*(1/categorical_dim)
    cat_samples = OneHotCategorical(probs=probs.cuda()).sample().view(-1, latent_
↪dim*categorical_dim)
    output = model.decode(cat_samples)
    return output.view(-1,28,28).detach().cpu().numpy()
```

[12]:
```
samples = generate_samples()
```

[13]:
```
def show_gray_image_grid(imgs, x=2, y=5, size=(8,8), path=None, save=False):
    fig, axs = plt.subplots(x, y, figsize=size)
    axs = axs.flatten()
    for img, ax in zip(imgs, axs):
        ax.imshow(np.squeeze(img), cmap='gray')
        #ax.imshow(img, cmap='gray')
        ax.set_axis_off()

    if save:
        plt.savefig(path)
    else:
        plt.show()

show_gray_image_grid(samples, 8,8)
```



4.54.4 Gumbel Straight-Through

In some instances we want to train models with discrete variables but do not want to pass relaxed values as inputs. This might be the case where we want to optimize a function that cannot be defined for relaxed inputs and must use categorical/discrete inputs. One heuristic for such cases is the Straight-Through estimator. Here given some pre-activation y for which we want the gradient we compute the sample z using the non-differentiable sampling operations such as with categorical or Bernoulli sampling. Then we compute the downstream function f on the hard sample. Then in the backward pass we ignore the non-differentiable operation and pass the gradient relative to z back as the gradient relative to y. That is we set.

$$\partial_y f := \partial_z f.$$

This is the straight-through gradient and gives a biased estimate of the gradient, but in many cases this can often allow us to train models with discrete variables.

Here we use the straight-through gradient with Gumbel-Softmax relaxation. In this case we compute the Gumbel-Softmax relaxation as before. From the relaxation we compute a 1-hot vector where the index with the largest value is set to 1 and all others are set to 0. This is used as the discrete value in the downstream network and we use the straight-through gradient in the backward pass.

Given a hard vector `y_hard` and a soft vector `y` there is a well-known trick that can be used to incorporate straight-through gradients. We compute

```
y = (y_hard - y).detach() + y
```

which simply uses the `y_hard` in the forward pass but the gradient relative to `y` in the backward pass.

[14]:
```
def gumbel_softmax(logits, temperature, evaluate=False, hard=False):
    if evaluate:
        d =  OneHotCategorical(logits=logits.view(-1, latent_dim, categorical_dim))
        return d.sample().view(-1, latent_dim * categorical_dim)

    y = gumbel_softmax_sample(logits, temperature)

    if hard:
        #Straight-through gradient
        #takes the index of the largest and insert a 1.
        #all others are set to 0 obtaining a 1-hot vector.
        shape = logits.size()
        _, k = y.max(-1)

        y_hard = torch.zeros_like(logits)
        y_hard = y_hard.zero_().scatter_(-1, k.view(shape[:-1] + (1,)), 1.0)

        #This a trick to use the 1-hot value in the forward pass and the
        #relaxed gradient in the backward pass
        y = (y_hard - y).detach() + y

    return y.view(-1, latent_dim * categorical_dim)
```

As an exercise you can train the VAE model given above using Gumbel-Straight-Through by using the above function in the model definition and setting `hard=True`.

In the next tutorials we will see how the basic Gumbel relaxation method can be used to differentiably sample other discrete structures such as subsets, permutations and graphs.

4.54.5 References

Categorical Reparameterization with Gumbel-Softmax

The Concrete Distribution: A Continuous Relaxation of Discrete Random Variables

4.55 SGA - Sampling Subsets with Gumbel-Top k Relaxations

Notebook:
Author: Adeel Pervez

In this part we show how to include a subset sampling component in differentiable models using Gumbel Top k relaxations. First we show how to build a differentiable subset sampler and then we show one application to differentiable k nearest neighbor classification.

Formally speaking we are given N elements with weights w_i. We would like to sample k elements from N without replacement. Stated otherwise, we want a k-element subset $S = \{w_{i_1}, w_{i_2}, \ldots, w_{i_k}\}$ from N elements.

Given total weight $Z = \sum w_i$, the first element is sampled with probability $\frac{w_{i_1}}{Z}$, the second with probability $\frac{w_{i_2}}{Z - w_{i_1}}$ and so on for k elements. Multiplying the factors gives the following distribution for k element subsets.

$$p(S) = \frac{w_{i_1}}{Z} \frac{w_{i_2}}{Z - w_{i_1}} \cdots \frac{w_{i_k}}{Z - \sum_{j=1}^{k-1} w_{i_j}}.$$

In the introduction we showed how sampling from a categorical distribution could be recast as choosing the argmax of a set of Gumbel random variables. Relaxing the argmax with a softmax allowed us to approximate sampling from the target categorical distribution. A temperature could be used to control the extent of relaxation. In this case the the categorical probabilities are given by the softmax distribution

$$p_i = \frac{exp(x_i)}{\sum_j exp(x_j)} = \frac{w_i}{\sum_j w_j}$$

It turns out that by selecting the k largest Gumbel random variables instead of just the largest we can sample subsets according to the sampling without replacement probability given above. This procedure is closely related to a procedure known by the name of weighted reservoir sampling.

Seen this way, the Gumbel-Argmax trick is a method for sampling subsets of size $k = 1$ with probabilities given by p_i. Replacing the argmax by a Top-k procedure for selecting the k largest elements generalizes the Gumbel-Argmax to sample size k subsets with probability $p(S)$. In this case we think of the Top-k procedure as returning a k-hot vector y where $y_i = 1$ if the ith element is selected and $y_i = 0$ otherwise. Thus we represent subsets as k-hot vectors which also generalizes the representation of categorical samples as 1-hot vectors.

The unrelaxed subset sampling procedure can then be written as follows given non-negative weights w_i.

1. Compute keys $\hat{r_i} = -\log(-\log(u_i)) + \log(w_i)$ for all i and $u_i \in U(0, 1)$.
2. Return k largest keys $\hat{r_i}$.

4.55.1 Top k Relaxation

We can construct an unrelaxed Top k by iteratively applying the softmax k times and sampling a 1-hot categorical sample at each step. The k 1-hot categorical samples are then combined into a single k-vector. When the categorical sample gives a particular element, the log probability for that element is set to $-\infty$ for the future iterations so that the element is never chosen again. We can relax this procedure by replacing samples from the softmax by the probabilities computed by softmax. When the softmax temperature is set to be small, the sampled and the relaxed outputs are close.

In more detail the procedure is as follows.

Unrelaxed Version

For $i = 1 \ldots n$ and $j = 1 \ldots k$, set \$ $\alpha_i^{`1} =: nbsphinx - math : hat\{r\_i\}`\$and\alpha_i^{j+1} = \alpha_i^j + \log(1 - a_i^j)$

Here a_i^j is a sample the categorical distribution with probabilities $p(a_i^j = 1) = \frac{\exp(\alpha_i^j/\tau)}{\sum_k \exp(\alpha_k^j/\tau)}$ and τ is a temperature.

Note that when a_i^j is a 1-hot categorical sample the $\log(1 - a_i^j)$ term in the first equation above sets the next α_i^{j+1} to $-\infty$ if $a_i^j = 1$ and leaves it unchanged otherwise. This ensures that the ith element once sampled is not sampled in the next steps. Finally we add all the k vectors as $\sum_j a^j$ and return the output as the sample.

Relaxed Version

To relax the above procedure we can replace the categorical sample at step by its expectation. In this case the update becomes

For $i = 1 \dots n$ and $j = 1 \dots k$, set \$ $\alpha_i^{`1} =: nbsphinx - math : hat\{r\_i\}`\$and\alpha_i^{j+1} = \alpha_i^j + \log(1 - p(a_i^j = 1))$

where $p(a_i^j = 1) = \frac{\exp(\alpha_i^j/\tau)}{\sum_k \exp(\alpha_k^j/\tau)}$ as above. At low values of τ the softmax distribution becomes close to deterministic outputs a value that is close to k-hot. The temperature variable is a hyperparameter and ideally should be annealed from larger to smaller values during the course of training. However, in most applications the temperature is left fixed per trial and tuned using cross validation. Proper tuning of temperature can have a significant effect on the performance of the model.

In the following we use code from [here]

[1]:
```
import os

import torch
import torch.nn as nn
import torch.nn.functional as F

from torchvision import datasets, transforms
from torch.utils.data import Dataset, DataLoader, TensorDataset, ConcatDataset, random_
↪split
from torch.utils.data.sampler import SubsetRandomSampler

import random
import time
from pathlib import Path

import numpy as np

import matplotlib
import matplotlib.pyplot as plt

%matplotlib inline
```

[2]:
```
gpu = torch.device('cuda')
```

4.55.2 Subset Sampler Class

The following `SubsetOperator` class implements the relaxed subset sampling procedure described above. As described the `forward` method takes a list of scores (unormalized log probs) of some fixed dimension. We add Gumbel noise with location 0 and scale 1 and divide by the temperature. Next we apply the Top-k relaxation and return the resulting k-hot vector as the sampled subset.

[3]:
```
EPSILON = np.finfo(np.float32).tiny

class SubsetOperator(torch.nn.Module):
    def __init__(self, k, tau=1.0, hard=False):
        super(SubsetOperator, self).__init__()
        self.k = k
        self.hard = hard
```

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```
        self.tau = tau

    def forward(self, scores):
        m = torch.distributions.gumbel.Gumbel(torch.zeros_like(scores), torch.ones_
↪like(scores))
        g = m.sample()
        scores = scores + g

        # continuous top k
        khot = torch.zeros_like(scores)
        onehot_approx = torch.zeros_like(scores)
        for i in range(self.k):
            khot_mask = torch.max(1.0 - onehot_approx, torch.tensor([EPSILON]).cuda())
            scores = scores + torch.log(khot_mask)
            onehot_approx = torch.nn.functional.softmax(scores / self.tau, dim=1)
            khot = khot + onehot_approx

        if self.hard:
            # straight through
            khot_hard = torch.zeros_like(khot)
            val, ind = torch.topk(khot, self.k, dim=1)
            khot_hard = khot_hard.scatter_(1, ind, 1)
            res = khot_hard - khot.detach() + khot
        else:
            res = khot

        return res
```

You can try the sampler on some example input and various temperatures. Note that the sum of the vectors elements is always k. At lower temperatures the output should be close to k-hot.

[4]:
```
sampler = SubsetOperator(k=2, tau=1.0)

x = torch.tensor([[1.,2.,3.,4.]]).to(gpu)
y = sampler(x)
print(y, y.sum())
```

```
tensor([[0.0236, 0.5672, 0.4200, 0.9892]], device='cuda:0') tensor(2., device='cuda:0')
```

4.55.3 Empirical Sampling Distribution

We empirically confirm that the k-hot relaxation generates subsets with the same distribution as the sampling without replacement distribution. For this we define a set with weights in `[1,2,3,4]` and generate 10000 subsets of size 2 using the true distribution (here with Gumbel Top k). Then we generate subsets using the relaxation given above with a fixed temperature. The samples are plotted side-by-side in a histogram.

[5]:
```
w = torch.tensor([[1.,2.,3.,4.]]).to(gpu)
w = w.tile((10000,1))
w_scores = torch.log(w)
```

Use Gumbel-Top-k to get true distribution samples.

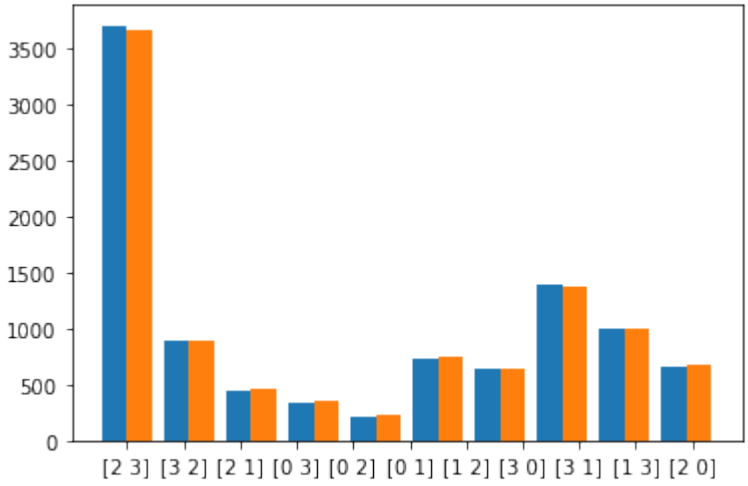
[6]:
```
#true samples
m = torch.distributions.gumbel.Gumbel(torch.zeros_like(w_scores), torch.ones_like(w_
↪scores))
g = m.sample()
scores = w_scores + g
samples = torch.topk(scores, 2)[1]
samples = samples.detach().cpu().numpy()
samples = [str(x) for x in samples]
```

To get samples of subsets from the relaxation, we first apply the relaxation and choose the Top k indices as the chosen subset.

[7]:
```
#relaxed samples
r_samples = sampler(w_scores)

r_samples = torch.topk(r_samples, 2)[1]
r_samples = r_samples.detach().cpu().numpy()
r_samples = [str(x) for x in r_samples]
```

[8]:
```
plt.hist([samples,r_samples], align='left')
plt.show()
```



4.55.4 Application: Differentiable k Nearest Neighbors

Now we apply the subset sampling procedure to a classification problem with differentiable k nearest neighbors. Recall that in k nearest neighbors classification we look at the labels of the k nearest neighbors and take the majority vote for classification. Unlike the classical form of nearest neighbors, we want to take the feature from a deep network. The k nearest neighbors loss is cannot be directly used in differentiable models so we relax it with our subset relaxation. Furthermore instead of looking for the nearest neighbors in the entire dataset (which can be large) we choose a random subset of data points for the distance calculations.

Given a query vector q and a set N of neighbors we compute the Euclidean distance between the q and each element $i \in N$. This gives us a list of scores (negative of the distances) and sample a k size subset of these scores as a relaxed k-hot vector.

Since this is a classification problem, during training we have the label y for the query vector q and for each of the neighbors y_i. If the labels are equal for a query, neighbor pair, we include the corresponding score otherwise we set it

to 0 and take the sum to compute the loss.

Given a subset of k neighbors the loss can be written as

$$L(S;q) = -\sum_{j \in S} I[y == y_i].$$

The actual loss is then the expectation of this expression over all subsets.

$$L(q) = E_S[L(S;q)].$$

The `SubsetsDKNN` class computes the scores between the queries and neighbors and returns the sampled subsets.

[9]:
```
class SubsetsDKNN(torch.nn.Module):
    def __init__(self, k, tau=1.0, hard=False, num_samples=-1):
        super(SubsetsDKNN, self).__init__()
        self.k = k
        self.subset_sample = SubsetOperator(k=k, tau=tau, hard=hard)
        self.num_samples = num_samples

    # query: batch_size x p
    # neighbors: 10k x p
    def forward(self, query, neighbors, tau=1.0):
        diffs = (query.unsqueeze(1) - neighbors.unsqueeze(0))
        squared_diffs = diffs ** 2
        l2_norms = squared_diffs.sum(2)
        norms = l2_norms  # .sqrt() # M x 10k
        scores = -norms

        top_k = self.subset_sample(scores)
        return top_k
```

The following is the convNet that we use to compute the features of the data examples.

[10]:
```
class ConvNet(nn.Module):
    def __init__(self):
        super(ConvNet, self).__init__()
        self.conv1 = nn.Conv2d(1, 20, kernel_size=5, stride=1)
        self.conv2 = nn.Conv2d(20, 50, kernel_size=5, stride=1)
        self.linear = nn.Linear(800, 500)

    def forward(self, x):
        out = F.relu(self.conv1(x))
        out = F.max_pool2d(out, 2)
        out = F.relu(self.conv2(out))
        out = F.max_pool2d(out, 2)
        out = out.view(out.size(0), -1)
        out = F.relu(self.linear(out))
        return out
```

Define hyperparameters.

Here we say that we are going to using 100 queries per minibatch and 100 neighbors for the distance computation. The embedding size for each data sample is set to 500.

[11]:
```
k = 9
tau = 1.0
NUM_TRAIN_QUERIES = 100
NUM_TEST_QUERIES = 10
NUM_TRAIN_NEIGHBORS = 100
LEARNING_RATE = 10 **-3
NUM_EPOCHS = 20
EMBEDDING_SIZE = 500
```

[12]:
```
dknn_layer = SubsetsDKNN(k, tau)
```

Data Sampler

In theory we could use the entire dataset as the set of data points from which to choose the k nearest neighbors for any query data point. This, however, is expensive so we instead use a random set of data points from which to select the k nearest neighbors.

In the following we define a data sampler class which samples a batch of query samples and a batch of neighbors from which to select the k nearest neighbors for each query. The size of the query set and the neighbor set is fixed by the `NUM_TRAIN_QUERIES` and the `NUM_TRAIN_NEIGHBORS` hyperparameters defined above.

[13]:
```
class ClassicDataset(Dataset):

    def __init__(self,
                 x,
                 y,
                 transform):

        self.xy = TensorDataset(x, y)
        self.transform = transform

    def __len__(self):

        return len(self.xy)

    def __getitem__(self, idx):

        x, y = self.xy[idx]
        if self.transform:
            x = self.transform(x)

        return x, y


class DataSplit(object):
    def __init__(self, dataset):
        if dataset == 'mnist':
            trva_real = datasets.MNIST(root='./data-mnist', download=True)
```

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```
            tr_real_ds, va_real_ds = random_split(trva_real, [55000, 5000])
            xtr_real = trva_real.train_data[tr_real_ds.indices].view(
                -1, 1, 28, 28)
            ytr_real = trva_real.train_labels[tr_real_ds.indices]
            xva_real = trva_real.train_data[va_real_ds.indices].view(
                -1, 1, 28, 28)
            yva_real = trva_real.train_labels[va_real_ds.indices]

            trans = transforms.Compose(
                [transforms.ToPILImage(), transforms.ToTensor()]
            )

            self.train_dataset = ClassicDataset(
                x=xtr_real, y=ytr_real, transform=trans)
            self.valid_dataset = ClassicDataset(
                x=xva_real, y=yva_real, transform=trans)
            self.test_dataset = datasets.MNIST(root='./data-mnist', train=False,␣
↪transform=transforms.Compose([
                transforms.ToTensor()
            ]))

    def get_train_loader(self, batch_size, **kwargs):
        train_loader = DataLoader(self.train_dataset,
                                  batch_size=batch_size, num_workers=4, shuffle=True,␣
↪**kwargs)
        return train_loader

    def get_valid_loader(self, batch_size, **kwargs):
        valid_loader = DataLoader(self.valid_dataset,
                                  batch_size=batch_size, shuffle=True, **kwargs)
        return valid_loader

    def get_test_loader(self, batch_size, **kwargs):
        test_loader = DataLoader(self.test_dataset,
                                 batch_size=batch_size, shuffle=False, **kwargs)
        return test_loader
```

Loss

Now we compute the loss given the sampled subsets for the queries using the labels for the queries and neighbors.

[14]:
```
def dknn_loss(query, neighbors, query_label, neighbor_labels):
    # query: batch_size x p
    # neighbors: 10k x p
    # query_labels: batch_size x [10] one-hot
    # neighbor_labels: n x [10] one-hot

    # num_samples x batch_size x n
    start = time.time()
    top_k_ness = dknn_layer(query, neighbors)
```

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```
    elapsed = time.time() - start
    correct = (query_label.unsqueeze(1) *
               neighbor_labels.unsqueeze(0)).sum(-1)  # batch_size x n
    correct_in_top_k = (correct.unsqueeze(0) * top_k_ness).sum(-1)
    loss = -correct_in_top_k

    return loss, elapsed
```

[15]:
```
h_phi = ConvNet().to(gpu)
```

[16]:
```
optimizer = torch.optim.SGD(
    h_phi.parameters(), lr=LEARNING_RATE, momentum=0.9, weight_decay=5e-4)
```

[17]:
```
split = DataSplit('mnist')

batched_query_train = split.get_train_loader(NUM_TRAIN_QUERIES)
batched_neighbor_train = split.get_train_loader(NUM_TRAIN_NEIGHBORS)

# labels is a 1-dimensional tensor
def one_hot(labels, l=10):
    n = labels.shape[0]
    labels = labels.unsqueeze(-1)
    oh = torch.zeros(n, l, device='cuda').scatter_(1, labels, 1)
    return oh
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torchvision/
↪datasets/mnist.py:498: UserWarning: The given NumPy array is not writeable, and␣
↪PyTorch does not support non-writeable tensors. This means you can write to the␣
↪underlying (supposedly non-writeable) NumPy array using the tensor. You may want to␣
↪copy the array to protect its data or make it writeable before converting it to a␣
↪tensor. This type of warning will be suppressed for the rest of this program.␣
↪(Triggered internally at  /opt/conda/conda-bld/pytorch_1623448224956/work/torch/csrc/
↪utils/tensor_numpy.cpp:180.)
  return torch.from_numpy(parsed.astype(m[2], copy=False)).view(*s)
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torchvision/
↪datasets/mnist.py:62: UserWarning: train_data has been renamed data
  warnings.warn("train_data has been renamed data")
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torchvision/
↪datasets/mnist.py:52: UserWarning: train_labels has been renamed targets
  warnings.warn("train_labels has been renamed targets")
```

Training

To train we sample a batch of queries and a batch of neighbors and compute the knn loss for each query and display the classification accuracy.

