Infra

Imahn Shekhzadeh imahn.shekhzadeh@unige.ch

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Note

The commands in this document might only run through if you use the .bashrc file provided in App. A

1 Baobab/Yggdrasil

• To connect to Baobab from your local machine, just type into a terminal:

```
eval $(ssh-agent)
ssh-add /home/imahn/.ssh/id_ed25519_unige_hpc
ssh shekhza2@login2.baobab.hpc.unige.ch
# ssh shekhza2@login1.yggdrasil.hpc.unige.ch
```

• Scp into yggdrasil:

```
scp file shekhza2@login1.yggdrasil.hpc.unige.ch:/home/users/s/shekhza2/
# scp -r folder_name shekhza2@login1.yggdrasil.hpc.unige.ch:/home/users/s/
shekhza2/
```

• To see all the machines that are occupied, just type

```
squeue
squeue -p cms-uhh # partition
squeue -u shekhza2 # user
```

Listing 1: Squeue commands

• To find out about your conda environment, just type (e.g. whether you use Anaconda2 or Anaconda3)

```
conda info
```

```
pip install ipykernel
python -m ipykernel install --user --name <environment_name> --display-name
"customStuff"
```

2 Bash

• Downloading file from URL and allowing for redirects,

```
curl -Lo output.out https://url.com
```

• For this directory structure,

```
infra_upd.tex
infra_upd.log
infra_upd.aux
infra_upd.out
infra_upd.pdf
```

rename all of them via

```
for file in infra_upd.*; do mv "$file" "${file/infra_upd/infra}"; done
```

What happens is called a substring replacement.

• Appending line to file,

```
echo "this is a line" | tee -a output.out # -a: appending, important
```

• Checking whether provided string (e.g. via an argument) is empty or not (typically used within conditional statements):

```
test_sth() {
  local env_name="$1" # bash starts counting indices from 1

if [ -z "$env_name" ]; then # spacing after '[' and before ']' needed
  echo "The string is empty."
  return 1 # return value of 1 indicates error
  fi
}
```

Listing 2: Check (e.g. in if-clause) whether string is empty or not

• For retrieving all but the first argument,

```
test_sth(){
shift

echo "all provided args (except the first): $@"
}
```

• And of course there is nothing stopping us from doing this $N \geq 1$ -times ... Pseudocode:

```
test_sth(){
shift
...
shift

echo "all provided args (except the first N): $@"
}
```

If N arguments are not provided, this is **not** a problem, the code will still run through.

• Example for an alias:

```
# forward output
ts(){
test_sth "$0"
}
```

• Finding out the size of a file or directory,

```
du -hs <path_to_file_or_dir> # du -hs file.ext

# for shorter summary (single quotation strings required)
du -hs <path_to_file_or_dir> | awk '{print $1}'
```

• When you want to create a new directory and you want all parent directories to be created as well (assuming they don't already exist), do

```
mkdir -p <dir>
```

The -p option is safe, since if the directory is already existent, no error will be outputted

• Searching for all files with a specific extension, e.g. .ext:

```
find . -name "*.ext"
    # find . -name "*.png"
```

Note that this can be nicely combined with *grep*.

- In Bash, using [[]] instead of [] is preferred, since [[]] is safer and more capable within Bash scripts. Also, within [] (where word splitting and filename expansion do occur), it's good practice to double-quote your variables. But it's safe to omit the double-quotes for e.g. \$# within [[]].
- Unzipping a file via the CLI,

```
unzip /path/to/file.zip -d /path/to/destination
```

• Opening a file and automatically scrolling to the bottom,

```
less +G /path/to/file.ext
```

• Comparing the contents of two directories,

```
diff -r --color directory1 directory2 # '-r' for recursive comparison
diff -rq --color directory1 directory2 # '-q' suppresses the output of
differences and only shows which files differ
```

Ignoring files only existent in one of the directories (which treats absent files as empty),

```
diff -rq --color --unidirectional-new-file directory1 directory2
```

3 Linux

• Under Ubuntu, listing all available kernels,

```
dpkg --list | grep linux-image
```

Listing 3: Find kernel versions in Ubuntu

Finding the currently active kernel version,

```
uname -a
```

Listing 4: Current kerel versions in Ubuntu

The -a option stands for appending, otherwise tee overwrites output.out (if existent).

- Better colors in CLI:
 - 1. Use monokai color scheme, i.e. dark gray background (#272822) with light peach color for the text (#F8F8F2)
 - 2. File paths are still displayed in blue, which is suboptimal, to change the color to the better readable cyan-blue color, click on the three horizontal lines in the CLI, then on **Preferences**, then choose the currently active color, switch to the **Colors** tab, then go to **Palette**, click on the blue color & instead use the color #66D9EF

where -h stands for human readability and -s for summarizing.

• Retrieving the number of available CPU resources,

```
echo "$(nproc)"
```

- It is possible to use colored outputs in Bash. Check the bash function str_diff in App. A. (Note that the -e option is mandatory to enable interpretation of the backslash escapes).
- Print day and time from CLI,

```
echo "$(date +%d_%m_%y-%H_%M_%S)"

# echo "$(date +%dp%mp%y-%Hp%Mp%S)"
```

• Seeing the resource consumption,

```
1 htop
```

• If you did an sshfs and the connection hung up, kill the connection via

```
fusermount -zu /path/to/dir
```

3.1 Opening Programs from CLI

• Opening the settings from CLI,

```
gnome-control-center
```

• Opening VSCode from CLI:

```
code path_to_file_name.ext
```

If a VSCode editor is already open, use the -n flag to open the file in a new editor:

code -n path_to_file/file_name.ext

A folder can also be opened directly:

code path_to_dir

Listing 5: Opening VSCode dir from CLI

• Opening LibreOffice from CLI:

libreoffice --writer path_to_dir/filename.odt

• Opening an image via the CLI:

eog /path/to/your/image.jpg

4 Anaconda

4.1 Installation of Environments

• Installing conda with specific python version,

```
# only 'myenv' needs to be specified (quotation marks necessary)
env_name="myenv" && conda create -n "$env_name" python=3.11.3 -y && conda
activate "$env_name"
```

As of Oct 16, I wouldn't recommend installing python 3.12.0 yet (I got a lot of unmet dependency problems when trying to install torch 2.1 with NVIDIA Cuda version 11.8 afterwards).

• Installation of conda environment from bash file:

```
conda deactivate # go into base environment
source conda/filename.sh
touch .env
```

• Completely remove conda environment,

```
conda deactivate && conda remove -n custom-env-name --all -y
```

4.2 Export

• Exporting an yml-file to share with others for reproducibility,

```
conda env export > environment.yml
```

At the end of the file, there will be a line starting with "Prefix:", you can safely delete it, for details see here

4.3 Installation & Removal of Packages

• Installation of packages from *pyproject.toml* file,

```
pip install -e .
```

• Installing specific conda package version:

```
conda install -c conda-forge custom-pkg-name -y
# conda install -c conda-forge cloudpathlib=0.15.1 -y
```

• Removing list of packages from conda environment:

```
conda remove -n custom-env-name pkg1 pkg2 ... pkgN -y
# conda remove -n google_jax matplotlib -y
```

4.4 Usage in VSCode

- Selecting a conda environment in VSCode, do Ctrl + Shift + P and type *Python: select interpreter*.
- Stepping into external code with Python debugger: https://stackoverflow.com/questions/53594900/visual-studio-code-python-debugging-step-into-the-code-of-external-function

- Creating a JSON file, here some instructions: https://code.visualstudio.com/docs/python/debugging
- Listing all installed environments,

```
conda env list
```

4.5 PyTorch

• Checking whether gpu version of PyTorch is installed, from python shell (for this, activate the right conda env first!):

```
import os

import torch

if __name__ == "__main__":
    os.path.dirname(torch.__file__)
```