[18]:
```
def train(epoch):
    timings = []
    h_phi.train()
    to_average = []
    # train
    for query, candidates in zip(batched_query_train, batched_neighbor_train):
        optimizer.zero_grad()
        cand_x, cand_y = candidates
        query_x, query_y = query

        cand_x = cand_x.to(device=gpu)
        cand_y = cand_y.to(device=gpu)
        query_x = query_x.to(device=gpu)
        query_y = query_y.to(device=gpu)

        neighbor_e = h_phi(cand_x).reshape(NUM_TRAIN_NEIGHBORS, EMBEDDING_SIZE)
        query_e = h_phi(query_x).reshape(NUM_TRAIN_QUERIES, EMBEDDING_SIZE)

        neighbor_y_oh = one_hot(cand_y).reshape(NUM_TRAIN_NEIGHBORS, 10)
        query_y_oh = one_hot(query_y).reshape(NUM_TRAIN_QUERIES, 10)

        losses, timing = dknn_loss(query_e, neighbor_e, query_y_oh, neighbor_y_oh)
        timings.append(timing)
        loss = losses.mean()
        loss.backward()
        optimizer.step()
        to_average.append((-loss).item() / k)

    print('Avg. train correctness of top k:',
          sum(to_average) / len(to_average))
```

For testing we can directly take the k nearest neighbors and do not sample.

[19]:
```
def majority(lst):
    return max(set(lst), key=lst.count)


def new_predict(query, neighbors, neighbor_labels):
    '''
    query: p
    neighbors: n x p
    neighbor_labels: n (int)
    '''
    diffs = (query.unsqueeze(1) - neighbors.unsqueeze(0))  # M x n x p
    squared_diffs = diffs ** 2
    norms = squared_diffs.sum(-1)  # M x n
    indices = torch.argsort(norms, dim=-1)
    labels = neighbor_labels.take(indices[:, :k])  # M x k
```

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```
    prediction = [majority(l.tolist()) for l in labels]
    return torch.Tensor(prediction).to(device=gpu).long()


def acc(query, neighbors, query_label, neighbor_labels):
    prediction = new_predict(query, neighbors, neighbor_labels)
    return (prediction == query_label).float().cpu().numpy()
```

[20]:
```
batched_query_val = split.get_valid_loader(NUM_TEST_QUERIES)
batched_query_test = split.get_test_loader(NUM_TEST_QUERIES)

def test(epoch, val=False):
    h_phi.eval()
    global best_acc
    with torch.no_grad():
        embeddings = []
        labels = []
        for neighbor_x, neighbor_y in batched_neighbor_train:
            neighbor_x = neighbor_x.to(device=gpu)
            neighbor_y = neighbor_y.to(device=gpu)
            embeddings.append(h_phi(neighbor_x))
            labels.append(neighbor_y)
        neighbors_e = torch.stack(embeddings).reshape(-1, EMBEDDING_SIZE)
        labels = torch.stack(labels).reshape(-1)

        results = []
        for queries in batched_query_val if val else batched_query_test:
            query_x, query_y = queries
            query_x = query_x.to(device=gpu)
            query_y = query_y.to(device=gpu)
            query_e = h_phi(query_x)  # batch_size x embedding_size
            results.append(acc(query_e, neighbors_e, query_y, labels))
        total_acc = np.mean(np.array(results))

    split = 'val' if val else 'test'
    print('Avg. %s acc:' % split, total_acc)
```

We can now train the model. After 20 epochs of training we can get about 99.3% test accuracy.

[21]:
```
for t in range(1, NUM_EPOCHS):
    print('Beginning epoch %d: ' % t)
    train(t)
test(-1, val=False)
```

```
Beginning epoch 1:
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torch/nn/
↪functional.py:718: UserWarning: Named tensors and all their associated APIs are an␣
↪experimental feature and subject to change. Please do not use them for anything␣
↪important until they are released as stable. (Triggered internally at  /opt/conda/
↪conda-bld/pytorch_1623448224956/work/c10/core/TensorImpl.h:1156.)
  return torch.max_pool2d(input, kernel_size, stride, padding, dilation, ceil_mode)
```

```
Avg. train correctness of top k: 0.798162693676322
Beginning epoch 2:
Avg. train correctness of top k: 0.9430294330673984
Beginning epoch 3:
Avg. train correctness of top k: 0.9600246477608737
Beginning epoch 4:
Avg. train correctness of top k: 0.9682177281620528
Beginning epoch 5:
Avg. train correctness of top k: 0.9722120181960283
Beginning epoch 6:
Avg. train correctness of top k: 0.9760807987174599
Beginning epoch 7:
Avg. train correctness of top k: 0.9786814417020248
Beginning epoch 8:
Avg. train correctness of top k: 0.9803707928127704
Beginning epoch 9:
Avg. train correctness of top k: 0.9808286046500168
Beginning epoch 10:
Avg. train correctness of top k: 0.9832377206436321
Beginning epoch 11:
Avg. train correctness of top k: 0.9841142041755441
Beginning epoch 12:
Avg. train correctness of top k: 0.9854074607232604
Beginning epoch 13:
Avg. train correctness of top k: 0.9857420248937129
Beginning epoch 14:
Avg. train correctness of top k: 0.9867219129234854
Beginning epoch 15:
Avg. train correctness of top k: 0.987558315161503
Beginning epoch 16:
Avg. train correctness of top k: 0.9883937643031893
Beginning epoch 17:
Avg. train correctness of top k: 0.988576520091355
Beginning epoch 18:
Avg. train correctness of top k: 0.9895413443054827
Beginning epoch 19:
Avg. train correctness of top k: 0.98968997531467
Avg. test acc: 0.9918
```

4.55.5 References

Reparameterizable Subset Sampling via Continuous Relaxations. [Code]

4.56 SGA: Learning Latent Permutations with Gumbel-Sinkhorn Networks

Notebook:
Author: David Knigge

Code in this tutorial was based on: https://github.com/perrying/gumbel-sinkhorn and https://github.com/google/gumbel_sinkhorn.

4.56.1 0. Introduction

In this notebook, we take a look at implementing a flavour of neural networks that can perform operations on discrete objects. More specifically, we look at **latent permutation**, where the objective is to find the correct **permutation** P of a latent variable without direct supervision. We make use of the **Gumbel-Sinkhorn operator** which allows us to pose the finding of a permutation P as a linear optimization problem. We recommend taking a look at the original paper by Mena, G., et al., (2018), though we will briefly introduce all necessary concepts in this notebook.

Questions and feedback may be forwarded to David Knigge; d.m.knigge@uva.nl.

0.1 Brief overview of the problem

Typically, we think of the characteristic of neural networks being flexible enough to learn arbitrarily complex mappings as favourable. However, in many practical applications of neural networks, we can restrict the space of learnable functions by incorporating **inductive biases**; things we a priori know to be true (and relevant) in our problem setting.

An example of the importance of incorporating such inductive biases in model design is in settings where we are performing operations on discrete objects. Think for example of sorting a list of numbers $\mathbf{n}$:

$$\mathbf{n}^T = \begin{bmatrix} 5 \\ 1 \\ 3 \\ 4 \end{bmatrix}$$

We could obtain a reordering of the numbers by left-multiplying with a permutation matrix P;

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

Applying such a permutation matrix to our input, we get:

$$P\mathbf{n}^T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 5 \\ 1 \\ 3 \\ 4 \end{bmatrix} \tag{4.104}$$

$$= \begin{bmatrix} 1 \\ 3 \\ 4 \\ 5 \end{bmatrix} \tag{4.105}$$

A natural first instinct would be to let our network learn the permutation matrix P directly. But what if we don't have the ground truth permutation matrix? We may instead optimize our network for the permuted input $P\mathbf{n}^T$.

However, next we should note that the matrix P has some special properties. It is what's known as an instance of a **doubly stochastic matrix**, essentially meaning both its rows and its columns sum to a value of 1. Each of its rows and columns are one-hot vectors, reflecting the fact that each value in the input $\mathbf{n}^T$ must occur once in the output $P\mathbf{n}^T$, and only at a single location.

How do we get our network do learn to map to such doubly stochastic matrices? This is exactly the focus of the Gumbel-Sinkhorn operator!

Note: - A permutation matrix is an instance of an orthogonal matrix. Remember that for such matrices, their inverses are given by their transpose. Hence $P^T P = \mathbf{I}$. We use this later on.

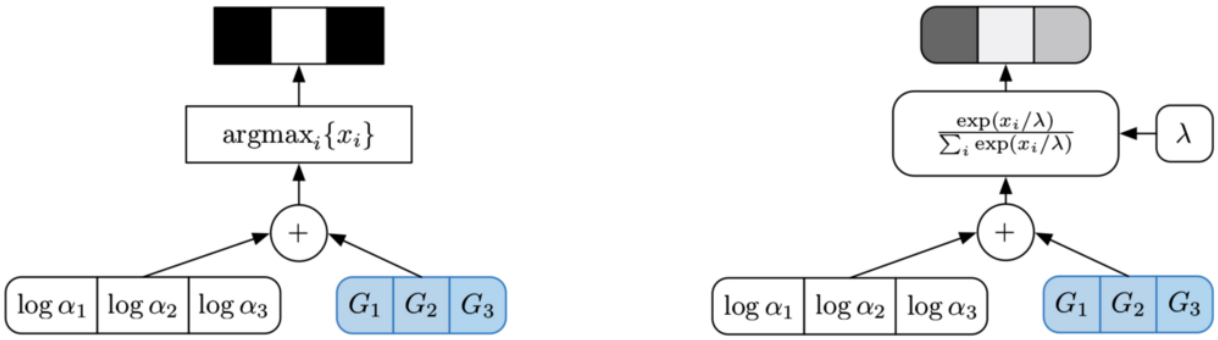
0.2 Refresher: The Gumbel-Softmax distribution

The authors introduce the Sinkhorn operator as permutation-friendly analogy to the **Gumbel-Softmax/Concrete** distribution; a differentiable approximation to sampling discrete data. Let's do a quick recap of the Gumbel-Softmax distribution.

Where the reparameterization trick as used in VAE's allows us to differentiably sample from continuous distributions, it is not straightforward to apply this to discrete distributions.

We can sample from a categorical distribution with class probabilities $\alpha = [\alpha_1, \alpha_2, \alpha_3]$ using the Gumbel-Max trick, by taking the argmax of $\log \alpha + \mathbf{G}$, where $\mathbf{G} = [G_1, G_2, G_3]$~$\mathrm{Gumbel}$. However, since the argmax operator isn't differentiable, we can't get gradients from this operation (visualized below in figure a).

Instead, we **relax** the discrete distribution by approximating a sampling from it through the Gumbel-Softmax trick. We replace the argmax operation by a softmax with temperature parameter λ. This operation is differentiable!



(a) Discrete(α) (b) Concrete(α, λ)

Where $G_i Gumbel = -log '(- : nbsphinx - math : log\{rmUnif\}'(0, 1))$.

0.3 Installing and importing some useful packages

Here we install and import some libraries that we will use throughout this tutorial. We use the `pytorch` as our deep learning framework of choice.

[1]:
```
## Standard libraries
import os
import numpy as np

## Imports for plotting
import matplotlib.pyplot as plt
import matplotlib

## PyTorch
import torch
import torch.nn as nn
import torch.utils.data as data
import torch.optim as optim
## Torchvision
import torchvision
from torchvision.datasets import MNIST
from torchvision import transforms
```

[2]:
```
# Download a pretrained model.
if not os.path.exists('saved_models'):
    os.mkdir('saved_models')
!wget -O 'saved_models/model.pth' https://raw.githubusercontent.com/david-knigge/uvadlc2-
↪tutorial-Gumbel-Sinkhorn-Networks/main/model.pth
```

```
--2022-04-22 12:23:42--  https://raw.githubusercontent.com/david-knigge/uvadlc2-tutorial-
↪Gumbel-Sinkhorn-Networks/main/model.pth
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.
↪199.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:
↪443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 31375 (31K) [application/octet-stream]
Saving to: ‘saved_models/model.pth’

100%[=====================================>] 31,375      --.-K/s   in 0.001s

2022-04-22 12:23:42 (39.1 MB/s) - ‘saved_models/model.pth’ saved [31375/31375]
```

[3]:
```
# Path to the folder where the datasets are be downloaded (e.g. MNIST)
DATASET_PATH = "./data"
# Path to the folder where the pretrained models are saved
CHECKPOINT_PATH = "./saved_models/"

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
```

4.56.2 1. The Gumbel-Sinkhorn operator

1.1 The Gumbel-Sinkhorn operator

In 0.2, we've seen how we can approximate a discrete distribution with continuous values by a temperature-dependent softmax function;

$$\text{softmax}_\tau(x_i) = \frac{\exp \frac{x_i}{\tau}}{\sum_j \exp \frac{x_j}{\tau}}$$

If we let the temperature parameter τ in this softmax approach 0, in the limit we obtain a one-hot vector corresponding to the largest x_i. We've found a differentiable way of approaching a categorical distribution! Extending this approximation to use for permutations is the point of the Sinkhorn operator.

The authors define the Sinkhorn operator S as follows:

$$S^0(X) = \exp(X) \tag{4.106}$$
$$S^l(X) = \mathcal{T}_c(\mathcal{T}_r(S^{l-1}(X))) \tag{4.107}$$
$$S(X) = \lim_{l \to \infty} S^l(X) \tag{4.108}$$

Where $\mathcal{T}_c(X) = X \oslash \mathbf{1}_N \mathbf{1}_N^T X$ and $\mathcal{T}_r(X) = X \oslash X \mathbf{1}_N \mathbf{1}_N^T$ with $\oslash$ denoting elementwise division. Essentially, we divide each row value by the sum of its row, and each column value by the sum of its column. Check if you understand these operations. The authors note that, in the limit, $S(X)$ converges to a doubly stochastic matrix! Just the kind we need.

Let's implement the sinkhorn operator!

Notes: - For numerical stability, the Sinkhorn operator is implemented in the log-space. Remember $\log(\frac{a}{b}) = \log(a) - \log(b)$! - To ensure positivity, the effective input to sinkhorn has to be `exp(log_alpha)` (elementwise). However, note that it is only at return time that entries are exponentiated. - We make use of the `logsumexp` function to first move α out of the log domain, then sum over α (rows and columns) and then return α to the log domain.

[4]:
```
def log_sinkhorn(log_alpha, n_iter):
    """Performs incomplete Sinkhorn normalization to log_alpha.
    By a theorem by Sinkhorn and Knopp [1], a sufficiently well-behaved  matrix
    with positive entries can be turned into a doubly-stochastic matrix
    (i.e. its rows and columns add up to one) via the successive row and column
    normalization.

    [1] Sinkhorn, Richard and Knopp, Paul.
    Concerning nonnegative matrices and doubly stochastic
    matrices. Pacific Journal of Mathematics, 1967
    Args:
      log_alpha: 2D tensor (a matrix of shape [N, N])
        or 3D tensor (a batch of matrices of shape = [batch_size, N, N])
      n_iters: number of sinkhorn iterations (in practice, as little as 20
        iterations are needed to achieve decent convergence for N~100)
    Returns:
      A 3D tensor of close-to-doubly-stochastic matrices (2D tensors are
        converted to 3D tensors with batch_size equals to 1)
    """
    for _ in range(n_iter):
```

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```
        log_alpha = log_alpha - torch.logsumexp(log_alpha, -1, keepdim=True)
        log_alpha = log_alpha - torch.logsumexp(log_alpha, -2, keepdim=True)
    return log_alpha.exp()
```

Let's see whether this function indeed yields a doubly stochastic matrix when we input the log of a matrix of unnormalized probabilities.

[5]:
```
# Create a matrix containing random numbers.
X = torch.rand((3, 3))
X
```

[5]:
```
tensor([[0.3834, 0.6550, 0.0086],
        [0.4759, 0.8863, 0.0279],
        [0.5294, 0.4645, 0.8727]])
```

[6]:
```
# Apply the Sinkhorn operator for 20 iterations.
S_X = log_sinkhorn(torch.log(X), n_iter=20)
S_X
```

[6]:
```
tensor([[0.4716, 0.4786, 0.0498],
        [0.4201, 0.4649, 0.1150],
        [0.1083, 0.0565, 0.8352]])
```

[7]:
```
# Check whether rows sum to 1.
assert torch.allclose(S_X.sum(dim=0), torch.ones(S_X.shape[0]))

# Check whether columns sum to 1.
assert torch.allclose(S_X.sum(dim=1), torch.ones(S_X.shape[1]))
```

1.2 Differentiably (deterministically) obtaining a permutation matrix

1.2.1 The problem with assignment probabilities

The Sinkhorn operator we defined above is only guaranteed to give us a doubly stochastic matrix X (rows and columns sum to 1) containing assignment probabilities. It is not directly clear how to get from this doubly stochastic matrix X to an actual permutation matrix P (where rows and columns are one-hot vectors). As illustration, given a doubly stochastic matrix X:

$$X = \begin{bmatrix} 0.3 & 0.3 & 0.4 \\ 0.2 & 0.3 & 0.5 \\ 0.5 & 0.4 & 0.1 \end{bmatrix}.$$

Simply taking the $\arg\max$ of every row would give us:

$$P = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix},$$

Which does not yield a valid permutation matrix.

1.2.2 From assignment probabilities a permutation matrix to as linear assignment problem

Taking a step back, the authors note that we can frame the assignment of a category $\mathbf{v}_i$ given a set of corresponding assignment probabilities $\mathbf{x}_i$ as a maximization problem. Given a one-hot vector $\mathbf{v}$ and a vector $\mathbf{x}$, we can pick the largest $\mathbf{x}_i$ by choosing $\mathbf{v}$ such that the inner product $\langle \mathbf{x}, \mathbf{v} \rangle$ is maximized.

In similar fashion, the authors note that we can frame the hard choice of a permutation matrix P given a doubly stochastic square matrix X as the solution to the linear assignment problem. Let $\mathcal{P}_N$ denote the set of all possible permutation matrices P and $\langle A, B \rangle_F$ the Frobenius inner product of matrices given by $\text{trace}(A^T B)$;

$$M(X) = \arg\max_{P \in \mathcal{P}_N} \langle P, X \rangle_F$$

The authors call this operator M the matching function. Intuitively; the best hard choice of permutation matrix P given a doubly stochastic matrix X of assignment probabilities is that P whose inverse most closely maps X to the identity matrix (as this would be the matrix with the largest trace).

We implement code for solving the assignment problem below, using a `scipy` implementation.

Notes: - Indeed, this way of finding a hard permutation matrix is non-differentiable, so it is of little use to us when training a neural net! We will only use this functionality at test time. - The `linear_sum_assignment` function expects a cost matrix as input. We instead have a probability matrix, hence we negate the probability matrix before inputting it - We go from `row` and `col` lists of the indices of our permutation matrix we should set to 1, to a permutation matrix P using `coo_matrix <https://docs.scipy.org/doc/scipy/reference/generated/scipy.sparse.coo_matrix.html>`__.

[8]:
```
## Scipy
from scipy.optimize import linear_sum_assignment
from scipy.sparse import coo_matrix


def matching(alpha):
    # Negate the probability matrix to serve as cost matrix. This function
    # yields two lists, the row and colum indices for all entries in the
    # permutation matrix we should set to 1.
    row, col = linear_sum_assignment(-alpha)

    # Create the permutation matrix.
    permutation_matrix = coo_matrix((np.ones_like(row), (row, col))).toarray()
    return torch.from_numpy(permutation_matrix)
```

Let's see whether we obtain a hard permutation matrix for the doubly stochastic matrix we created above.

[9]:
```
matching(S_X)
```

[9]:
```
tensor([[1, 0, 0],
        [0, 1, 0],
        [0, 0, 1]])
```

Cool! However, as mentioned above, this way of finding permutation matrices is **deterministic** and **non-differentiable** and hence will not do us much good when training a neural network to parameterize the variable α of a latent distribution.

1.3 Sampling a permutation matrix: the Gumbel-Matching distribution

The authors note that, in order to differentiably sample from a latent distribution such as the distribution of permutation matrices, we would like to apply techniques similar to the reparameterization trick that enable VAE's to learn. However, our latent distribution is discrete.

To set the stage, the authors recall the intuition behind the Gumbel-Softmax distribution; (1) with the Gumbel-max trick, we are able to sample from a categorical distribution but (2) since this reparameterization is non-differentiable (as we saw before) we instead relax the Gumbel distribution using the softmax operation, and thus obtain the Gumbel-Softmax distribution.

The authors introduce the Gumbel-Matching distribution $\mathcal{G}.\mathcal{M}.$, the distribution of permutation matrices we get when applying i.i.d. Gumbel noise to each of the entries of an assignment probability matrix X.

$$M(X + \epsilon) \quad \mathcal{G}.\mathcal{M}., \text{with } \epsilon \quad \text{Gumbel}$$

As in the categorical case, sampling from this distribution is still not differentiable however, as it still requires us to find the solution to a linear assignment problem.

1.3 Gumbel-Sinkhorn: Continuous relaxation of the Gumbel-Matching distribution

Now we come to the main theoretical contribution of the paper. The authors first show that the solution to the matching function $M(X)$ can in fact be obtained as the limit of the Sinkhorn operator $S(\frac{X}{\tau})$ with a small value of τ.

Finally, the authors introduce the Gumbel-Sinkhorn distribution $\mathcal{G}.\mathcal{S}.$ as the distribution obtained by applying the Sinkhorn operator on an unnormalized assignment probability matrix to which we add i.i.d. Gumbel noise:

$$S(\frac{X + \epsilon}{\tau}) \quad \mathcal{G}.\mathcal{S}., \text{with } \epsilon \quad \text{Gumbel}.$$

The authors show that in the limit, samples from the Gumbel-Sinkhorn distribution almost surely converge to the Gumbel-Matching distribution. The Sinkhorn operator is differentiable and may serve as a continuous relaxation for $M(X)$, allowing us to backpropagate through it!