Afterwards, do

```
ls -larht <path_from_prev_alg> | grep -E "cuda"
```

• If you had installed PyTorch via conda instead of pip, then this is easier, where the -E means we are searching for extended regular expressions (again activate the right conda env first!):

```
conda list | grep -E "torch|pytorch"

# or 'conda list | grep -E "torch|pytorch"'
```

5 CUDA

- When you need to find out the CUDA version installed, install *nvidia-cuda-toolkit*, but do NOT reboot. After its use, immediately remove this package and any package installed alongside with it!
- In case NVIDIA drivers do not allow for boot into Ubuntu (e.g. because you did not uninstall the *nvidia-cuda-toolkit* package):
 - 1. Boot into an older kernel version of Linux (in order to get there, do a "hard" reboot, and then go into "Advanced options for Ubuntu", and choose an older kernel version).
 - 2. Once booted into the older kernel version, I removed 'nvidia-cuda-toolkit' and rebooted.
 - 3. After a few more hard reboots and booting into the older kenel version, at some point, the newer kernel version was picked up and worker again.
 - 4. Now to fix the monitors (because dual-monitor setup didn't work), I had to open the program "Additional Drivers" and change the driver from the open-source version to an NVIDIA proprietary one.
 - 5. Then I had to install CUDA according to https://docs.nvidia.com/cuda/cuda-installation-index.html again.
 - 6. For PyTorch to recognize the GPU, I had to reboot.

6 Docker

6.1 Installation

- Follow this great tutorial by DigitalOcean.
- To use NVIDIA GPUs (both in PyTorch & Jax), install the NVIDIA Container Toolkit
- Once done with the installation of the NVIDIA Container Toolkit, proceed with the configuration. During the configuration, it will be necessary to restart the docker daemon, which you can achieve as follows:

```
sudo systemctl restart docker
```

6.2 Basics

• Interactive start of containers:

```
d ps -a # find out ID (also docker container name)
d start -i ID
```

• Copying files from local system to docker container and vice versa; **run both commands from local CLI**

```
d cp file_name container_ID:/target_dir # local -> docker
d cp container_ID:/file_name dir_name # docker -> local
```

6.3 Dockerfile

• When you find the command for pulling a docker image on https://hub.docker.com, e.g.

```
d pull ubuntu:jammy-20231004
```

then in the Dockerfile, just write

```
FROM ubuntu:jammy-20231004
```

When no tag is specified, by default the *latest* one will be taken. However, using the *latest* tag can potentially cause issues with reproducibility and consistency, because you might pull a different version of the image at different times without knowing it if the latest tag gets updated. For more predictable builds, it is advised to use a specific version tag.

• Note that the structure of the docker pull command is

```
d pull [OPTIONS] NAME[:TAG|@DIGEST]
```

In general, the *NAME* is in the format *repository/image*. If *repository* is not specified, Docker assumes the image is located in the default DockerHub library repository. However, many images (like PyTorch) are hosted under a specific user or organization's namespace on DockerHub, rather than the top-level library. That's why the command for the docker pull (for the latest tag) reads

```
d pull pytorch/pytorch
```

- If using a Docker image like *pytorch/pytorch:latest*, conda is already installed. In this case, the default environment is named *base*, which is a common practice in Docker images with conda unless otherwise stated.
- Copying local scripts into docker container,

```
COPY relative/path/to/script.py .
```

From the documentation:

Multiple (src) resources may be specified but the paths of files and directories will be interpreted as relative to the source of the context of the build.

It is also important to put the . at the end, since it represents the destination in the Docker image where the file should be copied. The dot . refers to the current working directory inside the Docker image, which is determined by the WORKDIR command in the Dockerfile. If WORKDIR is not set, it defaults to the root directory (/) of the image.

Also, each time the script relative/path/to/script.py changes, the Dockerfile needs to be rebuilt – however, a cached version will be used, which speeds things up.