For proof of this finding, we kindly refer you to appendix A of the paper.

Let's implement the Gumbel-Sinkhorn distribution!

[10]:
```
def sample_gumbel(shape, device='cpu', eps=1e-20):
    """Samples arbitrary-shaped standard gumbel variables.
    Args:
      shape: list of integers
      eps: float, for numerical stability
    Returns:
      A sample of standard Gumbel random variables
    """
    u = torch.rand(shape, device=device)
    return -torch.log(-torch.log(u + eps) + eps)
```

Let's sample some Gumbel noise.

[11]:
```
sample_gumbel((3, 3))
```

[11]:
```
tensor([[ 0.1238,  0.9551, -0.6666],
        [ 1.1801, -0.8376, -0.1454],
        [-0.9623,  3.0603,  0.2785]])
```

[12]:
```
def gumbel_sinkhorn(log_alpha, tau, n_iter):
    """ Sample a permutation matrix from the Gumbel-Sinkhorn distribution
    with parameters given by log_alpha and temperature tau.

    Args:
      log_alpha: Logarithm of assignment probabilities. In our case this is
        of dimensionality [num_pieces, num_pieces].
      tau: Temperature parameter, the lower the value for tau the more closely
        we follow a categorical sampling.
    """
    # Sample Gumbel noise.
    gumbel_noise = sample_gumbel(log_alpha.shape, device=log_alpha.device)

    # Apply the Sinkhorn operator!
    sampled_perm_mat = log_sinkhorn((log_alpha + gumbel_noise)/tau, n_iter)
    return sampled_perm_mat
```

Let's sample some permutation matrices.

[13]:
```
# For low values of tau the sampled matrices are closer to actual
# permutation matrices.
gumbel_sinkhorn(X, tau=0.01, n_iter=20)
```

[13]:
```
tensor([[1.0931e-15, 1.0000e+00, 1.6772e-38],
        [0.0000e+00, 2.3445e-10, 1.0000e+00],
        [1.0000e+00, 0.0000e+00, 0.0000e+00]])
```

[14]:
```
# For higher values of tau the sampled matrices are 'less categorical'
gumbel_sinkhorn(X, tau=10, n_iter=20)
```

[14]:
```
tensor([[0.3739, 0.3147, 0.3113],
        [0.3008, 0.3512, 0.3480],
        [0.3252, 0.3341, 0.3407]])
```

Importantly, this operation is differentiable!

[15]:
```
# Create a matrix containing random numbers. Let PyTorch know we want gradients.
X = torch.rand((3, 3), requires_grad=True)

# Sample a permutation matrix from the Gumbel-Sinkhorn distribution.
P = gumbel_sinkhorn(X*1000, tau=1, n_iter=2000)
P.sum().backward()

X.grad
```

[15]:
```
tensor([[ 0.0000e+00,  0.0000e+00,  0.0000e+00],
        [ 1.2052e-11, -1.2052e-11,  3.0366e-38],
        [ 0.0000e+00,  0.0000e+00,  0.0000e+00]])
```

4.56.3 2. Implementing a Sinkhorn Network for learning latent permutations

We now have everything in place to build our own Sinkhorn network! We will be solving the task of unscrambling MNIST digits. First, let's implement the network.

2.1 Sinkhorn Convolutional Network

We replicate the convolution-based Sinkhorn network that the authors visualize in figure 1 (see below).

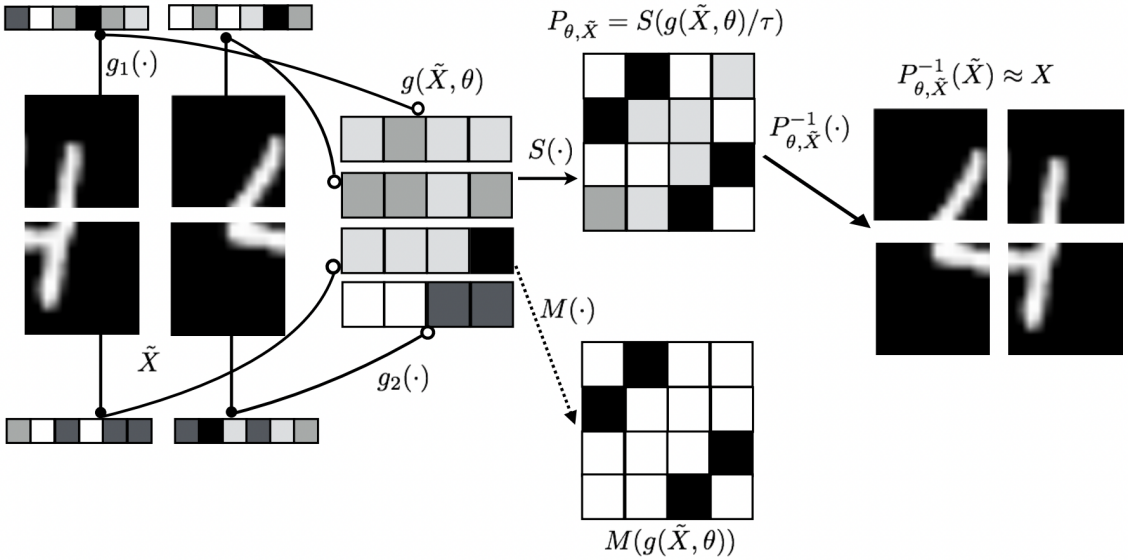

Figure 1: Schematic of Sinkhorn Network for Jigsaw puzzles. Each piece of the scrambled digit $\tilde{X}$ is processed with the same (convolutional) network g_1 (arrows with solid circles). The outputs lying on a latent space (rectangles surrounding $\tilde{X}$) are then connected through g_2 (arrows with empty circles) to conform the rows of the matrix $g(\tilde{X},\theta)$; $g(\tilde{X},\theta)_i = g_1 \circ g_2(\tilde{X}_i)$. Rows may be interpreted as unnormalized assignment probabilities, indicating individual unnormalized likelihoods of pieces of $\tilde{X}$ to be at every position in the actual image. Applying $S(\cdot)$ leads to a 'soft-permutation' $P_{\theta,\tilde{X}}$ that resolves inconsistencies in $g(\tilde{X},\theta)$. $P_{\theta,\tilde{X}}$ is then used to recover the actual X at training, although at test time one may use the actual $M(g(\tilde{X},\theta))$.

[16]:
```
import torch
import torch.nn as nn

class SinkhornConvNet(nn.Module):
    def __init__(
        self,
        in_channels: int,
        num_pieces: int,
        image_size: int,
        hidden_channels: int,
        kernel_size: int,
        tau: float = 1.0,
        n_sink_iter: int = 20,
    ):
```

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```
        super().__init__()

        # store these for later use.
        self.tau = tau
        self.n_sink_iter = n_sink_iter

        self.g_1 = nn.Sequential(
            nn.Conv2d(in_channels, hidden_channels, kernel_size, padding=kernel_size//2),
            nn.MaxPool2d(2),
            nn.ReLU(True),
            nn.BatchNorm2d(hidden_channels)
        )

        # calculate the size of a single piece in pixels
        piece_size = image_size // num_pieces

        # calculate the size of a single piece in pixels after 1 max pooling
        piece_size_after_conv = (piece_size) // (2 * 1)

        self.g_2 = nn.Linear(piece_size_after_conv**2 * hidden_channels, num_pieces**2,␣
↪bias=False)

    def forward(self, batch_pieces):
        batch_size = batch_pieces.shape[0]

        # Switch batch and piece dimensions. We want to apply the same network
        # to each of the pieces.
        pieces = batch_pieces.transpose(0, 1).contiguous()

        # Apply g_1 to each of the pieces.
        conv_pieces = []
        for piece in pieces:
            piece = self.g_1(piece)
            conv_piece = piece.reshape(batch_size, -1)
            conv_pieces.append(conv_piece)

        # Apply g_2 to each of the pieces.
        latent_pieces = []
        for piece in conv_pieces:
            latent_piece = self.g_2(piece)
            latent_pieces.append(latent_piece)

        # Create a matrix of log unnormalized assignment probabilities. After this
        # the batch dimension is batch in the first position.
        log_alphas = torch.stack(latent_pieces, 1)

        # During training, we sample from the Gumbel-Sinkhorn distribution.
        if self.training:
            permutation_matrices = gumbel_sinkhorn(log_alphas, tau=self.tau, n_iter=self.
↪n_sink_iter)

        # During eval, we solve the linear assignment problem.
```

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```
        else:
            permutation_matrices = torch.stack([
                matching(log_alpha)
                for log_alpha in log_alphas.cpu().detach().numpy()]
            ).float().to(log_alphas.device)

        # We obtain the ordered pieces as predicted by our network
        ordered_pieces = inverse_permutation_for_image(batch_pieces, permutation_
↪matrices)

        # Return the ordered pieces, along with the predicted permutation.
        # We will inspect the predicted permutation matrices during test time.
        return ordered_pieces, permutation_matrices
```

2.2 Unscrambling MNIST digits

2.2.1 Scrambling MNIST.

First, we will define some utility functions for chunking and scrambling the images.

[17]:
```
def chunk_image(image: torch.Tensor, num_pieces: int):
    """Randomly chunk a single image.
    Args:
      image: Image [channels, height, width].

    Returns:
      pieces: Image chunks in their original positions. [num_pieces, channels,
        height // num_pieces, width // num_pieces]
      random_pieces: Image chunks in their randomly permuted positions.
      permute_index: List of permuted indices.
    """
    # Get image dimensions.
    height, width = image.shape[-2:]

    # Get piece dimensions.
    piece_height = height // num_pieces
    piece_width  = width // num_pieces
    pieces = []

    # Obtain indices for each of the image chunks.
    for p_h in range(num_pieces):
        for p_w in range(num_pieces):
            left   = p_w * piece_width
            right  = left + piece_width
            top    = p_h * piece_height
            bottom = top + piece_height
            piece  = image[:,top:bottom,left:right]
            pieces.append(piece)

    pieces = torch.stack(pieces, 0)
```

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```
    # Randomly permute the index of the pieces.
    permute_index = torch.randperm(num_pieces**2)
    random_pieces = pieces[permute_index]
    return pieces, random_pieces, permute_index

def batch_chunk_image(images: torch.Tensor, num_pieces: int):
    """Randomly chunk a batch of images.
    Args:
      image: Images [batch, channels, height, width].

    Returns:
      pieces: Batch of image chunks in their original positions. [batch,
        num_pieces, channels, height // num_pieces, width // num_pieces]
      random_pieces: Batch of image chunks in their randomly permuted positions.
         [batch, num_pieces, channels, height // num_pieces, width // num_pieces]
      permute_index: Batch of permutation lists. [batch, num_pieces**2]
    """
    batch_pieces, batch_random_pieces, batch_permute_index = [], [], []
    for image in images:
        pieces, random_pieces, permute_index = chunk_image(image, num_pieces)

        batch_pieces.append(pieces)
        batch_random_pieces.append(random_pieces)
        batch_permute_index.append(permute_index)
    return torch.stack(batch_pieces, 0), torch.stack(batch_random_pieces, 0), torch.
↪stack(batch_permute_index, 0)


def inverse_permutation_for_image(X, permutation_matrix):
    """Apply the inverse of a permutation (its transpose) to a batch of image
       chunks.
    Args:
      X: Batched sets of image chunks. [batch, num_pieces, channels, height, width]
      permutation_matrix: float, for numerical stability

    Returns:
      Permuted set of image chunks.
    """
    return torch.einsum("bpq,bpchw->bqchw", (permutation_matrix, X)).contiguous()
```

Let's load the MNIST dataset and have a look.

[18]:
```
from torchvision import datasets
from torchvision import transforms

from torch import optim
from torch.utils.data import DataLoader

device = torch.device('cuda')

transform = transforms.Compose([
```

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```
    transforms.ToTensor(),
    transforms.Normalize((0.1307,), (0.3081,))
])

trainset = datasets.MNIST(root='./data', train=True, download=True, transform=transform)
testset = datasets.MNIST(root='./data', train=False, transform=transform)

train_loader = DataLoader(trainset, 64, drop_last=True, shuffle=True)
test_loader = DataLoader(testset, 64, drop_last=False, shuffle=True)
```

```
Downloading http://yann.lecun.com/exdb/mnist/train-images-idx3-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/train-images-idx3-ubyte.gz to ./data/MNIST/
↪raw/train-images-idx3-ubyte.gz
```

```
  0%|          | 0/9912422 [00:00<?, ?it/s]
```

```
Extracting ./data/MNIST/raw/train-images-idx3-ubyte.gz to ./data/MNIST/raw

Downloading http://yann.lecun.com/exdb/mnist/train-labels-idx1-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/train-labels-idx1-ubyte.gz to ./data/MNIST/
↪raw/train-labels-idx1-ubyte.gz
```

```
  0%|          | 0/28881 [00:00<?, ?it/s]
```

```
Extracting ./data/MNIST/raw/train-labels-idx1-ubyte.gz to ./data/MNIST/raw

Downloading http://yann.lecun.com/exdb/mnist/t10k-images-idx3-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/t10k-images-idx3-ubyte.gz to ./data/MNIST/
↪raw/t10k-images-idx3-ubyte.gz
```

```
  0%|          | 0/1648877 [00:00<?, ?it/s]
```

```
Extracting ./data/MNIST/raw/t10k-images-idx3-ubyte.gz to ./data/MNIST/raw

Downloading http://yann.lecun.com/exdb/mnist/t10k-labels-idx1-ubyte.gz
Downloading http://yann.lecun.com/exdb/mnist/t10k-labels-idx1-ubyte.gz to ./data/MNIST/
↪raw/t10k-labels-idx1-ubyte.gz
```

```
  0%|          | 0/4542 [00:00<?, ?it/s]
```

```
Extracting ./data/MNIST/raw/t10k-labels-idx1-ubyte.gz to ./data/MNIST/raw
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torchvision/
↪datasets/mnist.py:498: UserWarning: The given NumPy array is not writeable, and␣
↪PyTorch does not support non-writeable tensors. This means you can write to the␣
↪underlying (supposedly non-writeable) NumPy array using the tensor. You may want to␣
↪copy the array to protect its data or make it writeable before converting it to a␣
↪tensor. This type of warning will be suppressed for the rest of this program.␣
↪(Triggered internally at  /opt/conda/conda-bld/pytorch_1623448224956/work/torch/csrc/
↪utils/tensor_numpy.cpp:180.)
  return torch.from_numpy(parsed.astype(m[2], copy=False)).view(*s)
```

[19]:
```
image_batch, _ = next(iter(test_loader))

# Chunk the images into 2 pieces
num_pieces = 2
```

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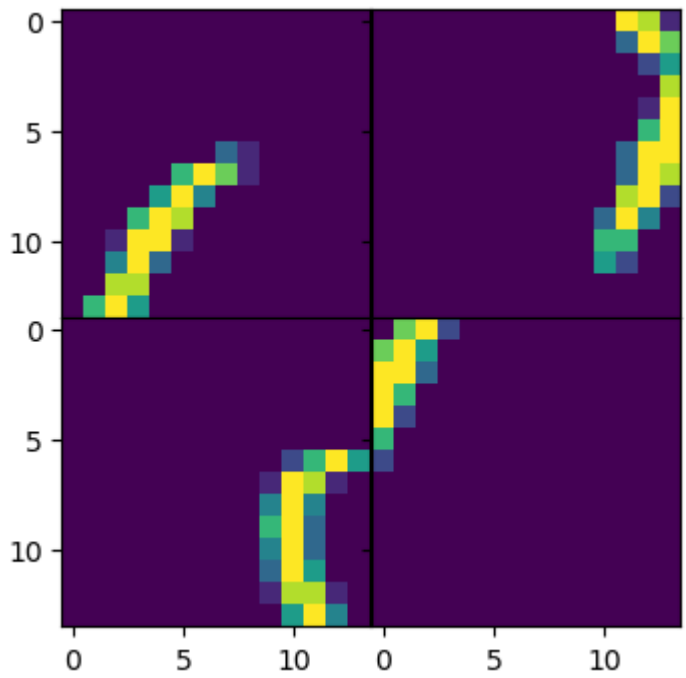
```
# Select an image from the batch
batch_idx = 0

pieces, random_pieces, perm_list = batch_chunk_image(image_batch, num_pieces=num_pieces)
pieces, random_pieces = pieces.to(device), random_pieces.to(device)

# Plot the original scrambed image.
figs, axs = plt.subplots(num_pieces, num_pieces, figsize=(4,4), sharex=True, sharey=True)
for idx, piece in enumerate(random_pieces[batch_idx]):
    axs[idx // num_pieces, idx % num_pieces].imshow(piece.cpu().squeeze())

plt.subplots_adjust(wspace=0, hspace=0)
plt.show()
```



2.2.2 Training the model

Let's set the hyperparameters for our model.

[20]:
```
tau = 0.1 # Temperature parameter.
n_sink_iter = 20 # Number of iterations of Sinkhorn operator.

num_pieces = 2 # Number of pieces each side.
image_size = 28 # Original image size.

in_channels = 1
hidden_channels = 32
kernel_size = 5
```

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```
epochs = 5
learning_rate = 1e-4
train = False # Set this to false if you only want to evaluate the model
```

[21]:
```
model = SinkhornConvNet(
    in_channels=in_channels,
    num_pieces=num_pieces,
    image_size=image_size,
    hidden_channels=hidden_channels,
    kernel_size=kernel_size,
    tau=tau,
    n_sink_iter=n_sink_iter
).to(device)

optimizer = optim.Adam(model.parameters(), learning_rate, eps=1e-8)
```

Next, we train the model. With a small number of pieces, after 5 epochs the network already obtains remarkable accuracy.

[22]:
```
if train:
    model.train()
    for epoch in range(epochs):
        sum_loss = 0
        for i, data in enumerate(train_loader):
            inputs, _ = data

            # Chunk the images into pieces
            pieces, random_pieces, _ = batch_chunk_image(inputs, num_pieces)
            pieces, random_pieces = pieces.to(device), random_pieces.to(device)

            # Predict the ordering of the pieces using the Sinkhorn Network
            ordered_pieces, _ = model(random_pieces)

            # Apply MSE Loss
            loss = torch.nn.functional.mse_loss(ordered_pieces, pieces, reduction='sum')

            optimizer.zero_grad()
            loss.backward()
            optimizer.step()

            sum_loss += loss.item()

        print(f"epoch {epoch}|  mean loss {round(sum_loss/len(train_loader.dataset), 4)}
↪")

    if not os.path.exists('./saved_models/'):
        os.mkdir('./saved_models')
    torch.save(model.state_dict(), "./saved_models/model.pth")
```

2.2.2 Evaluating the networks predictions.

To evaluate the network's predicted permutation matrices, we follow the authors in using the Kendall-Tau correlation coefficient. We measure how correlated the predicted list of permutation indices is to the original list of permutation indices.

[23]:
```
# Scipy
from scipy.stats import kendalltau

model = SinkhornConvNet(
    in_channels=in_channels,
    num_pieces=num_pieces,
    image_size=image_size,
    hidden_channels=hidden_channels,
    kernel_size=kernel_size,
    tau=tau,
    n_sink_iter=n_sink_iter
).to(device)

model.load_state_dict(torch.load(os.path.join("./saved_models/model.pth")))
model = model.to(device)
model.eval()

with torch.no_grad():

    kendall_taus = []

    for data in test_loader:
        inputs, _ = data
        pieces, random_pieces, perm_list = batch_chunk_image(inputs, num_pieces)
        pieces, random_pieces = pieces.to(device), random_pieces.to(device)

        ordered_pieces, predicted_permutation_matrices = model(random_pieces)

        # Create the list of inverse permutation indices from the predicted
        # permutation matrix.
        predicted_perm_list = predicted_permutation_matrices.transpose(1, 2).max(1)[1]

        # Obtain the Kendall-Tau correlation coefficient for the target
        # and predicted list of permutation matrices.
        for p1, p2 in zip(perm_list, predicted_perm_list):
            kendall_taus.append(
                kendalltau(p1.cpu(), p2.cpu())[0]
            )

    print(f"Mean Kendall-Tau: {np.mean(kendall_taus)}")
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/torch/nn/
↪functional.py:718: UserWarning: Named tensors and all their associated APIs are an␣
↪experimental feature and subject to change. Please do not use them for anything␣
↪important until they are released as stable. (Triggered internally at  /opt/conda/
↪conda-bld/pytorch_1623448224956/work/c10/core/TensorImpl.h:1156.)
  return torch.max_pool2d(input, kernel_size, stride, padding, dilation, ceil_mode)
```

```
Mean Kendall-Tau: 0.9930666666666667
```

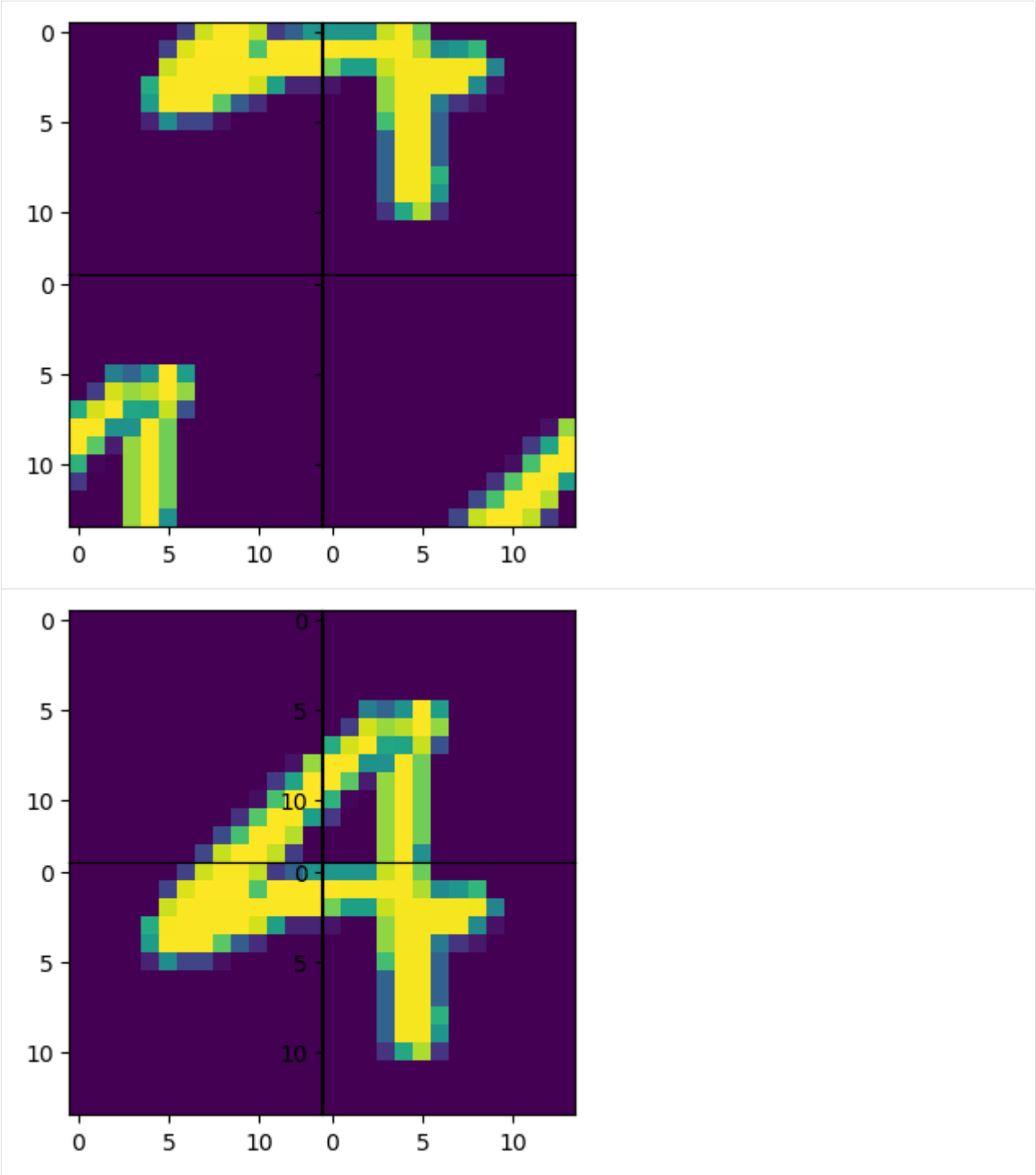
For small numbers of pieces, the correlation coefficient is close to 1! This means our Sinkhorn network is able to correctly find the correct permutation in almost all cases.

Finally, let's inspect model predictions!

[24]:
```
image_batch, _ = next(iter(test_loader))
pieces, random_pieces, perm_list = batch_chunk_image(image_batch, num_pieces)
pieces, random_pieces = pieces.to(device), random_pieces.to(device)

# Make sure we are evaluating!
model.eval()

# Predict the correctly ordered pieces.
predicted_pieces, _ = model(random_pieces)
```

[25]:
```
# Select an image from the batch.
batch_idx = 3
```

[26]:
```
# Plot the original scrambed image.
figs, axs = plt.subplots(num_pieces, num_pieces, figsize=(4,4), sharex=True, sharey=True)
for idx, piece in enumerate(random_pieces[batch_idx]):
    axs[idx // num_pieces, idx % num_pieces].imshow(piece.cpu().squeeze())
plt.subplots_adjust(wspace=0, hspace=0)
plt.show()

# Plot the predicted reconstructed image.
figs, axs = plt.subplots(num_pieces, num_pieces, figsize=(4,4))
for idx, piece in enumerate(predicted_pieces[batch_idx]):
    axs[idx // num_pieces, idx % num_pieces].imshow(piece.cpu().squeeze())
plt.subplots_adjust(wspace=0, hspace=0)
plt.show()
```


0
5
10
0
5
10
0
5
10
0
5
10
0
5
10
0
5
10
0
5
10
0
5
10

4.57 SGA - Graph Sampling for Neural Relational Inference

Notebook:
Author: Adeel Pervez

In this tutorials we show an example of a variational autoencoder model with graph structured latent spaces. This model is called Neural Relational Inference and is described in this paper. This tutorial uses code from the associated code base available here

The problem dealt by this model is one of predicting particle trajectories. Suppose that we have N interacting particles (say, charges) with some interaction structure (say, attractive/repulsive forces) that are moving about in space. For each particle we are observe its trajectory (say, position and velocity) as it moves about over some period of time T. Each new state in the trajectory of a particle will depend on the current state (position and velocity) and on the interaction with other particles. Our data consists of a set of N particle trajectories but the actual interactions are unknown. The task of our model is to learn the dynamics of the particles to predict future trajectories given example trajectories only.

Notice that the task of predicting particle dynamics would become easier if we knew the form of the interactions between particles. which we think of as a graph of interactions. Each particle in the system would occupy a node in the graph and the strength of the interaction could be represented by the weight of the graph. The interaction graph could be fed to a neural network along with the currently known trajectory which could then predict the next steps of the particles.

However, since in this problem we are not given the interaction graph, the approach taken by Neural Relational Inference is to use the encoder of a variational autoencoder to sample a graph using the given trajectory as input. For this the method uses a graph neural network as encoder.

4.57.1 Graph Network Encoder

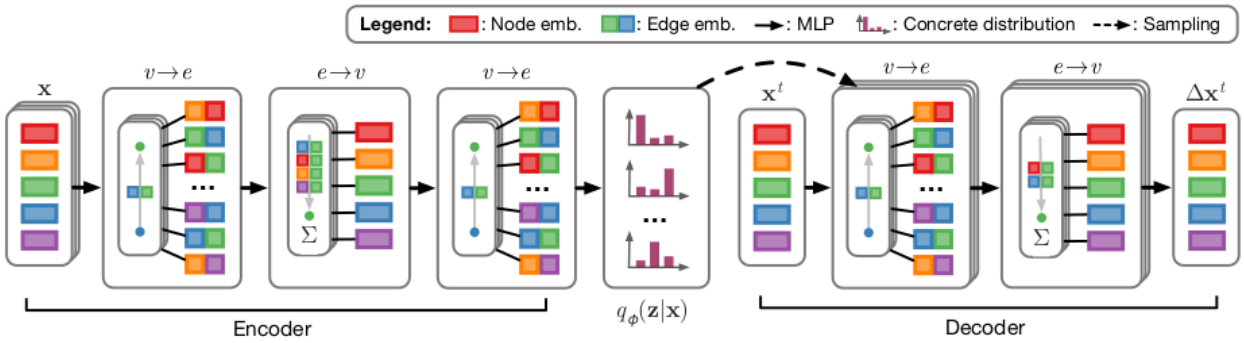
Since graph neural networks already require a graph over which to pass messages, the encoder starts with a fully connected graph with each node representing a particle. The entire trajectory information for a particle is used as the input feature for each node. Node features are transformed and passed over edges and concatenated to form edge features. This process can be repeated to get a deeper network with edge features as the output.

The edge features are then transformed into edge weights (as (unnormalized) log probabilities). Finally from these edge weights we can sample an interaction graph by sample edges according to their weights. This interaction graph then serves as a latent variable z to be used in the decoder where z_{ij} indicates whether edge (i, j) is present in the graph. Since we need to backpropagate into the encoder we relax the edge sampling operation using the Gumbel-Softmax relaxation.

4.57.2 Graph Network Decoder

In the decoder we use another graph network which uses the graph sampled by the encoder and the input trajectory to predict the next step in the trajectory for some predefined number of steps. The models uses a gaussian likelihood loss for the trajectory which is fed into the VAE loss for optimization.

The model structure can be seen in the following figure from the paper linked above.



4.57.3 Neural Relational Inference

Now we build a model to learn the dynamics of a 5 particle system connected by springs. The trajectory data for this system has been generated synthetically using the dynamical equations of motion and a ground truth interaction graph. The code to load the data is given in the `load_data` function in `utils.py`.

As the first step we begin with downloading loading the data.

[2]:
```
!wget -O 'nri_springs.zip' https://surfdrive.surf.nl/files/index.php/s/LXV9iJjxfu5jhdD/
↪download
```

```
--2022-06-21 17:04:34--  https://surfdrive.surf.nl/files/index.php/s/LXV9iJjxfu5jhdD/
↪download
Resolving surfdrive.surf.nl (surfdrive.surf.nl)... 145.100.27.67, 2001:610:108:203b:0:
↪a11:da7a:5afe
Connecting to surfdrive.surf.nl (surfdrive.surf.nl)|145.100.27.67|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 586393709 (559M) [application/zip]
Saving to: 'nri_springs.zip'

100%[=====================================>] 586,393,709 21.9MB/s   in 21s

2022-06-21 17:04:55 (26.1 MB/s) - 'nri_springs.zip' saved [586393709/586393709]
```

[2]:
```
!unzip -u nri_springs.zip -d data
```

```
Archive:  nri_springs.zip
```

[3]:
```
import time
import argparse
import pickle
import os
import datetime

import torch
import torch.nn as nn
import torch.nn.functional as F
import numpy as np
#import math
```

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```
from torch.utils.data.dataset import TensorDataset
from torch.utils.data import DataLoader
import torch.nn.functional as F
from torch.autograd import Variable


import torch.optim as optim
from torch.optim import lr_scheduler
import networkx
import matplotlib
import matplotlib.pyplot as plt

try:
    import networkx
except ModuleNotFoundError:
    !pip install --quiet networkx
    import networkx

%matplotlib inline
```

Loading and Exmaining Data

Next we load the data, convert the arrays into torch tensors and return the loader objects.

[4]:
```
def load_data(batch_size=1, suffix=''):
    loc_train = np.load('data/loc_train' + suffix + '.npy')
    vel_train = np.load('data/vel_train' + suffix + '.npy')
    edges_train = np.load('data/edges_train' + suffix + '.npy')

    loc_valid = np.load('data/loc_valid' + suffix + '.npy')
    vel_valid = np.load('data/vel_valid' + suffix + '.npy')
    edges_valid = np.load('data/edges_valid' + suffix + '.npy')

    loc_test = np.load('data/loc_test' + suffix + '.npy')
    vel_test = np.load('data/vel_test' + suffix + '.npy')
    edges_test = np.load('data/edges_test' + suffix + '.npy')

    # [num_samples, num_timesteps, num_dims, num_atoms]
    num_atoms = loc_train.shape[3]

    loc_max = loc_train.max()
    loc_min = loc_train.min()
    vel_max = vel_train.max()
    vel_min = vel_train.min()

    # Normalize to [-1, 1]
    loc_train = (loc_train - loc_min) * 2 / (loc_max - loc_min) - 1
    vel_train = (vel_train - vel_min) * 2 / (vel_max - vel_min) - 1

    loc_valid = (loc_valid - loc_min) * 2 / (loc_max - loc_min) - 1
    vel_valid = (vel_valid - vel_min) * 2 / (vel_max - vel_min) - 1
```

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```
    loc_test = (loc_test - loc_min) * 2 / (loc_max - loc_min) - 1
    vel_test = (vel_test - vel_min) * 2 / (vel_max - vel_min) - 1

    # Reshape to: [num_sims, num_atoms, num_timesteps, num_dims]
    loc_train = np.transpose(loc_train, [0, 3, 1, 2])
    vel_train = np.transpose(vel_train, [0, 3, 1, 2])
    feat_train = np.concatenate([loc_train, vel_train], axis=3)
    edges_train = np.reshape(edges_train, [-1, num_atoms ** 2])
    edges_train = np.array((edges_train + 1) / 2, dtype=np.int64)

    loc_valid = np.transpose(loc_valid, [0, 3, 1, 2])
    vel_valid = np.transpose(vel_valid, [0, 3, 1, 2])
    feat_valid = np.concatenate([loc_valid, vel_valid], axis=3)
    edges_valid = np.reshape(edges_valid, [-1, num_atoms ** 2])
    edges_valid = np.array((edges_valid + 1) / 2, dtype=np.int64)

    loc_test = np.transpose(loc_test, [0, 3, 1, 2])
    vel_test = np.transpose(vel_test, [0, 3, 1, 2])
    feat_test = np.concatenate([loc_test, vel_test], axis=3)
    edges_test = np.reshape(edges_test, [-1, num_atoms ** 2])
    edges_test = np.array((edges_test + 1) / 2, dtype=np.int64)

    feat_train = torch.FloatTensor(feat_train)
    edges_train = torch.LongTensor(edges_train)
    feat_valid = torch.FloatTensor(feat_valid)
    edges_valid = torch.LongTensor(edges_valid)
    feat_test = torch.FloatTensor(feat_test)
    edges_test = torch.LongTensor(edges_test)

    # Exclude self edges
    off_diag_idx = np.ravel_multi_index(
        np.where(np.ones((num_atoms, num_atoms)) - np.eye(num_atoms)),
        [num_atoms, num_atoms])
    edges_train = edges_train[:, off_diag_idx]
    edges_valid = edges_valid[:, off_diag_idx]
    edges_test = edges_test[:, off_diag_idx]

    train_data = TensorDataset(feat_train, edges_train)
    valid_data = TensorDataset(feat_valid, edges_valid)
    test_data = TensorDataset(feat_test, edges_test)

    train_data_loader = DataLoader(train_data, batch_size=batch_size)
    valid_data_loader = DataLoader(valid_data, batch_size=batch_size)
    test_data_loader = DataLoader(test_data, batch_size=batch_size)

    return train_data_loader, valid_data_loader, test_data_loader, loc_max, loc_min, vel_
↪max, vel_min
```

We specify the batch size and the data file suffix to load.

[5]:
```
train_loader, valid_loader, test_loader, _, _, _, _ = load_data(128, "_springs5")
```

Let's now examine this data. We get an iterator from the data loader and retrieve the first minibatch. The dataset is in the form of tuples of trajectory information and the ground truth interaction graph.

[6]:
```
(x_sample,rel_sample) = next(iter(train_loader))
print(x_sample.shape)
print(rel_sample.shape)
```

```
torch.Size([128, 5, 49, 4])
torch.Size([128, 20])
```

Let's look at the interaction graph first. This dataset consists of trajectories of systems of 5 particles. The interaction graph then specifies for each particle whether or not it interacts with every other particle. For 5 particles this gives us 20 interaction pairs.

[7]:
```
idx=0
print(rel_sample[idx])
```

```
tensor([0, 0, 0, 1, 0, 1, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 1, 0, 0, 0])
```

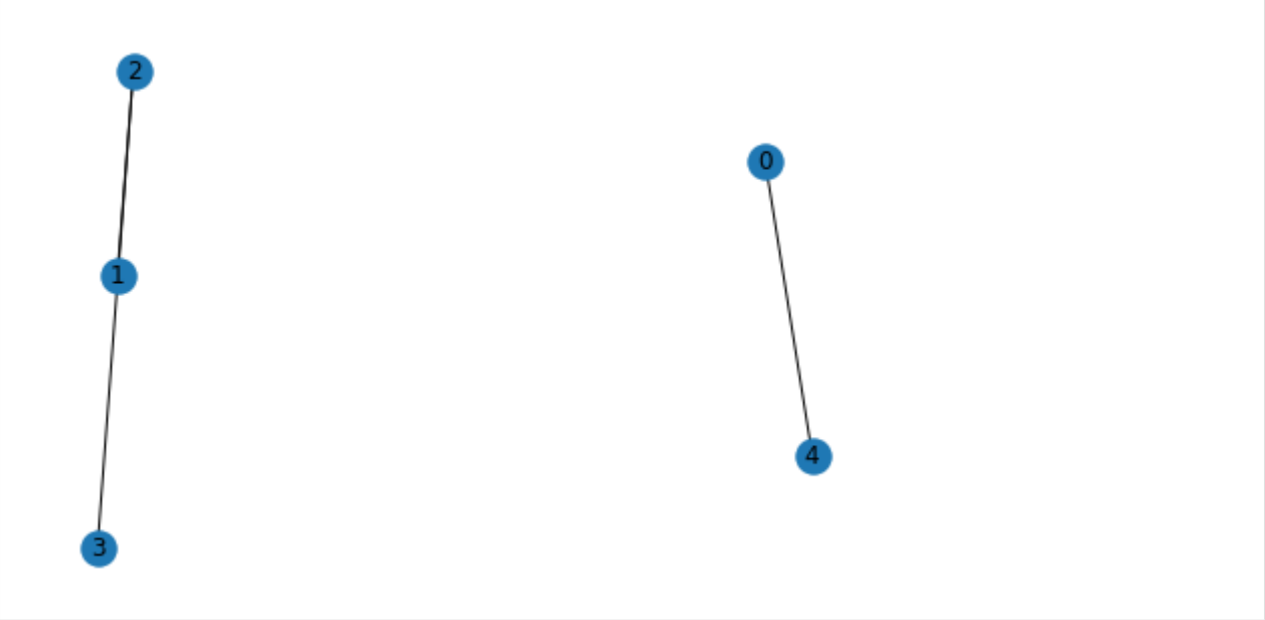
This interaction is in the form of a list of interactions pairs. We can convert one such list to an interaction graph adjacency matrix as follows. Here we specify that a particle does not interact with itself by setting the diagonal to 0.

[8]:
```
def list_to_adj(rel):
    b = torch.zeros((5*5))
    for i in range(4):
        b[i*5+i+1:(i+1)*5+(i+1)] = rel[i*5:(i+1)*5]
    return b.reshape((5,5))
b=list_to_adj(rel_sample[idx])
print(b.reshape((5,5)))
```

```
tensor([[0., 0., 0., 0., 1.],
        [0., 0., 1., 0., 0.],
        [0., 1., 0., 1., 0.],
        [0., 0., 1., 0., 0.],
        [1., 0., 0., 0., 0.]])
```

We can draw the graph

[9]:
```
def show_graph(b):
    g = b.reshape((5,5)).cpu().numpy()
    graph = networkx.from_numpy_array(g)
    networkx.draw(graph, with_labels=True)
    plt.show()
show_graph(b)
```



Let's now examine the trajectory data for the first data point.

[10]:
```
x_sample[idx].shape
```

[10]:
```
torch.Size([5, 49, 4])
```

The shape of the data above specifies that each entry consists of 5 particles with trajectories given for 49 time steps. Furthermore, each state in the trajectory is specified by a 4 dimensional vector. In this case the state is a 2d position and 2d velocity pair specifying the position and velocity of each particle at each time step. We examine the position and velocity of the first particle in the first trajectory for a couple of time steps.

[11]:
```
x_sample[idx,0,0:2,:]
```

[11]:
```
tensor([[-0.1272, -0.0987, -0.3305,  0.1197],
        [-0.1380, -0.0945, -0.3275,  0.1196]])
```

Next we define some hyperparameters.

[12]:
```
dims=4
num_atoms=5
timesteps=49
lr=0.0005
temp=0.5
output_var=5e-5

_EPS = 1e-10
```

Recall that we mentioned above that the encoder of the model works on the fully connected graph in order to predict the interaction graph. To pass messages over the fully connected graph, it is useful to define some relational masks specifying which vertices receive messages from which other ones.

[13]:
```
def encode_onehot(labels):
    classes = set(labels)
    classes_dict = {c: np.identity(len(classes))[i, :] for i, c in
```

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```
                    enumerate(classes)}
    labels_onehot = np.array(list(map(classes_dict.get, labels)),
                             dtype=np.int32)
    return labels_onehot

off_diag = np.ones([num_atoms, num_atoms]) - np.eye(num_atoms)

rel_rec = np.array(encode_onehot(np.where(off_diag)[0]), dtype=np.float32)
rel_send = np.array(encode_onehot(np.where(off_diag)[1]), dtype=np.float32)
rel_rec = torch.FloatTensor(rel_rec)
rel_send = torch.FloatTensor(rel_send)
```

We can convert edge features into node features and node features into edge features by passing messages over the fully connected graph using these masks.

[14]:
```
print(rel_rec.t(), rel_rec.shape)
```

```
tensor([[1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
         0., 0.],
        [0., 0., 0., 0., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
         0., 0.],
        [0., 0., 0., 0., 0., 0., 0., 0., 1., 1., 1., 1., 0., 0., 0., 0., 0.,
         0., 0.],
        [0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 1., 1., 1., 1., 0.,
         0., 0.],
        [0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 1.,
         1., 1.]]) torch.Size([20, 5])
```

For example to convert edge features for the 20 interactions into node features we can multiply the above matrix with the edge feature vector as

```
torch.matmul(rel_rec.t(), x)
```

which collects the messages from all neighboring nodes for each vertex and adds the messages.

Next we define a simple MLP class to be used for the nonlinear feature transformations.