• Copying local dirs into docker container,

```
COPY relative/path/to/dir/ .
```

• Running a Dockerfile:

```
d build -f file_name -t img_name .

d build -f file_name -t img_name:tag_name . # tag name optional, but recommended, e.g. 1.0 (no quotes required)

# d build -f file_name --no-cache -t [...] # forcing to rebuild from scratch, no cached version is used (only do if really required)
```

where $Image_name$ will be the name of the newly created image, Tag_name the tag name and $file_name$ the name of the docker file.

• Via

```
EXPOSE custom-port-number
# EXPOSE 80
```

it is possible to expose a port. Note that port exposure is related to network access. Note that even though network access might not be needed, there is still no harm in exposing a port (since an exposure of the port does not make the docker container more vulnerable).

6.4 Docker images

• A Dockerfile does not necessarily need to have the name *Dockerfile*. To pass another name when building the img, do

```
d build -f custom_docker_file .
```

The . specifies the context of the build, which is the current directory in this case. I would recommend running this command from the same dir in which <code>custom_docker_file</code> is located.

• Check all available Docker images via

```
d images
```

• Cleaning up dangling docker images (these are the entries with $\langle none \rangle$ in the repository or tag name in the output of the previous algo):

```
d image prune -f
```

• Removing a Docker image – only do this when finished with using the image

```
d image rm Image_name:Tag

# d container rm <container_id> # in case some containers are using the image
```

6.5 Docker containers

6.5.1 Basics

• Running Docker images – without being able to utilize NVIDIA GPUs:

```
d run -it img_name # if 'tag_name' was not provided
d run -it img_name:tag_name # if 'tag_name' was provided during build (
recommended)
```

• Running Docker images & utilizing GPUs:

```
d run --gpus all -it img_name
d run --gpus all -it img_name:tag_name # recommended
```

• To mount a local file to the container at runtime, do

```
d run -v /absolute/path/to/script.py:/path/to/workdir/script.py --gpus all
-it img_name
d run -v /absolute/path/to/script.py:/path/to/workdir/script.py --gpus all
-it img_name:tag_name # recommended, provide 'img_name' & 'tag_name'
```

The mounting expects **absolute** file paths on the side of the host machine.

 Note that you can include the bash command pwd to avoid having to manually pass absolute paths for the mounting

```
d run -v $(pwd)/script.py:/path/to/workdir/script.py --gpus all -it img_name:tag_name # recommended, provide 'img_name' & 'tag_name'
```

If you need the container to reflect changes made to the scripts on the host without rebuilding the image every time, you would use the -v flag to mount the directory. If the scripts won't change, or you don't need to reflect changes in real-time, you don't need to mount the directory, as the necessary scripts have already been copied into the image during the build process.

• It is also possible to directly mount directories:

```
d run -v $(pwd)/dir_path:/path/to/workdir --gpus all -it img_name:tag_name
```

Note that the specified directory from the host is mounted into the container at the specified mount point. If there are any existing files or directories in the container at the mount point, they become obscured by the mount.

- In several cases it can be useful to remove the docker container right after execution: When you...
 - ... are running many short-lived containers, like during development or testing,
 - ... want to avoid manual cleanup of stopped containers later on,
 - ... are running containers for one-off tasks that do not need to persist any state after they are finished.

In this case,

```
d run --rm -v $(pwd)/dir_path:/path/to/workdir --gpus all -it img_name: tag_name
```

• It is also possible to mount two separate host directories to two separate directories within the container,

```
d run --rm -v $(pwd)/dir_path1:/path/to/workdir1 -v $(pwd)/dir_path2:/path
   /to/workdir2 --gpus all -it img_name:tag_name
```

This will not cause any overwriting as each -v flag creates a unique mount point inside the container.

• Finding out the python version of the Docker image

```
d run -it --rm img_name:tag_name python3 --version
```

This command will immediately remove the container after execution.