[15]:
```
class MLP(nn.Module):
    """Two-layer fully-connected ELU net with batch norm."""

    def __init__(self, n_in, n_hid, n_out, do_prob=0.):
        super(MLP, self).__init__()
        self.fc1 = nn.Linear(n_in, n_hid)
        self.fc2 = nn.Linear(n_hid, n_out)
        self.bn = nn.BatchNorm1d(n_out)
        self.dropout_prob = do_prob

        self.init_weights()

    def init_weights(self):
        for m in self.modules():
            if isinstance(m, nn.Linear):
                nn.init.xavier_normal(m.weight.data)
                m.bias.data.fill_(0.1)
```

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```
            elif isinstance(m, nn.BatchNorm1d):
                m.weight.data.fill_(1)
                m.bias.data.zero_()

    def batch_norm(self, inputs):
        x = inputs.view(inputs.size(0) * inputs.size(1), -1)
        x = self.bn(x)
        return x.view(inputs.size(0), inputs.size(1), -1)

    def forward(self, inputs):
        # Input shape: [num_sims, num_things, num_features]
        x = F.elu(self.fc1(inputs))
        x = F.dropout(x, self.dropout_prob, training=self.training)
        x = F.elu(self.fc2(x))
        return self.batch_norm(x)
```

Encoder

Next we specify the VAE encoder as a graph neural network. For each particle we construct a single feature vector by using the entire trajectory information. We include three graph neural network layers that convert the node features into edge features into node features and finally into edge features. The final edge features are then used to parameterize the edge probabilities for the graph sampling operation.

[16]:
```
class MLPEncoder(nn.Module):
    def __init__(self, n_in, n_hid, n_out=2, do_prob=0.,):
        super(MLPEncoder, self).__init__()

        self.mlp1 = MLP(n_in, n_hid, n_hid, do_prob)
        self.mlp2 = MLP(n_hid * 2, n_hid, n_hid, do_prob)
        self.mlp3 = MLP(n_hid, n_hid, n_hid, do_prob)
        self.mlp4 = MLP(n_hid * 3, n_hid, n_hid, do_prob)

        self.fc_out = nn.Linear(n_hid, n_out)
        self.init_weights()

    def init_weights(self):
        for m in self.modules():
            if isinstance(m, nn.Linear):
                nn.init.xavier_normal(m.weight.data)
                m.bias.data.fill_(0.1)

    def edge2node(self, x, rel_rec, rel_send):
        # NOTE: Assumes that we have the same graph across all samples.
        incoming = torch.matmul(rel_rec.t(), x)
        return incoming / incoming.size(1)

    def node2edge(self, x, rel_rec, rel_send):
        # NOTE: Assumes that we have the same graph across all samples.
        receivers = torch.matmul(rel_rec, x)
        senders = torch.matmul(rel_send, x)
```

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```
        edges = torch.cat([senders, receivers], dim=2)
        return edges

    def forward(self, inputs, rel_rec, rel_send):
        # Input shape: [num_sims, num_atoms, num_timesteps, num_dims]
        x = inputs.view(inputs.size(0), inputs.size(1), -1)
        # New shape: [num_sims, num_atoms, num_timesteps*num_dims]

        x = self.mlp1(x)  # 2-layer ELU net per node

        x = self.node2edge(x, rel_rec, rel_send)
        x = self.mlp2(x)
        x_skip = x

        x = self.edge2node(x, rel_rec, rel_send)
        x = self.mlp3(x)
        x = self.node2edge(x, rel_rec, rel_send)
        x = torch.cat((x, x_skip), dim=2)  # Skip connection
        x = self.mlp4(x)

        return self.fc_out(x)
```

Decoder

In the decoder we take the initial state and attempt to predict the remaining trajectory. To predict a single time step the function `single_step_forward` takes as input the current state and the proposed interaction graph. From the states of the nodes as node features we produce edge features by passing messages over all neighbors and then zero out the messages corresponding to edges not present in the proposed graph. The edge messages are then sent to the corresponding nodes after which we apply an MLP to compute the next prediction as a difference with the current state. The process is then repeated for all timesteps.

[17]:
```
class MLPDecoder(nn.Module):
    """MLP decoder module."""

    def __init__(self, n_in_node, edge_types, msg_hid, msg_out, n_hid,
                 do_prob=0.):
        super(MLPDecoder, self).__init__()

        self.msg_fc1 = (nn.Linear(2 * n_in_node, msg_hid))
        self.msg_fc2 = (nn.Linear(msg_hid, msg_out))
        self.msg_out_shape = msg_out

        self.out_fc1 = nn.Linear(n_in_node + msg_out, n_hid)
        self.out_fc2 = nn.Linear(n_hid, n_hid)
        self.out_fc3 = nn.Linear(n_hid, n_in_node)

        print('Using learned interaction net decoder.')

        self.dropout_prob = do_prob

    def single_step_forward(self, single_timestep_inputs, rel_rec, rel_send,
```

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```
                            single_timestep_rel_type):

        # single_timestep_inputs has shape
        # [batch_size, num_timesteps, num_atoms, num_dims]

        # single_timestep_rel_type has shape:
        # [batch_size, num_timesteps, num_atoms*(num_atoms-1), num_edge_types]

        # Node2edge
        receivers = torch.matmul(rel_rec, single_timestep_inputs)
        senders = torch.matmul(rel_send, single_timestep_inputs)
        pre_msg = torch.cat([senders, receivers], dim=-1)

        msg = F.relu(self.msg_fc1(pre_msg))
        msg = F.dropout(msg, p=self.dropout_prob)
        msg = F.relu(self.msg_fc2(msg))
        msg = msg * single_timestep_rel_type[:, :, :, 1:2]

        # Aggregate all msgs to receiver
        agg_msgs = msg.transpose(-2, -1).matmul(rel_rec).transpose(-2, -1)
        agg_msgs = agg_msgs.contiguous()

        # Skip connection
        aug_inputs = torch.cat([single_timestep_inputs, agg_msgs], dim=-1)

        # Output MLP
        pred = F.dropout(F.relu(self.out_fc1(aug_inputs)), p=self.dropout_prob)
        pred = F.dropout(F.relu(self.out_fc2(pred)), p=self.dropout_prob)
        pred = self.out_fc3(pred)

        # Predict position/velocity difference
        return single_timestep_inputs + pred

    def forward(self, inputs, rel_type, rel_rec, rel_send, pred_steps=1):
        # NOTE: Assumes that we have the same graph across all samples.

        inputs = inputs.transpose(1, 2).contiguous()

        sizes = [rel_type.size(0), inputs.size(1), rel_type.size(1),
                 rel_type.size(2)]
        rel_type = rel_type.unsqueeze(1).expand(sizes)

        time_steps = inputs.size(1)
        assert (pred_steps <= time_steps)
        preds = []

        # initial step
        last_pred = inputs[:, 0:1, :, :]
        # NOTE: Assumes rel_type is constant (i.e. same across all time steps).
        curr_rel_type = rel_type[:, 0:1, :, :]

        # Run n prediction steps
```

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```
        for step in range(0, pred_steps):
            last_pred = self.single_step_forward(last_pred, rel_rec, rel_send,
                                                 curr_rel_type)
            preds.append(last_pred)

        sizes = [preds[0].size(0), preds[0].size(1) * pred_steps,
                 preds[0].size(2), preds[0].size(3)]

        #output = Variable(torch.zeros(sizes))
        output = torch.zeros(sizes)
        if inputs.is_cuda:
            output = output.cuda()

        # Re-assemble correct timeline
        for i in range(len(preds)):
            output[:, i:i+1, :, :] = preds[i]

        pred_all = output[:, :(inputs.size(1) - 1), :, :]

        return pred_all.transpose(1, 2).contiguous()
```

Now we make a few helper arrays to specify the sending and receiving nodes in a message passing step. These simply correspond to the neighbors in a fully connected graph.

[18]:
```
# Generate off-diagonal interaction graph
off_diag = np.ones([num_atoms, num_atoms]) - np.eye(num_atoms)

rel_rec = np.array(encode_onehot(np.where(off_diag)[0]), dtype=np.float32)
rel_send = np.array(encode_onehot(np.where(off_diag)[1]), dtype=np.float32)
rel_rec = torch.FloatTensor(rel_rec)
rel_send = torch.FloatTensor(rel_send)
```

[19]:
```
#edge weights have dim 2
encoder = MLPEncoder(timesteps * dims, 256, 2)
decoder = MLPDecoder(n_in_node=dims,
                         edge_types=2,
                         msg_hid=256,
                         msg_out=256,
                         n_hid=256, )
```

```
Using learned interaction net decoder.
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/ipykernel_launcher.
↪py:16: UserWarning: nn.init.xavier_normal is now deprecated in favor of nn.init.xavier_
↪normal_.
  app.launch_new_instance()
```

[20]:
```
encoder.cuda()
decoder.cuda()
rel_rec = rel_rec.cuda()
rel_send = rel_send.cuda()
```

[21]:
```
optimizer = optim.Adam(list(encoder.parameters()) + list(decoder.parameters()),
                       lr=lr)
train_loader, valid_loader, test_loader, loc_max, loc_min, vel_max, vel_min = load_data(
    128, "_springs5")
```

Discrete Sampling

We will sample graphs by selecting a subset of the fully connected graph using the weights output by the encoder by using Gumbel softmax. We define the Gumbel softmax routines below as from the earlier tutorial.

[22]:
```
def my_softmax(input, axis=1):
    trans_input = input.transpose(axis, 0).contiguous()
    soft_max_1d = F.softmax(trans_input)
    return soft_max_1d.transpose(axis, 0)

def sample_gumbel(shape, eps=1e-10):
    U = torch.rand(shape).float()
    return - torch.log(eps - torch.log(U + eps))

def gumbel_softmax_sample(logits, tau=1, eps=1e-10):
    gumbel_noise = sample_gumbel(logits.size(), eps=eps)
    if logits.is_cuda:
        gumbel_noise = gumbel_noise.cuda()
    y = logits + Variable(gumbel_noise)
    return my_softmax(y / tau, axis=-1)


def gumbel_softmax(logits, tau=1, hard=False, eps=1e-10):
    y_soft = gumbel_softmax_sample(logits, tau=tau, eps=eps)
    if hard:
        shape = logits.size()
        _, k = y_soft.data.max(-1)
        y_hard = torch.zeros(*shape)
        if y_soft.is_cuda:
            y_hard = y_hard.cuda()
        y_hard = y_hard.zero_().scatter_(-1, k.view(shape[:-1] + (1,)), 1.0)
        y = Variable(y_hard - y_soft.data) + y_soft
    else:
        y = y_soft
    return y
```

Next we define some helper functions for computing accuracies, prediction loss and KL divergence.

[23]:
```

def kl_categorical_uniform(preds, num_atoms, num_edge_types, add_const=False,
                           eps=1e-16):
    kl_div = preds * torch.log(preds + eps)
    if add_const:
        const = np.log(num_edge_types)
        kl_div += const
```

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```
    return kl_div.sum() / (num_atoms * preds.size(0))


def nll_gaussian(preds, target, variance, add_const=False):
    neg_log_p = ((preds - target) ** 2 / (2 * variance))
    if add_const:
        const = 0.5 * np.log(2 * np.pi * variance)
        neg_log_p += const
    return neg_log_p.sum() / (target.size(0) * target.size(1))

def edge_accuracy(preds, target):
    _, preds = preds.max(-1)
    correct = preds.float().data.eq(
        target.float().data.view_as(preds)).cpu().sum()
    return np.float(correct) / (target.size(0) * target.size(1))
```

We can now train the model. This runs the encoder to get the latent graph parameters and samples the edges using the `gumbel_softmax` function to get a latent graph which is then passed to the decoder. We use the uniform categorical prior to compute the KL divergence for the VAE loss and a Gaussian likelihood loss with a fixed various for the predictions.

[24]:
```
def train(epoch, best_val_loss):
    t = time.time()
    nll_train = []
    acc_train = []
    kl_train = []
    mse_train = []

    encoder.train()
    decoder.train()
    #scheduler.step()
    for batch_idx, (data, relations) in enumerate(train_loader):

        #if args.cuda:
        data, relations = data.cuda(), relations.cuda()
        #data, relations = Variable(data), Variable(relations)

        optimizer.zero_grad()

        logits = encoder(data, rel_rec, rel_send)
        edges = gumbel_softmax(logits, tau=temp, hard=False)
        prob = my_softmax(logits, -1)

        output = decoder(data, edges, rel_rec, rel_send, timesteps)

        target = data[:, :, 1:, :]

        loss_nll = nll_gaussian(output, target, output_var)

        loss_kl = kl_categorical_uniform(prob, num_atoms, 2)
```

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```
        loss = loss_nll + loss_kl

        acc = edge_accuracy(logits, relations)
        acc_train.append(acc)

        loss.backward()
        optimizer.step()

        mse_train.append(F.mse_loss(output, target).item())
        nll_train.append(loss_nll.item())
        kl_train.append(loss_kl.item())

    nll_val = []
    acc_val = []
    kl_val = []
    mse_val = []

    encoder.eval()
    decoder.eval()
    for batch_idx, (data, relations) in enumerate(valid_loader):
        #if args.cuda:
        data, relations = data.cuda(), relations.cuda()

        logits = encoder(data, rel_rec, rel_send)
        edges = gumbel_softmax(logits, tau=temp, hard=True)
        prob = my_softmax(logits, -1)

        # validation output uses teacher forcing
        output = decoder(data, edges, rel_rec, rel_send, timesteps)

        target = data[:, :, 1:, :]
        loss_nll = nll_gaussian(output, target, output_var)

        loss_kl = kl_categorical_uniform(prob, num_atoms, 2)

        acc = edge_accuracy(logits, relations)
        acc_val.append(acc)

        mse_val.append(F.mse_loss(output, target).item())
        nll_val.append(loss_nll.item())
        kl_val.append(loss_kl.item())

    print('Epoch: {:04d}'.format(epoch),
          'nll_train: {:.10f}'.format(np.mean(nll_train)),
          'kl_train: {:.10f}'.format(np.mean(kl_train)),
          'mse_train: {:.10f}'.format(np.mean(mse_train)),
          'acc_train: {:.10f}'.format(np.mean(acc_train)),
          'nll_val: {:.10f}'.format(np.mean(nll_val)),
          'kl_val: {:.10f}'.format(np.mean(kl_val)),
          'mse_val: {:.10f}'.format(np.mean(mse_val)),
          'acc_val: {:.10f}'.format(np.mean(acc_val)),
```

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```
            'time: {:.4f}s'.format(time.time() - t))
    return np.mean(nll_val)
```

[25]:
```
t_total = time.time()
best_val_loss = np.inf
best_epoch = 0
for epoch in range(10):
    val_loss = train(epoch, best_val_loss)
    if val_loss < best_val_loss:
        best_val_loss = val_loss
        best_epoch = epoch
```

```
/home/apervez/anaconda3/envs/pytorch1.9_2/lib/python3.7/site-packages/ipykernel_launcher.
↪py:3: UserWarning: Implicit dimension choice for softmax has been deprecated. Change␣
↪the call to include dim=X as an argument.
  This is separate from the ipykernel package so we can avoid doing imports until
Epoch: 0000 nll_train: 82207.3378531610 kl_train: -0.4316625203 mse_train: 0.0428163237␣
↪acc_train: 0.5102473625 nll_val: 13553.7608163568 kl_val: -0.5440562605 mse_val: 0.
↪0070592507 acc_val: 0.5207624604 time: 39.0780s
Epoch: 0001 nll_train: 10482.0866405750 kl_train: -0.8068965521 mse_train: 0.0054594203␣
↪acc_train: 0.5672370524 nll_val: 9608.4652764043 kl_val: -0.9848571722 mse_val: 0.
↪0050044091 acc_val: 0.6150959256 time: 38.8682s
Epoch: 0002 nll_train: 7622.5237534467 kl_train: -0.9681852530 mse_train: 0.0039700646␣
↪acc_train: 0.6575051950 nll_val: 7999.2846617880 kl_val: -0.9407296845 mse_val: 0.
↪0041662942 acc_val: 0.6889833861 time: 38.9219s
Epoch: 0003 nll_train: 6435.7686271180 kl_train: -0.8848858903 mse_train: 0.0033519629␣
↪acc_train: 0.7282261029 nll_val: 6645.1351859177 kl_val: -0.8726646719 mse_val: 0.
↪0034610081 acc_val: 0.7700009889 time: 38.9155s
Epoch: 0004 nll_train: 5131.3655265945 kl_train: -0.7572590768 mse_train: 0.0026725863␣
↪acc_train: 0.8130400815 nll_val: 4324.9007367484 kl_val: -0.6718307175 mse_val: 0.
↪0022525526 acc_val: 0.8733831092 time: 38.8255s
Epoch: 0005 nll_train: 3077.5661589874 kl_train: -0.5434278285 mse_train: 0.0016028991␣
↪acc_train: 0.8900433584 nll_val: 3308.9670224733 kl_val: -0.4739881709 mse_val: 0.
↪0017234204 acc_val: 0.9016811709 time: 38.8303s
Epoch: 0006 nll_train: 2414.1095929158 kl_train: -0.4157265660 mse_train: 0.0012573488␣
↪acc_train: 0.9119279492 nll_val: 2641.4135803995 kl_val: -0.3809240079 mse_val: 0.
↪0013757363 acc_val: 0.9172320016 time: 38.7057s
Epoch: 0007 nll_train: 2069.5431726168 kl_train: -0.3398666841 mse_train: 0.0010778871␣
↪acc_train: 0.9245336477 nll_val: 2234.7316940887 kl_val: -0.3186675578 mse_val: 0.
↪0011639228 acc_val: 0.9260087025 time: 38.7296s
Epoch: 0008 nll_train: 1849.1151079339 kl_train: -0.2847137487 mse_train: 0.0009630808␣
↪acc_train: 0.9329048114 nll_val: 2150.2909862663 kl_val: -0.2708904545 mse_val: 0.
↪0011199433 acc_val: 0.9309285997 time: 38.5185s
Epoch: 0009 nll_train: 1702.6682693989 kl_train: -0.2453164980 mse_train: 0.0008868064␣
↪acc_train: 0.9392786925 nll_val: 1745.5321894778 kl_val: -0.2299301707 mse_val: 0.
↪0009091314 acc_val: 0.9383850870 time: 38.7678s
```

Visualizing Discovered Graphs

We can now visualize the actual and predicted interaction graphs for some examples.

[26]:
```
data,relations = next(iter(valid_loader))
data=data.cuda()
relations=relations.cuda()
```

[27]:
```
logits = encoder(data, rel_rec, rel_send)
_, rel = logits.max(-1)
```

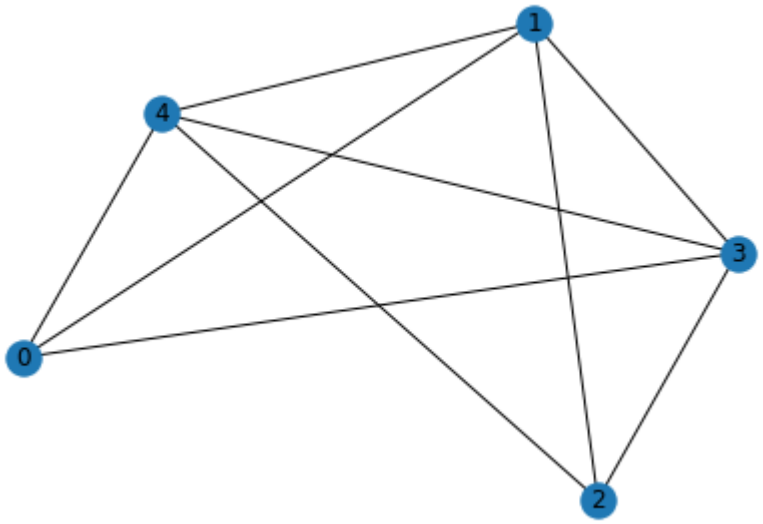
[28]:
```
print(rel[0])
print(relations[0])
```