6.5.2 Passing Arguments

It is possible to pass arguments when running a docker container.

1. Assuming you have a bash script run_scripts.sh, in which a Python script, e.g.

```
#!/bin/sh
isort /app/scripts/*.py
black /app/scripts/*.py

python3 -B /app/scripts/test_script.py
python3 -B /app/scripts/test_anil.py
```

Modify this bash script s.t. any arguments passed to the CLI when running the docker container are picked up,

```
python3 -B /app/scripts/test_anil.py "$@"

# python3 -B /app/scripts/test_script.py "$@" # alternative
```

- 2. Rebuild (!) the docker image.
- 3. Now run the docker container as follows:

```
d run --rm -v $(pwd)/dir_path:/path/to/workdir --gpus all -it img_name:
    tag_name arg1 arg2

# d run --rm -v $(pwd)/dir_path:/path/to/workdir --gpus all -it img_name:
    tag_name --n_ways 1 --k_shots 1 # example
```

6.5.3 Listing & Stopping

• Listing all running containers,

```
d ps
```

Listing only the container ID (of all running containers),

```
d ps -q
```

• Stopping a running container,

```
d stop container-ID
```

• Stopping a running container and removing it,

```
d stop container-ID && d rm container-ID
```

6.6 Pushing to DockerHub & HPC

1. First login to Docker via

```
d login -u user_name -p password
```

- 2. Then follow the instructions from this tutorial (from minute 17:05 on)
- 3. And then follow the HPC tutorial from UNIGE

7 Python

7.1 Config File & JSON Files

• When using argparse in combination with a JSON configuration file, the JSON keys need to match the long option names specified in *parser.add_argument* method calls. The argparse module itself does not automatically recognize abbreviated forms from a JSON file.

7.2 Jupyter Notebooks

• Converting jupyter notebooks into PDFs:

```
for nb in /path/one/Notebook1.ipynb /path/two/Notebook2.ipynb [...]

do

jupyter nbconvert --to pdf "$nb"

done
```

If you have several notebooks in the same directory,

```
for nb in *.ipynb
do
jupyter nbconvert --to pdf "$nb"
done
```

7.3 Map (Built-In Function)

• Function signature:

```
map(function, iterable, *iterables)
```

Description provided in the documentation:

Return an iterator that applies function to every item of iterable, yielding the results. If additional iterables arguments are passed, function must take that many arguments and is applied to the items from all iterables in parallel. With multiple iterables, the iterator stops when the shortest iterable is exhausted. For cases where the function inputs are already arranged into argument tuples, see *itertools.starmap()*.

• Example usage: Natively multiplying Python lists elementwise,

```
from typing import List

def multiply(x: List, y: List):
    return x * y

list_one = [i for i in range(1000)]

list_two = [j for j in range(1000, 2000)]

result = list(map(multiply, list_one, list_two)) # 'map' is a built-in function, do not use '(list_one, list_two)' in this case
```

• Example usage: Converting NumPy arrays into PyTorch tensors,

```
a = np.array([1, 2, 3, 4])
tensor_list = list(map(torch.from_numpy, (a,))) # list containing tensor,
use of additional brackets necessary
```

• Example usage: Converting NumPy arrays into PyTorch tensors,

```
a = np.array([1, 2, 3, 4])
b = np.array([5, 6, 7, 8])
a, b = map(torch.from_numpy, (a, b)) # tuple unpacking
```

7.4 PyTorch

7.4.1 Leaf Tensors

- If requires_grad=False, then the tensor will be leaf by convention. If requires_grad=True, then the tensor will be leaf if it was created directly by the user and is **not** the result of an operation, e.g. .to(device) when the tensor is on cpu and device="cuda:0".
- However, by definition, leaf tensors themselves do not have a **gradient function** .grad_fn because they are not the result of a differentiable operation applied to other tensors, i.e. grad_fn on such tensors will return None. The gradient function in neural network libraries like PyTorch or TensorFlow is associated with tensors that are outputs of differentiable operations.
- The .grad attribute on leaf tensors that require gradients, i.e. those for which requires_grad=True, stores the gradient computed during backpropagation. (For leaf tensors that have requires_grad=False, calling the .grad attribute outputs None.) Note that for non-leaf tensors, calling .grad results in a UserWarning, since non-leaf tensors are generally intermediate results in the computation graph, and their gradients are usually not needed once the gradients of the leaf tensors have been obtained. However, there are cases where those gradients are needed, which can be enforced by setting retain_grad=True on those tensors,

Note that in the example of this code snippet, doing y.grad means that we access the gradient of the scalar loss function y.sum() — on which we performed .backward(). Correspondingly, doing x.grad implies the gradient of the scalar loss function y.sum() with respect to x.

• In general, it is **not** possible to perform **in-place** operations on leaf tensors for which requires_grad=True, since PyTorch dynamically builds a computational graph during the forward pass, which is used during backpropagation to calculate the gradients. If leaf tensors that have requires_grad=True are changed in-place, then the values used during the forward pass are changed, which will affect the gradient calculations in the backward pass. However, note that when no gradients are required for the operations, e.g. when performing parameter updates manually, one can use the context manager with torch.no_grad(), in which case in-place operations on leaf tensors can be performed, since inside the context manager, requires_grad=False.

7.4.2 Autograd & Backward

- The function torch.autograd.grad() computes the gradient. If the gradient of a scalar (loss function) wrt a (weight) matrix is taken, then the output will also be a matrix, where each element corresponds to the partial derivative of the scalar (loss function) wrt to the (weight) matrix element.
- torch.autograd.grad() is particularly useful if more direct control over the gradient computation is desired, in particular compared to .backward().
- Note that the default behavior of .backward() accumulates gradients in the .grad attribute of tensors,

```
x = torch.tensor([1., 2., 3.], requires_grad=True, device=torch.device("
          cuda:0"))
       # fwd pass
3
       y = 2 * x
       # first backward pass
6
       y.sum().backward(retain_graph=True)
       print(f"Gradients of 'x' after first backward pass: {x.grad}") # 'torch.
          tensor([2., 2., 2.])'
9
       # second backward pass
10
       y.sum().backward()
       print(f"Gradients of 'x' after second backward pass: {x.grad}") # 'torch.
12
          tensor([4., 4., 4.])', notice how gradients have accumulated
```

However, this behavior can be suppressed by simply zeroing the gradients, i.e. x.grad.zero_() — note that x.grad returns a tensor, and <tensor>.zero_() is a general PyTorch function that sets all elements in-place to 0.

8 AWS S3

8.1 Installation & Configuration

- 1. Installation instructions
- 2. The CLI will display the path under which the aws package was installed, but it might be sufficient to simply run

```
1 aws
```

Double check by running

```
which aws
```

3. After installation, configuration is necessary. For this run

```
aws configure
```

You can leave these fields empty:

```
Default region name [None]:
Default output format [None]:
```

A configuration file will be saved under

```
\sim/.aws/credentials
```

4. In the case you are a member of UNIGE, you can obtain the AWS access key ID and the secret access key as follows:

```
echo -n "$user_name" | base64 # the '-n' is important in this context
echo -n "$passwd" | md5sum
```

where \$user_name and \$passwd need to be provided

Otherwise, you need login to the AWS Management Console.

5. To test the configuration was successful, do this:

```
aws s3 ls --endpoint-url https://your-custom-s3-endpoint.com
```

where you replace the endpoint-url https://your-custom-s3-endpoint.com with yours.