```
tensor([1, 0, 1, 1, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       device='cuda:0')
tensor([1, 0, 1, 1, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       device='cuda:0')
```

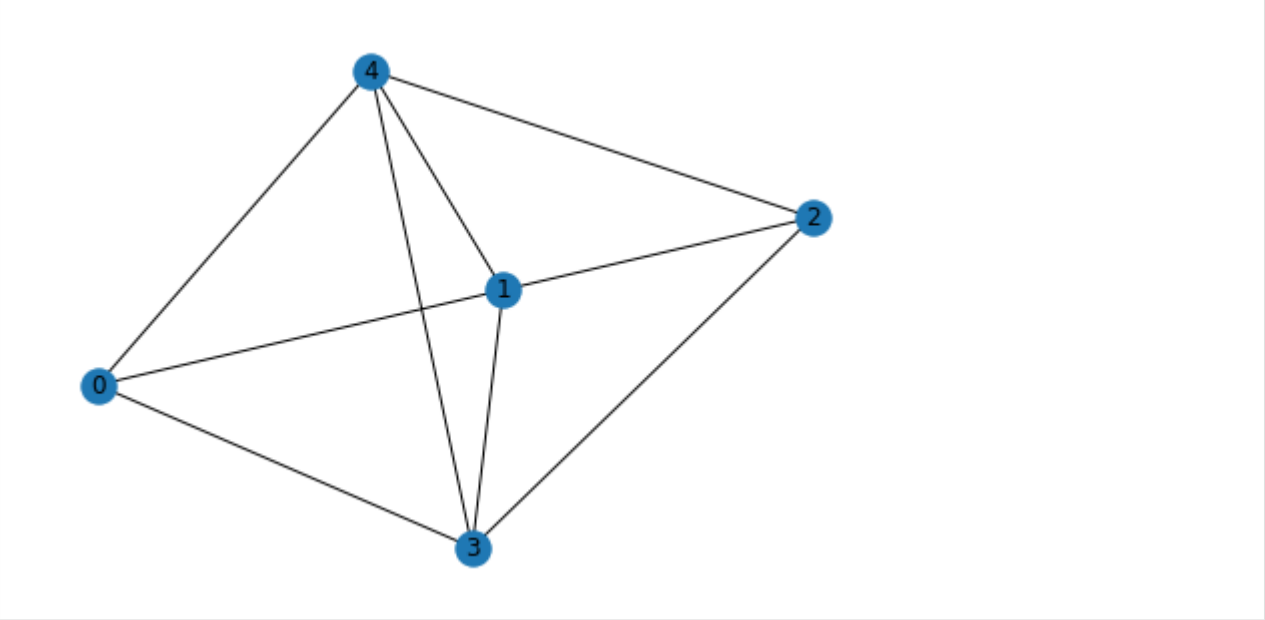
[29]:
```
for i in range(5):
    g_act = list_to_adj(relations[i])
    g_pred = list_to_adj(rel[i])

    print("Original")
    show_graph(g_act)
    print("Predicted")
    show_graph(g_pred)
```

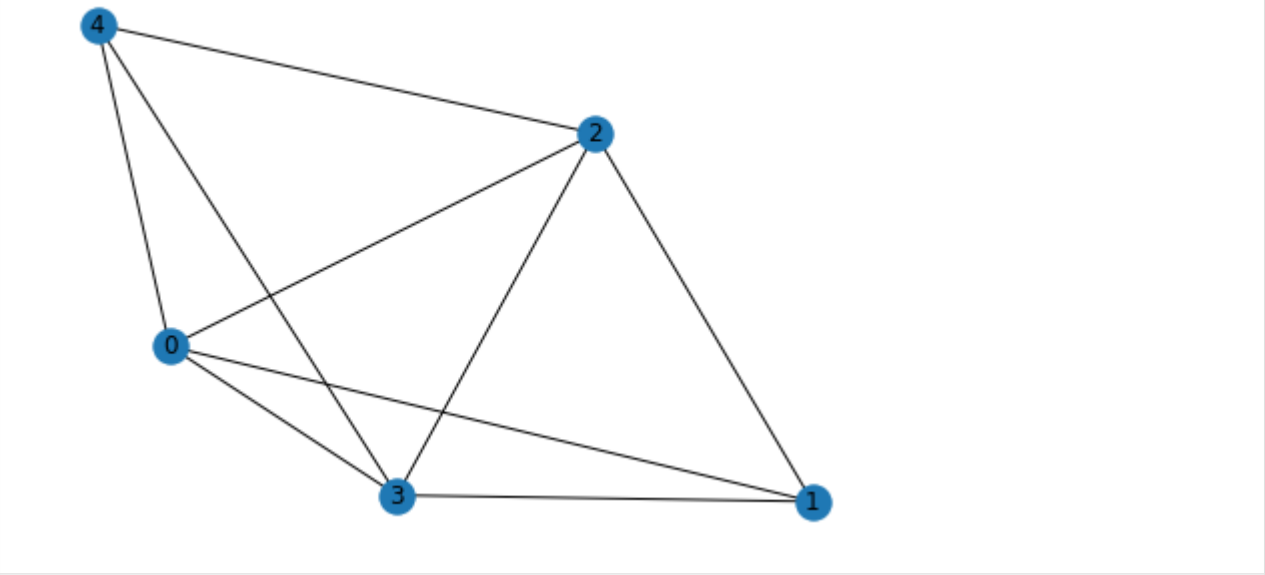
```
Original
```



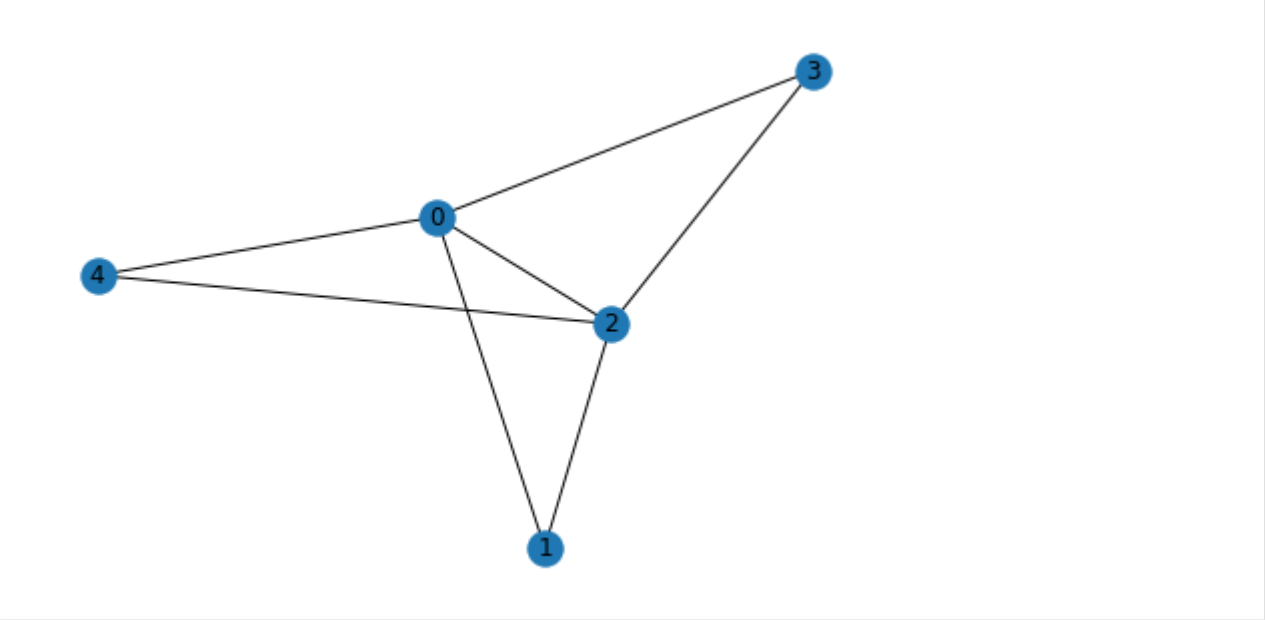

```
Predicted
```



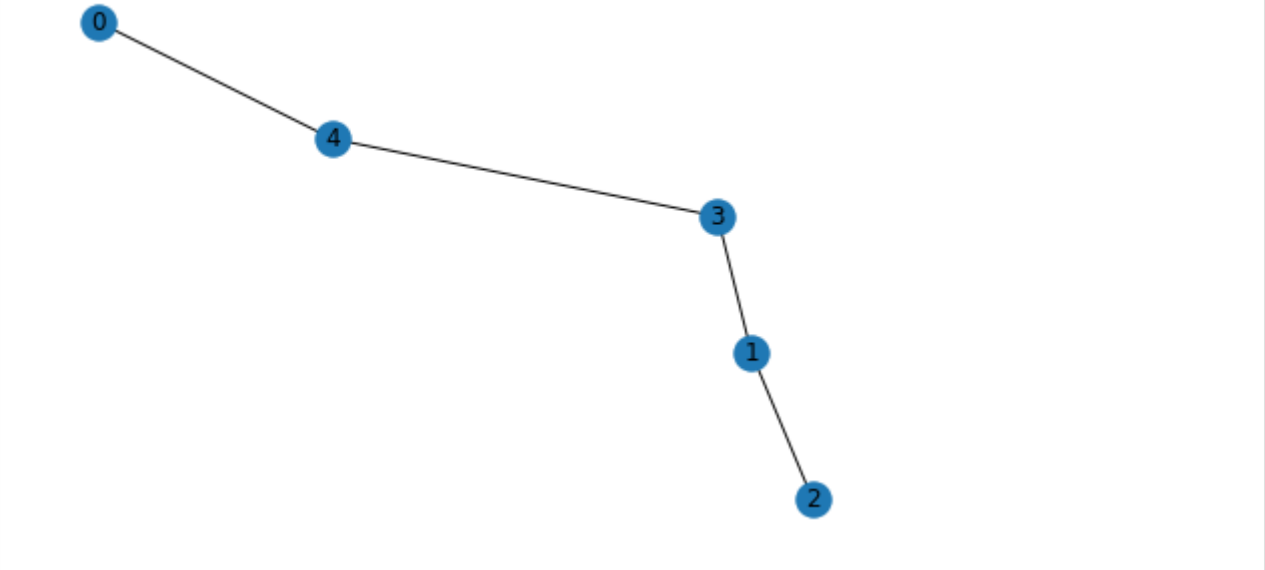
Original



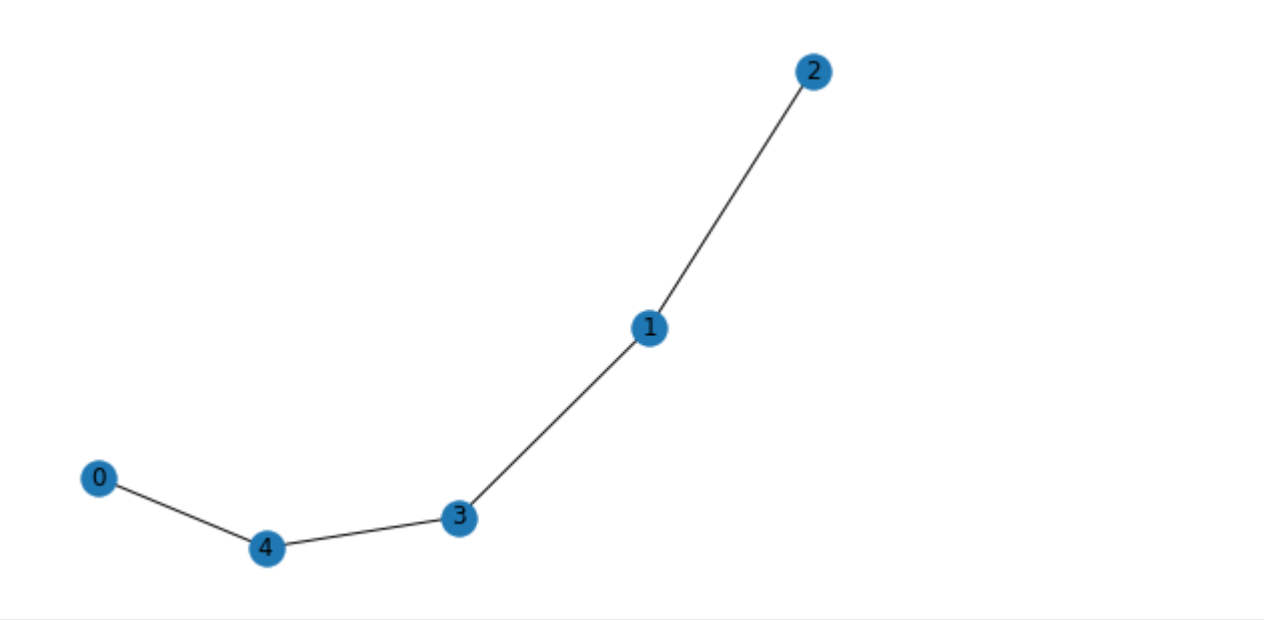
Predicted



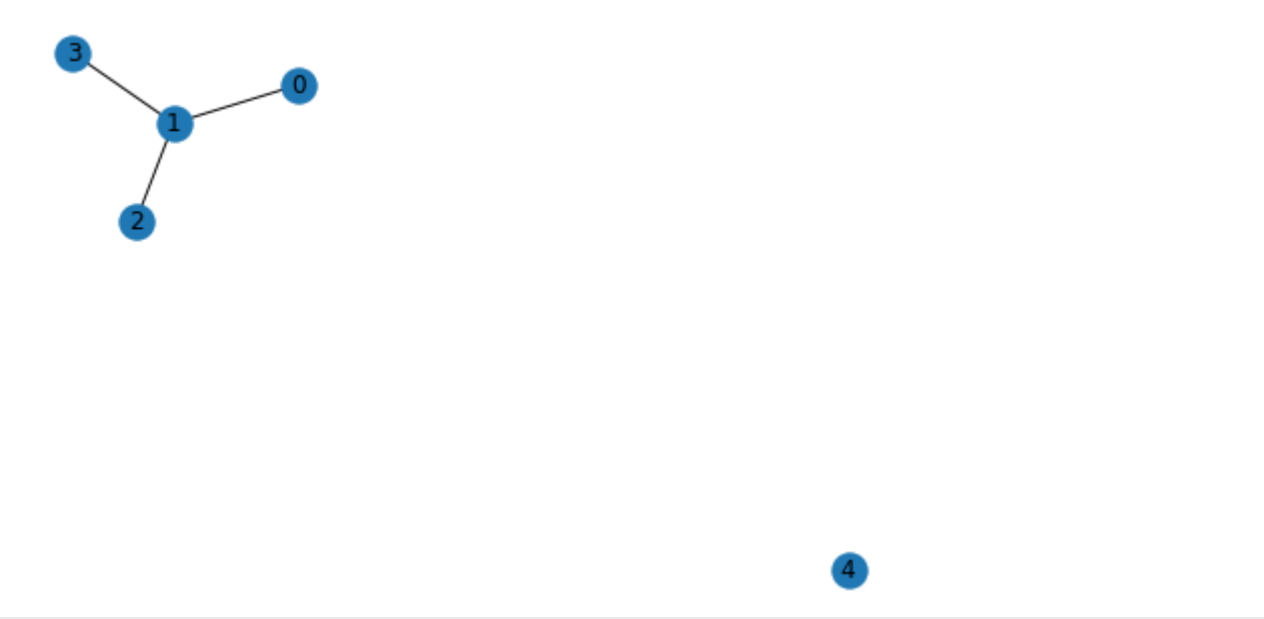
Original



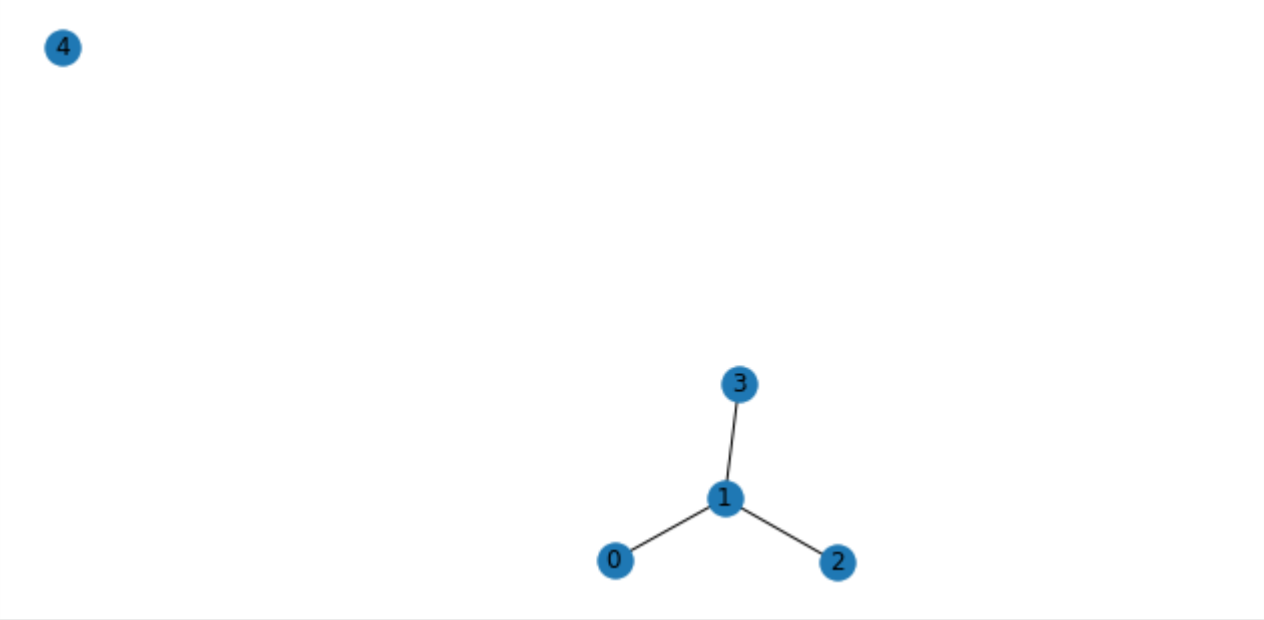
Predicted



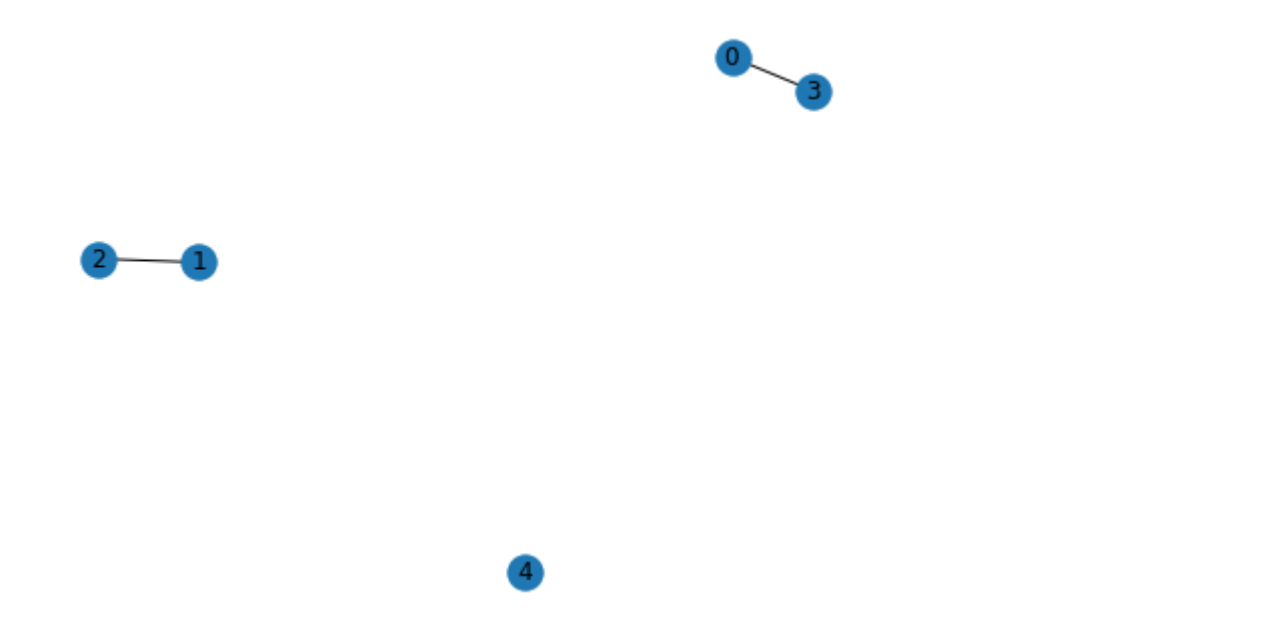
Original



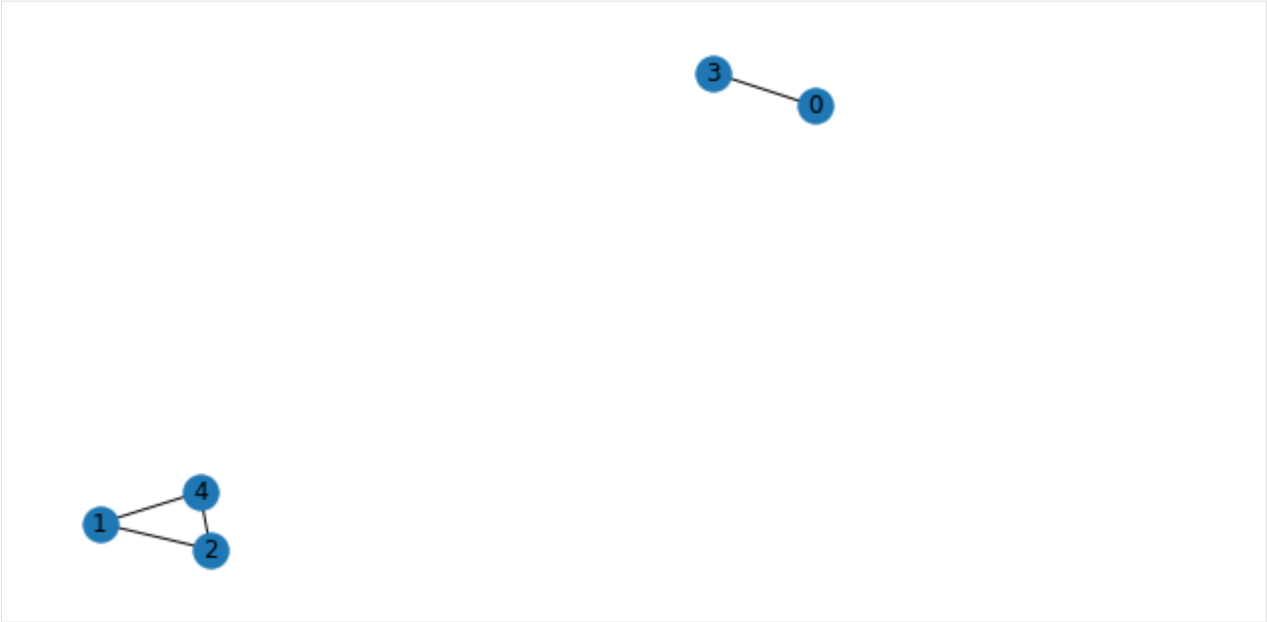
Predicted



Original



Predicted



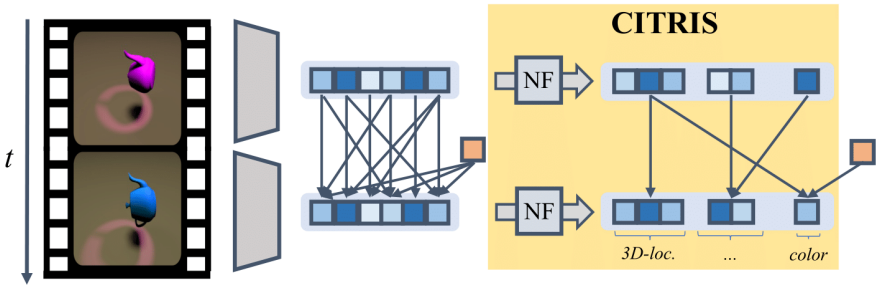
4.57.4 References

Neural Relational Inference for Interacting Systems

4.58 CRL - Causal Identifiability from Temporal Intervened Sequences

Filled notebook:
Pre-trained models:
Authors: Angelos Nalmpantis, Danilo de Goede

Understanding the latent causal factors of a dynamical system from visual observations is a crucial step towards agents reasoning in complex environments. In this tutorial, we will have a closer look at CITRIS (Lippe et al., 2022a), a variational autoencoder framework that learns causal representations from temporal sequences of images in which underlying causal factors have possibly been intervened upon. As shown in the figure below, CITRIS utilizes both temporal consistency and interventions (orange) in order to identify causal variables (blue) from an image sequence. In contrast to previous work in causal representation learning, CITRIS considers causal variables as potentially multi-dimensional vectors. Furthermore, by introducing a normalizing flow, CITRIS can be easily extended to leverage and disentangle representations obtained by already pretrained autoencoders.



In the remainder of this tutorial, we first provide a brief introduction to the recently emerging field of causal representation learning (CRL). Then, we will look into the inner workings of CITRIS in greater detail, before performing a number of experiments to demonstrate its capabilities.

Let's start with importing our standard libraries here.

[1]:
```
## Standard libraries
import os
import sys
import importlib
import numpy as np