8.2 AWS Credentials (Profiles)

- It is possible to use several profiles in the file \sim /.aws/credentials.
- For example:

```
[default]
aws_access_key_id = YOUR_DEFAULT_ACCESS_KEY
aws_secret_access_key = YOUR_DEFAULT_SECRET_KEY

[profile1]
aws_access_key_id = ANOTHER_ACCESS_KEY_ID
aws_secret_access_key = ANOTHER_SECRET_ACCESS_KEY
```

```
[profile2]
aws_access_key_id = YET_ANOTHER_ACCESS_KEY_ID
aws_secret_access_key = YET_ANOTHER_SECRET_ACCESS_KEY
```

Using specific profile when running aws cli commands via --profile option in the command:

```
aws s3 --profile profile1 [...]
# aws s3 --profile default [...]
```

8.3 Buckets

One can have several buckets.

8.3.1 Creation

• To create a new bucket:

```
aws s3api create-bucket --bucket custom-bucket-name --endpoint-url https://custom-s3-endpoint.com --profile default
```

8.3.2 Listings

• Directly "folder" contents of an s3 bucket,

```
aws s3 ls s3://custom-bucket-name --recursive --endpoint-url https://custom-s3-endpoint.com --profile default # '--recursive' optional
```

• Showing file contents,

```
aws s3 ls s3://custom-bucket-name/prefix/ --recursive --endpoint-url https
://custom-s3-endpoint.com --profile default # '--recursive' optional
```

Note that the / at the end of the prefix ("folder") is necessary.

8.3.3 File Copying

• Local machine \longrightarrow S3:

```
aws s3 cp path/to/custom_file.ext s3://custom-bucket-name/path/to/
    custom_file.ext --endpoint-url https://custom-s3-endpoint.com --profile
    default
```

• S3 \longrightarrow local machine:

```
aws s3 cp s3://custom-bucket-name/path/to/s3_file.ext custom/destination -- endpoint-url https://custom-s3-endpoint.com --profile default
```

8.3.4 Directory Copying

• Local machine \longrightarrow S3:

```
aws s3 sync path/to/dir s3://custom-bucket-name/path/to --endpoint-url https://custom-s3-endpoint.com --profile default
```

8.3.5 Directory/File Deletion

• Deleting a folder (which is essentially a prefix in S3) and its contents in an S3 bucket,

```
aws s3 rm s3://your-bucket-name/path-to-your-folder --recursive --endpoint-
url https://custom-s3-endpoint.com --profile default
```

• Deleting a file,

```
aws s3 rm s3://your-bucket-name/path-to-your-file.out --recursive --
endpoint-url https://custom-s3-endpoint.com --profile default
```

8.4 Cloudpathlib

• When you use the cloudpathlib module, and you want to specify a profile, do this:

```
from cloudpathlib import S3Path, S3Client

# Create an S3 client with a specific AWS profile
s3_client = S3Client(
aws_access_key_id=aws_access_key_id,
aws_secret_access_key=aws_secret_access_key,
endpoint_url=endpoint_url,
profile_name="profile1", # specify profile here

# Make 'client' default:
client.set_as_default_client()
```

9 Git

9.1 Cloning

• Cloning a repository via sshfs and adjusting the folder name,

```
git clone <ssh_url> <folder_name>

git clone <https_path> <folder_name>
```

• After moving into the ¡folder name; via cd, do

```
git switch <desired_branch>
```

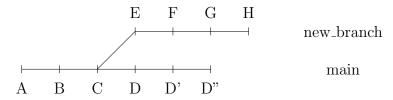
9.2 Remote Branch

Creating a local branch and then pushing it remotely,

```
git push origin <local-branch>
git push origin code-dev
```

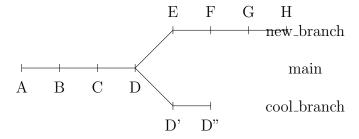
9.3 Merging

• Assuming the following commit-history is given,



when merging main and new_branch, the two branches will be either auto-merged or there will be a merge conflict.