## Imports for plotting
import matplotlib.pyplot as plt
plt.set_cmap('cividis')
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('svg', 'pdf') # For export
import matplotlib
matplotlib.rcParams['lines.linewidth'] = 2.0
import seaborn as sns
sns.set()
import ipywidgets as widgets

## tqdm for loading bars
from tqdm.notebook import tqdm

## PyTorch
import torch
import torch.nn as nn
import torch.nn.functional as F

# PyTorch Lightning
try:
    import pytorch_lightning as pl
except ModuleNotFoundError: # Google Colab does not have PyTorch Lightning installed by␣
↪default. Hence, we do it here if necessary
    !pip install --quiet pytorch-lightning>=1.4
    import pytorch_lightning as pl

try:
    from scipy.stats import norm
except ModuleNotFoundError: # The DL2022 environment does not have Scipy installed by␣
↪default. Hence, we do it here if necessary.
    !pip install --quiet scipy
    from scipy.stats import norm

try:
    import networkx as nx
except ModuleNotFoundError: # The DL2022 environment does not have NetworkX installed by␣
↪default. Hence, we do it here if necessary.
    !pip install --quiet networkx
    import networkx as nx
```

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```
DATASET_PATH = "../data"
CHECKPOINT_PATH = "../../saved_models/DL2/CRL"

# Setting the seed
pl.seed_everything(42)

# Ensure that all operations are deterministic on GPU (if used) for reproducibility
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False

device = torch.device("cuda:0") if torch.cuda.is_available() else torch.device("cpu")
print("Device:", device)

# Import a minimized version of the code implementation of CITRIS
if not os.path.exists('CITRIS_DL2'):
    !git clone https://github.com/danilodegoede/CITRIS_DL2

sys.path.append('CITRIS_DL2')
module_name = 'CITRIS_DL2.models.citris_nf'
importlib.invalidate_caches()
CITRISNF = importlib.import_module(module_name).CITRISNF
```

```
/tmp/ipykernel_37834/2678719819.py:12: DeprecationWarning: `set_matplotlib_formats` is␣
↪deprecated since IPython 7.23, directly use `matplotlib_inline.backend_inline.set_
↪matplotlib_formats()`
  set_matplotlib_formats('svg', 'pdf') # For export
Global seed set to 42
```

```
Device: cuda:0
```

We also have a few pre-trained models, which we download below.

[2]:
```
import urllib.request
from urllib.error import HTTPError

base_url = "https://raw.githubusercontent.com/phlippe/saved_models/main/DL2/CRL/"
pretrained_files = ['ae.ckpt', 'citris.ckpt']
os.makedirs(CHECKPOINT_PATH, exist_ok=True)

# For each file, check whether it already exists. If not, try downloading it.
for file_name in pretrained_files:
    file_path = os.path.join(CHECKPOINT_PATH, file_name)
    if "/" in file_name:
        os.makedirs(file_path.rsplit("/", 1)[0], exist_ok=True)
    if not os.path.isfile(file_path):
        file_url = base_url + file_name
        print(f"Downloading {file_url}...")
        try:
            urllib.request.urlretrieve(file_url, file_path)
        except HTTPError as e:
            print("Something went wrong. Please try later again, or contact the author␣
↪with the full output including the following error:\n", e)
```

4.58.1 Causal Representation Learning

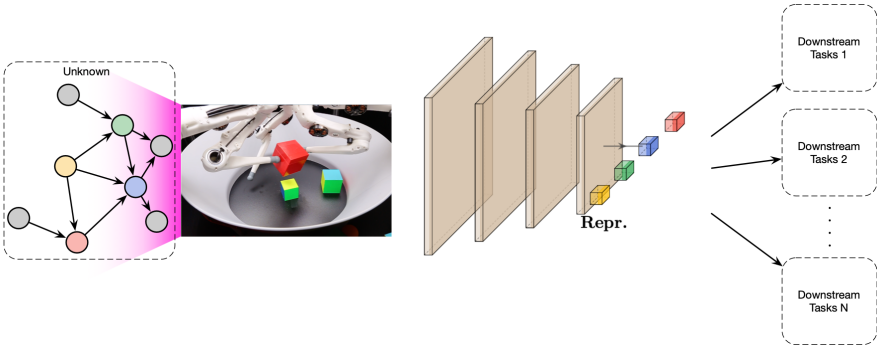
Over the last decades, machine learning has become one of the most prominent approaches in artificial intelligence. One major advantage of machine learning approaches over earlier AI paradigms is their ability to automatically learn useful features from high-dimensional observations. However, in doing so, machine learning methods generally only leverage statistical information in data, and not the causal process that underlies how that data was generated in the first place. Consequently, they often struggle to perform tasks that involve out-of-domain generalization and planning.

Causal inference, on the other hand, goes beyond the statistical description of data, and instead aims to reason about the effect of *interventions* in the system underlying the data. In order to perform such causal reasoning, it is required that the causal variables and their relations are provided beforehand. However, many real-world observations, such as objects in images, are not structured into such variables to begin with.

Thus, an emerging field of research is *causal representation learning* (CRL), in which the task is to identify such causal variables including their relations from low-level data such as images or videos (Schölkopf et al., 2021). The central idea here is that a low-level observation X is merely a view on the state of a causal system $C_1, \dots, C_n$:

$$X = h(C_1, \dots, C_n),$$

where $h : \mathcal{C} \to \mathcal{X}$ is some non-linear function that maps from the causal system's state space to the observational space. In CRL, we are then interested in approximating the inverse of G (e.g. with a neural network) in order to map a low-level observation to high-level causal variables that are useful for a set of downstream tasks of interest, as shown in the figure below.



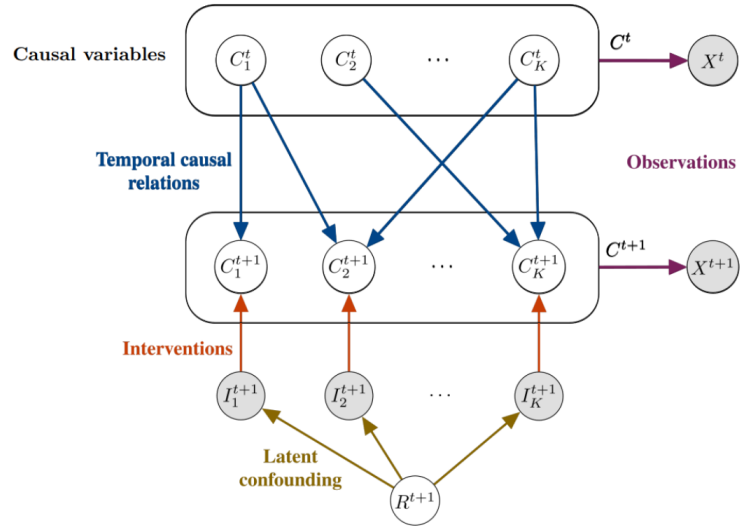
4.58.2 Causal Setting: TempoRal Intervened Sequences (TRIS)

The setting in which CITRIS aims to identify causal variables is TempoRal Intervented Sequences (TRIS). In TRIS, we assume that the underlying latent causal process is a dynamic Bayesian network (DBN) over a set of K causal factors $(C_1, C_2, \dots, C_K)$. In the corresponding causal graph $G = (V, E)$, each node $i \in V$ is associated with the causal factor C_i, which can be scalar or vector-valued, and each edge $(i, j) \in E$ represents a causal relation from C_i to C_j: $C_i \to C_j$.

TRIS further assumes that each causal factor C_i is instantiated at each time step t, denoted C_i^t, and its causal parents can only be causal factors at time $t-1$. In other words, we assume that DBN resembles a temporal latent causal process with K causal factors $(C_1^t, C_2^t, \dots, C_K^t)_{t=1}^T$ that change over time according to the temporal dynamics governed by the DBM. Crucially, in TRIS, some causal factors might have been intervened upon at each time step, and we have access to the corresponding intervention targets (but not the intervention values). We denote these intervention targets by the binary vector $I^t \in \{0, 1\}^K$, whose i-th component is 1 if and only if the causal factor C_i has been intervened upon at time t (i.e., C_i^t has been intervened upon).

It is important to note that we never observe the causal factors $(C^t)_{t=1}^T$ in TRIS, and instead only have access to a temporal sequence of high-level observations $(X^t)_{t=1}^T$ along with the corresponding intervention targets $(I^t)_{t=2}^T$. Each high-level observation represents a noisy and entangled view of all causal factors. Formally, $X^t = h(C_1^t, C_2^t, \dots, C_K^t, E_o^t)$, where E_o^t represents noise, and $h : \mathcal{C} \times \mathcal{E} \to \mathcal{X}$ is a function from the causal factor space $\mathcal{C}$ and the space of the noise

variables $\mathcal{E}$ to the observation space $\mathcal{X}$. The overall set-up of TRIS is illustrated below, with observed variables shown in gray and latent variables in white.



It is noteworthy that the set-up of TRIS is general enough to be able to describe many dynamical systems. In fact, CITRIS (and iCITRIS (Lippe et al., 2022b), which we do not discuss in this notebook) have been successful in identifying the causal structure in settings that range from 3D rendered objects to pinball and pong.

In the remainder of this tutorial, we will focus on the Causal3DIdent dataset, which we will describe in further detail next.

Causal3DIdent

Now we will look into the Causal3DIdent dataset. It contains a sequence of images with the intervention targets at each time-step. In the below cell, we will load a small sample of the dataset.

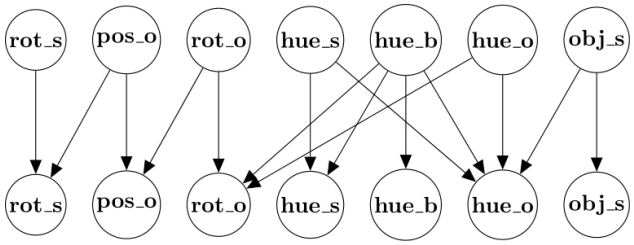
[3]:
```
causal3d_dataset = dict(np.load(os.path.join('CITRIS_DL2', 'data', 'causal3d.npz')))
print(causal3d_dataset.keys())
```

```
dict_keys(['images', 'interventions'])
```

The intervention targets declare which causal variables were intervened upon. In Causal3DIdent, we consider the following 7 causal variables (with 11 causal dimensions in total):

Variable	Values
Object position (pos_o)	$[x, y, z] \in [-2, 2]^3$
Object rotation (rot_o)	$[\alpha, \beta] \in [0, 2\pi)^2$
Spotlight rotation (rot_s)	$\theta \in [0, 2\pi)$
Object hue (hue_o)	$h_{\text{obj}} \in [0, 2\pi)$
Spotlight hue (hue_s)	$h_{\text{light}} \in [0, 2\pi)$
Background hue (hue_b)	$h_{\text{bg}} \in [0, 2\pi)$
Object shape (obj_s)	$s \in \{\text{teapot, cow, head, horse, armadillo, dragon, hare}\}$

Note that in our experiments, we will use a variant of Causal3DIdent that only contains the teapot as a possbile object shape. The relations among these causal variables are shown in the figure below.



Below you can see what causal variables were intervened at each time-step. The i-th intervention targets imply that the causal variables of the $(i-1)$-th image were intervened, resulting in the i-th image.

[4]:
```
time_steps = 4
print(causal3d_dataset['interventions'][0:time_steps])
```

```
[[0 0 0 0 0 0 0 0 0 0 0 0]
 [0 0 0 0 1 0 1 0 1 0 0 0]
 [0 0 0 1 1 0 0 0 0 0 0 0]
 [0 0 0 0 0 0 0 0 1 0 0 0]]
```

Note that each interention target has 12 dimensions instead of 11. This is because the last dimension is the object material, which is not modeled by CITRIS.

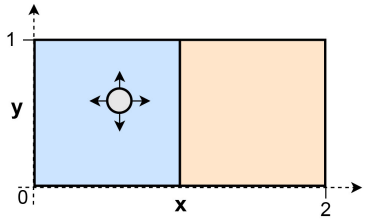
In the next cell, we will plot a sequence of images. Note how the intervention targets, printed above, affect the object and the surrounding environment.

[5]:
```
plt.rcParams['figure.figsize'] = [10, 5]
for i in range(time_steps):
    plt.subplot(1, time_steps, i+1)
    plt.imshow(causal3d_dataset['images'][i])
    plt.xlabel(f't = {i}')
    plt.xticks([])
    plt.yticks([])
plt.show()
```

4.58.3 Theoretical Framework of CITRIS

Minimal Causal Variables

In TRIS, we generally cannot disentangle two causal factors if they are always intervened upon jointly, or, on the contrary, if they are never intervened upon. Furthermore, multidimensional causal variables are not always identifiable in TRIS as interventions might only affect a subset of its dimensions. Instead, we may only be able to identify *minimal causal variables*, which only model the information of a causal factor that is strictly affected by a provided intervention. For example, consider the causal process illustrated below, where a ball can move freely within the box it is currently in, but can only jump into another box under an intervention (which keeps the relative position of the ball within the box intact).



If we were to model this process by two causal variables, the relative position within the box x' (on which we never intervene) and the current box b, we are only able to identify the causal variable b, since x' is not affected by the

interventions. In other words, b is the minimal causal variable in this example.

To formalize the notion of minimal causal variables, consider an invertible map $s_i : \mathcal{D}_i^{M_i} \to \mathcal{D}_i^{\text{var}} \times \mathcal{D}_i^{\text{inv}}$ that splits each causal variable C_i^t into an *intervention-dependent* part $s_i^{\text{var}}(C_i^t)$ and an *intervention-independent* part $s_i^{\text{inv}}(C_i^t)$ (note that this invertible map is not unique). We are interested in identifying the split where $s_i^{\text{var}}(C_i^t)$ *only* contains information that truly depends on the intervention. Under this split, $s_i^{\text{var}}(C_i^t)$ is defined as the *minimal causal variable* and denoted by $s_i^{\text{var}^*}(C_i^t)$.

Learning the Minimal Causal Variables

In order to learn the minimal causal variables in TRIS, CITRIS approximates the inverse of the observation function based on data triplets $\{x^t, x^{t+1}, I^{t+1}\}$ by learning two components. 1. An invertible mapping from observations to latent space: $g_\theta : \mathcal{X} \to \mathcal{Z}$. 2. An assignment function $\psi : [\![1..M]\!] \to [\![0..K]\!]$ that maps each dimension of $\mathcal{Z}$ to a causal factor in $\mathcal{C}$.

For the assignment function, $\psi(j) = 0, j \in [\![1..M]\!]$ indicates that the latent dimension z_j does not correspond to any dimension of the minimal causal variable, but rather to some dimension of $s_i^{\text{inv}}(C_i^t)$, and $z_{\psi_i} = \{z_j \mid j \in [\![1..M]\!], \psi(j) = i\}$ denotes the set of latent variables that ψ assigns to the causal variable C_i.

To encourage a disentanglement of the causal factors, CITRIS model a **transition prior** in the latent space that conditions each latent variable on exactly one of the intervention targets:

$$p_\phi\left(z^{t+1}|z^t, I^{t+1}\right) = \prod_{i=0}^{K} p_\phi\left(z_{\psi_i}^{t+1}|z^t, I_i^{t+1}\right),$$

where $I_0^{t+1} = 0$. Combining the transition prior and the invertible mapping g_θ, the objective of CITRIS is to maximize the following likelihood:

$$p_{\phi,\theta}(x^{t+1}|x^t, I^{t+1}) = \left|\frac{\partial g_\theta(x^{t+1})}{\partial x^{t+1}}\right| p_\phi(z^{t+1}|z^t, I^{t+1})$$

If a model $\mathcal{M}$ maximizes the information content of z_{ψ_0} under the constraint of maximizing this likelihood $\mathcal{L}_{\phi,\theta}(x^{t+1}|x^t, I^{t+1})$ and no intervention variable is a deterministic function of any other intervention variable, then $\mathcal{M}$ is shown to identify any causal system $\mathcal{S}$ (i.e., it identifies the minimal causal variables of $\mathcal{S}$ up to an invertible transformation). Intuitively, this means that the latent variables z_{ψ_i} only model the information of C_i that strictly depends on the intervention targets I_i^{t+1}.

4.58.4 Practical Implementation of CITRIS

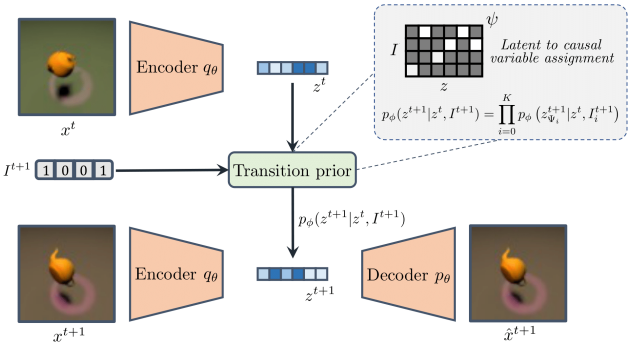
Thus far, we have sketched a theoretical framework to identify causal variables from an image sequence with known intervention targets. We are now ready to provide a practical implementation of the model $\mathcal{M}$. The original paper proposes two variants for such a model: CITRIS-VAE and CITRIS-NF.

CITRIS-VAE

Recall that CITRIS approximates $h^{-1} : \mathcal{X} \to \mathcal{C} \times \mathcal{E}$ by learning two components: the intertible mapping $g_\theta : \mathcal{X} \to \mathcal{Z}$, and the assignment function $\psi : [\![1..M]\!] \to [\![0..K]\!]$. CITRIS-VAE approximate g_θ via a variational autoencoder (AE), with encoder q_θ and decoder p_θ, that optimizes the following Evidence Lower Bound (ELBO):

$$\mathcal{L}_{\text{ELBO}} = -\mathbb{E}_{z^{t+1}}\left[\log \underbrace{p_\theta\left(x^{t+1}|z^{t+1}\right)}_{\text{Decoder}}\right] + \mathbb{E}_{z^t,\psi}\left[\sum_{i=0}^{K} D_{\text{KL}}\left(\underbrace{q_\theta(z_{\psi_i}^{t+1}|x^{t+1})}_{\text{Encoder}} || \underbrace{p_\phi(z_{\psi_i}^{t+1}|z^t, I_i^{t+1})}_{\text{Transition Prior}}\right)\right]$$

To ensure that blocks of latent variables that are assigned to different causal variables are independent conditioned on the latent variables of the previous time steps and the interventions (i.e., the $z_{\psi_i}^{t+1}$'s are independent conditioned on z^t and I_i^{t+1}), the KL divergence term utilizes the prior definition of the transition prior. Thereby, the assignment function ψ is learned via a Gumbel-Softmax distribution per latent variable. The overall setup of CITRIS-VAE is visualized below.



Now that we have discussed CITRIS-VAE in detail, we can implement a simplified version of it:

[6]:
```
class CITRISVAE_MINIMAL(nn.Module):
    """
    This is a minimal implementation of CITRIS-VAE and is meant for educational purposes.
    Several steps and details have been omitted for clarity.
    You can find the full version at:
    https://github.com/phlippe/CITRIS/blob/main/models/citris_vae/lightning_module.py
    """

    def __init__(self, encoder, decoder, transition_prior):
        super().__init__()

        # Encoder-Decoder
        self.encoder, self.decoder = encoder, decoder

        # Transition prior
        self.prior_t1 = transition_prior

    def forward(self, x):
        """ Returns the reconstruction of x"""
        # Encode
        z_mean, z_logstd = self.encoder(x)

        # Reparameterization trick
        z_sample = z_mean + torch.randn_like(z_mean) * z_logstd.exp()

        # Decode
        x_rec = self.decoder(z_sample)

        return x_rec, z_sample, z_mean, z_logstd

    def _get_loss(self, batch):
        """ Returns the loss for a batch of data"""
        # Unpack batch
        imgs, labels, target = batch
```

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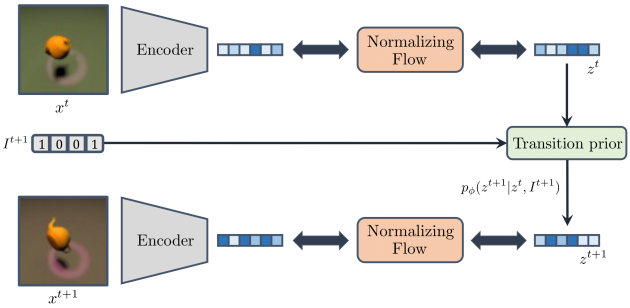
```
        # Encode
        z_mean, z_logstd = self.encoder(imgs)

        # Reparameterization trick
        z_sample = z_mean + torch.randn_like(z_mean) * z_logstd.exp()

        # Decode
        x_rec = self.decoder(z_sample)

        # Calculate KL divergence between every pair of frames
        kld = self.prior_t1.kl_divergence(z_t=z_mean[:, :-1],
                                          target=target,
                                          z_t1_mean=z_mean[:, 1:],
                                          z_t1_logstd=z_logstd[:, 1:],
                                          z_t1_sample=z_sample[:, 1:])

        # Reconstruction loss
        rec_loss = F.mse_loss(x_rec, labels[:, 1:], reduction='none').sum()

        # Get the full loss
        loss = (kld + rec_loss.sum(dim=1)).mean()

        return loss
```

CITRIS-NF

One disadvantage of using a VAE is that it may struggle to model complex images that contain many details that are small yet relevant to model the causal system. CITRIS-NF overcomes this issue by separating the learning process of g_θ into the following two components: 1. **(Pretrained) Autoencoder (AE)**: Learns to encode the high-dimensional observations *without* disentangling the dimensions in the latent space. 2. **Normalizing Flow (NF)**: Learns to map the entangled latent representation of the autoencoder into a disentangled one.

In contrast to the VAE setup, the autoencoder does not require the latent distribution to be similar to a transition prior, thus allowing it to model more complex marginal distributions. We visualize the setup of CITRIS-NF below.



While it is not strictly necessary the understand normalizing flows to follow the remainder of this tutorial, we highly recommend having a look at Tutorial 11 or the following video for readers that are interested in learning more about them.

Similar to the VAE setup, we implement a simplified version of CITRIS-NF below:

[7]:
```
class CITRISNF_MINIMAL(nn.Module):
    """
    This is a minimal implementation of CITRIS-NF and is meant for educational purposes.
    Several steps and details have been omitted for clarity.
    You can find the full version at:
    https://github.com/phlippe/CITRIS/blob/main/models/citris_nf/lightning_module.py
    """

    def __init__(self, encoder, decoder, transition_prior, flow):
        super().__init__()

        # Encoder-Decoder
        self.encoder, self.decoder = encoder, decoder

        # Transition prior
        self.prior_t1 = transition_prior

        # Normalizing Flow
        self.flow = flow

    def forward(self, x, noise_level=0.0):
        """ Returns the reconstruction of x
            Note that we do not use the flow in the forward pass.
            The flow is used only to disentangle the latent space.
        """
        # Encode
        z = self.encoder(x)

        # Add some noise
        z = z + torch.randn_like(z) * noise_level

        # The decoder expects the original latent space.
        # Executing the flow and then reversing has no effect.
        # Thus, we skip the flow here.
        # # Execute the flow to disentangle the latent space
        # z, _ = self.flow(z)
        # # Reverse the flow to get the original latent space
        # z = self.flow.reverse(z)

        # Decode
        x_rec = self.decoder(z)

        return x_rec, z

    def _get_loss(self, batch, noise_level=0.0):
        """ Returns the loss for a batch of data"""

        # Unpack batch
        imgs, target = batch

        # Encode
        z = self.encoder(imgs)
```

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```
        # Add some noise
        z = z + torch.randn_like(z) * noise_level

        # Execute the flow
        z_sample, ldj = self.flow(z)  # ldj = log(det(Jacobian))

        # Calculate the negative log likelihood of the transition prior
        nll = self.prior_t1.sample_based_nll(z_t=z_sample[:, :-1],
                                             z_t1=z_sample[:, 1:],
                                             target=target)

        # Add LDJ and prior NLL for full loss
        loss = nll + ldj

        return loss
```

Target Classifier (optional)

To further guide the disentanglement in latent space, both CITRIS-VAE and CITRIS-NF can make use of a target classifier that is trained to predict the intervention targets from the latent variables over time, *i.e.*, $p(I^{t+1}|z^t, z_{\psi_i}^{t+1})$ for $i \in [\![0..K]\!]$. To achieve this, we can train $z_{\psi_i}^{t+1}$ to have higher mutual information with the intervention target I_i^{t+1} of its intended causal variable C_i.

4.58.5 Experiments

Now that we have discussed how CITRIS works, we are ready to perform some experiments to gain a better understanding of its capabilities. First, we will study CITRIS' capabilities to disentangle the causal factors on the Causal3DIdent dataset. Then, we will demonstrate how we can use the learned latent dimensions of CITRIS to perform interventions in the image space, and conversely analyze how these latent dimensions are affected if we change a single causal variable in the input image.

For our experiments, we will use variant of CITRIS-NF that has been pre-trained on the Causal3DIdent dataset discussed previously.

[8]:
```
pretrained_CITRIS_path = os.path.join(CHECKPOINT_PATH, "citris" + ".ckpt")

if os.path.isfile(pretrained_CITRIS_path):
    print(f"Found pretrained model at {pretrained_CITRIS_path}, loading...")
    model = CITRISNF.load_from_checkpoint(pretrained_CITRIS_path)
    model.eval()
```

```
Found pretrained model at ../../saved_models/DL2/CRL/citris.ckpt, loading...
```

Triplet Evaluation

To reveal complex dependencies between latent variables, we first perform a parameter-free evaluation involving triplets of images. The first two elements of the triplets are randomly sampled from the original test dataset, and the third element is created based on a random combination of causal factors of the first two images.

Let's first inspect what a single image triplet might look like:

[9]:
```
triplets = dict(np.load(os.path.join('CITRIS_DL2', 'data', 'causal3d_triplets.npz')))

image_triplet = triplets['images'][0]

plt.rcParams['figure.figsize'] = [10, 5]
labels = ['Image 1', 'Image 2', 'Combination of Causal Factors']
for i in range(3):
    plt.subplot(1, 3, i+1)
    plt.imshow(image_triplet[i])
    plt.xlabel(labels[i])
    plt.xticks([])
    plt.yticks([])

plt.show()
```

The triplet dataset further stores a binary mask $\mathbf{m} \in \mathbb{R}^K$, whose k-th element is 1 if C_k was taken from image 2, and 0 if it was taken from image 1.

[10]:
```
triplet_mask = triplets['mask'][0]
mask_names = ['x_position', 'y_position', 'z_position', 'alpha_rotation', 'beta_rotation
↪', 'gamma_rotation', 'theta_spot_light', 'hue_object', 'hue_spot_light', 'hue_
↪background', 'shape', 'material']

assigned_to = {0: [], 1: []}
for mask_name, mask in zip(mask_names, triplet_mask):
    assigned_to[mask].append(mask_name)

print(f"Assigned to image 1: {assigned_to[0]}")
print(f"Assigned to image 2: {assigned_to[1]}")
```

```
Assigned to image 1: ['y_position', 'z_position', 'alpha_rotation', 'beta_rotation',
↪'theta_spot_light', 'hue_spot_light', 'hue_background']
Assigned to image 2: ['x_position', 'gamma_rotation', 'hue_object', 'shape', 'material']
```

For evaluation, we encode the two test images independently, perform the combination of ground-truth causal factors as is done for the third image in latent space, and use the decoder to generate a new image, which ideally resembles the ground-truth third image.

[11]:
```
@torch.no_grad()
def encode(imgs):
    imgs = torch.from_numpy(imgs)[...,:3]
    if len(imgs.shape) == 5:
        imgs = imgs.permute(0, 1, 4, 2, 3)
        imgs = imgs.flatten(0, 1)
    else:
        imgs = imgs.permute(0, 3, 1, 2)
        imgs = imgs.flatten(0)
    print(imgs.shape)
    imgs = imgs.float() / 255.0
    imgs = imgs * 2.0 - 1.0
    encs = model.autoencoder.encoder(imgs)
    encs = encs.unflatten(0, (-1, triplets['images'].shape[1]))
    return encs
```

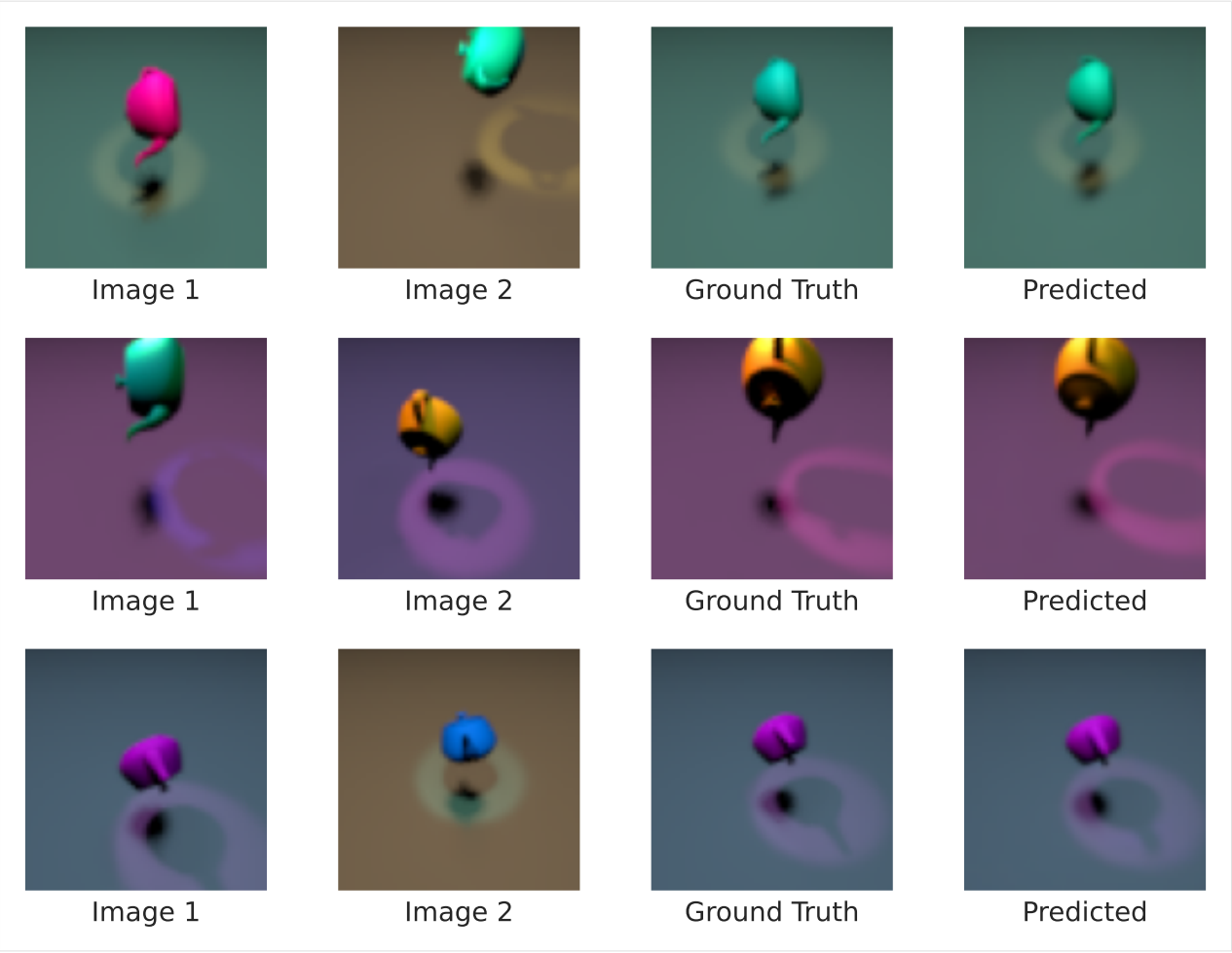
[12]:
```
@torch.no_grad()
def triplet_reconstruction(imgs, source):
    # Encode Images
    x_encs = encode(imgs)

    # Pass through the normalizing flow to disentagle the latent space
    input_samples, _ = model.flow(x_encs[:,:2].flatten(0, 1))
    input_samples = input_samples.unflatten(0, (-1, 2))

    # Get the assignment of the latent variables to the causal ones
    target_assignment = model.prior_t1.get_target_assignment(hard=True)

    # Take the latent variables from the encoding of image 1 respective to the mask
    mask_1 = (target_assignment[None,:,:] * (1 - source[:,None,:])).sum(dim=-1)
    # Take the rest from image 2
    mask_2 = 1 - mask_1

    # Create an encoding with the combination of causal variables from image 1 and image␣
↪2
    triplet_samples = mask_1 * input_samples[:,0] + mask_2 * input_samples[:,1]

    # Reverse the flow from the triplet_samples
    triplet_samples = model.flow.reverse(triplet_samples)

    # Decode and get the new image
    triplet_rec = model.autoencoder.decoder(triplet_samples)

    return triplet_rec
```

[13]:
```
triplet_rec = triplet_reconstruction(triplets['images'][0:3], triplets['mask'][0:3, [0,1,
↪2,3,4,6,7,8,9,10]])
```

```
torch.Size([9, 3, 64, 64])
```

Finally, we plot reconstructed triplet images next to the original image triplets.

[14]:
```
def normalize(imgs):
    imgs = imgs.numpy().transpose(1,2,0)
    imgs = (imgs + 1)/2
    imgs = imgs*255
    return imgs.astype(int)


fig, axs = plt.subplots(3, 4, figsize=(8, 6))

for i in range(3):
    axs[i, 0].imshow(triplets['images'][i][0])
    axs[i, 0].set_xlabel('Image 1')

    axs[i, 1].imshow(triplets['images'][i][1])
    axs[i, 1].set_xlabel('Image 2')

    axs[i, 2].imshow(triplets['images'][i][2])
    axs[i, 2].set_xlabel('Ground Truth')

    axs[i, 3].imshow(normalize(triplet_rec[i]))
    axs[i, 3].set_xlabel('Predicted')

for ax in axs.flat:
    ax.set_xticks([])
    ax.set_yticks([])

plt.tight_layout()
plt.show()
```



The resulting triplet image that is reconstructed by CITRIS based solely on the combined latent dimensions closely resembles the true combined image. This shows that the latent dimensions learned by CITRIS do not only capture the distribution of the image space, but are also disentangled in the sense each latent dimension only models a single causal variable, and contains no information about any of the other causal variables.

Performing interventions

The results above indicate that CITRIS can learn causal representations from temporal sequences, and suggest that we can use its latent dimensions to control what values each causal variable takes in the generated images. In other words, we can use its latent dimensions to perform interventions in the underlying data generation process. To verify whether this is indeed the case, we implement a function that performs an intervention on the rotation of the object through the latent space learned by CITRIS.

[15]:
```
@torch.no_grad()
def encode(imgs):
    imgs = torch.from_numpy(imgs)[...,:3]
    imgs = imgs.permute(0, 3, 1, 2)
    imgs = imgs.float() / 255.0
    imgs = imgs * 2.0 - 1.0
    encs = model.autoencoder.encoder(imgs)
    return encs
```

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```
@torch.no_grad()
def rotate_image(img):
    x_rotation_target = 3

    # Encode Images
    x_encs = encode(img)

    # Pass through the normalizing flow to disentagle the latent space
    input_samples, _ = model.flow(x_encs)

    # Get the assignment of the latent variables to the causal ones
    target_assignment = model.prior_t1.get_target_assignment(hard=True)

    # Get the number of latents mapped to x rotation
    num_x_rotation_latents = input_samples[:, target_assignment[:, x_rotation_target] ==␣
↪1].shape[-1]

    # Replace them with a random tensor
    input_samples[:, target_assignment[:, x_rotation_target] == 1] = torch.randn(1, num_
↪x_rotation_latents)*3

    # Reverse the flow from the triplet_samples
    input_samples = model.flow.reverse(input_samples)

    # Decode and get the new image
    rotated_image = model.autoencoder.decoder(input_samples)

    return rotated_image.squeeze(0)
```

Let us inspect what the intervened images look like.

[16]:
```
fig, axs = plt.subplots(1, 5)
img = causal3d_dataset['images'][0]
for i in range(5):
    if i ==0:
        axs[i].imshow(img)
        axs[i].set_xlabel('Original Image')
    else:
        axs[i].imshow(normalize(rotate_image(img[None, :])))
        axs[i].set_xlabel(f'Randomly Rotated {i}')

for ax in axs.flat:
    ax.set_xticks([])
    ax.set_yticks([])

plt.tight_layout()
plt.show()
```

The above results indicate that, since the normalizing flow is invertible, we can indeed use CITRIS' latent dimensions to perform interventions on the causal mechanisms by which the data was generated to answer '*what if*' type of questions; in this case: *What would the generated image look like if we change the rotation of the object*. All of this is possible even though CITRIS has learned these causal variables without ever having access to their ground-truth labels.

Analyzing the latent space

In order to gain further intuition on how the latent space of CITRIS is affected by isolated changes in the values of the causal variables, we generate an image sequence where we first change the position of the teapot in the image, then the rotation of the spotlight, and finally the color of the background.

[17]:
```
data_slider = dict(np.load(os.path.join('CITRIS_DL2', 'data', 'data_slider.npz')))
```

We then pass the image sequence through the encoder and normalizing flow of CITRIS-NF, obtain the target assignments of each latent dimension, and finally group the latent dimensions that are assigned to the same causal variables.

[18]:
```
@torch.no_grad()
def get_causal_latents(img):
    # Encode Images
    x_encs = encode(np.expand_dims(img, axis=0))

    # Pass through the normalizing flow to disentagle the latent space
    causal_latents, _ = model.flow(x_encs)

    # Get the target assignments
    target_assignment = torch.argmax(model.prior_t1.get_target_assignment(hard=True),␣
↪dim = -1)

    # Keep the causal latents that will be visualized, i.e., position, spotlight␣
↪rotation and background hue
    causal_latents_to_keep = torch.where((target_assignment==0) |
                                         (target_assignment==1) |
                                         (target_assignment==2) |
                                         (target_assignment==5) |
                                         (target_assignment==8))

    causal_latents = causal_latents.squeeze(0)[causal_latents_to_keep]
    target_assignment = target_assignment[causal_latents_to_keep]

    # Just to sort them based on the assignment
    indices = torch.argsort(target_assignment)

    return causal_latents[indices], target_assignment[indices]
```

We then visualize what happens to the latent space by these isolated changes using a bar plot. You can use the slider to control for which frame the latent dimensions are visualized (note that you might have to open the notebook in Colab in order to use the slider, the GIF below iterates through the different images).

[19]:
```
@widgets.interact(img_id=(0, 29))
def visualize_latents(img_id=0):
    img = data_slider['imgs'][img_id]

    causal_latents, assignments = get_causal_latents(img)
    assignments[assignments <= 2] = 0
    assignments[assignments == 5] = 1
    assignments[assignments == 8] = 2


    labels = ['Object position', 'Spotlight Rotation', 'Background Hue']
    groups = [labels[i] for i in assignments]
    colors = [f'C{assignment}' for assignment in assignments]
    fig, axs = plt.subplots(1, 2)

    axs[0].imshow(img)

    axs[1].bar(np.arange(causal_latents.shape[0]), height=causal_latents, color=colors,␣
↪label=groups)
    axs[1].set_ylim(-25, 25)

    for ax in axs.flat:
        ax.set_xticks([])
        ax.set_yticks([])

    handles, labels = plt.gca().get_legend_handles_labels()
    by_label = dict(zip(labels, handles))
    plt.legend(by_label.values(), by_label.keys(), loc='upper right')
    plt.tight_layout()
    plt.show()

visualize_latents.widget.children[0].layout.width = '100%'
```

```
interactive(children=(IntSlider(value=0, description='img_id', max=29), Output()), _dom_
↪classes=('widget-inter...
```

When experimenting with the slider, you should observe that only the latent dimensions that CITRIS assigns to the causal variable of interest are affected by changes in that causal variable. This provides more empirical evidence that the latent dimensions of CITRIS are indeed properly disentangled.

4.58.6 Conclusion

In this tutorial, we have taken a closer look at CITRIS, a recent CRL method that learns causal variables from an image sequence with interventions. We first discussed what causal representation learning comprehends, and why this recently emerging field of research is exciting. We then described the causal setting in which we aim to identify unknown causal variables, before explaining how CITRIS works in greater detail. Our experiments highlighted that CITRIS can disentangle the causal factors relatively well in the setting of 3D-rendered objects, and showed how we can use such a causal representation to perform interventions in a high-dimensional image space. Overall, considering that causality has great potential to address existing gaps in ML methods with a statistical basis, we believe that it will play an increasingly important role in machine learning in the coming decade.

4.58.7 References

In case you are interested to learn more about causal representation learning, we provide a non-exhaustive list of relevant works to check out.

- Towards Causal Representation Learning (Schölkopf et al., 2021);
- Disentanglement via Mechanism Sparsity Regularization: A New Principle for Nonlinear ICA (Lachapelle et al., 2021);
- iCITRIS: Causal Representation Learning for Instantaneous and Temporal Effects in Interactive Systems (Lippe et al., 2022a);
- Self-Supervised Learning with Data Augmentations Provably Isolates Content from Style (von Kügelgen et al., 2022);
- Weakly supervised causal representation learning (Brehmer et al., 2022).