• Assuming the following commit history is given,



- After merging main with new_feature, which happens via a fast-forward, you can delete it. New commit structure:
- A B C D E F G H branch ; main;
- Merging new feature into master, do

```
git switch main
git merge <new_feature>
```

9.4 Merge Conflicts

To resolve a merge conflict, type

```
git mergetool
```

Afterwards, confirm with Enter that you want to use vimdiff as default editing tool. The vimdiff display will now resemble the following structure:

```
| LOCAL | BASE | REMOTE |
| MERGED
```

If the file has not already existed in BASE, then we need this view:

```
| LOCAL | MERGED | REMOTE |
| LOCAL -- Current branch
| BASE -- Common ancestor (how did the file look like before both changes?)
| REMOTE -- File that I am merging into the current branch
| MERGED -- Merge result
```

It is probably easiest to take the merged view and edit it directly. In the vim editor, an entire line can be deleted by pressing D (no control before!). If I instead wanted the changes from either LOCAL, BASE or REMOTE, you have to do one of these,

```
:diffg LO
:diffg BA
:diffg LO
```

Of course, the merged view can also be edited directly. Regardless of the chosen method, type

```
ı :wqa
```

into vim. Afterwards, do not forget to commit and push. And if you want, do

```
git clean -f
```

Locally restore file

```
git restore --source <commit SHA> file
git restore --source HEAD file
```

qit restore does not overwrite HEAD, though. For that, a push would be necessary.

It can sometimes also be useful to run dry merges to proactively check for conflicts during a merge; for this, run

```
git merge --no-commit --no-ff <branch_name>
```

Afterwards, type

```
git merge --abort
```

to abort, and no changes will occur.

If you only want to do a fast-forward, do

```
git merge <branch_to_be_merged> --ff-only
```

9.5 Checking History

• Viewing the history of commits,

```
git log
```

• Viewing a specific file,

```
git show <commit-hash>:<file-name>

# git show 123abc:example.txt
```

9.6 Removing a File/Folder

• To remove a file/folder that is already tracked, adding it to .gitignore won't remove it (though this also needs to happen). For this, do:

```
git rm --cached <file>
git rm -r --cached <folder>
```

• Adding the file/folder to *.gitignore* is still a good idea, though, since the file/dir won't be removed locally with the commands.

9.7 Renaming a Repository

- 1. Rename the repository remotely first (by going to your repository's URL),
- 2. then go to the locally cloned version of the repository and do

```
git remote set-url origin <new-url>
# git remote set-url origin https://github.com/username/new-repo-name.git
```

3. and finally

```
git remote -v
```

which lists the remote names and their URLs.

9.8 Restore File

Resetting specific file to state of previous commit,

```
git restore --source=<commit-hash> <file-path>
git restore --source=HEAD <file_path>
```

Replace (commit-hash) with the commit SHA and (file-path) with the path to the file. This change is local and you would need to commit it if you want it to be reflected in the repository history.

9.9 Delete Branches

• Local git branch,

```
git branch -d <branch_name>
# git branch -d testing
```

Regardless of merge status,

```
git branch -D <branch_name>
# git branch -D testing
```

• Remote branch,

```
git push origin --delete <branch_name>
# git push origin --delete testing
```

9.10 List Branches

Listing all local and remote branches,

```
git branch -a
```

9.11 Remote URL

Obtaining the remote URL,

```
git remote get-url origin
git remote get-url origin | sed 's/\.git$//' # optional: trim output
```

10 Remote Development

10.1 Connection

- 1. When connecting two machines remotely, install this extension on local machine (also directly in VSCode possible),
- 2. open VSCode on local machine,
- 3. press F1-button, choose "Remote-SSH: Connect to Host..." and type for the SSH host (optionally save it in the SSH config file) the same as in Algo. (B),
- 4. enter the passwd for the remote SSH host.

10.2 Troubleshooting

• If you find you are getting a permission error for saving a file on the remote machine (in VSCode when doing the local coding), try

sudo chown custom-username path/to/custom/script.ext

The *custom-username* here refers to the username on the remote machine.

11 Jax

Try to install via pip first. Only if this doesn't work use conda!

• To put a Jax array onto a specific device, use this:

```
import jax
from jax import devices, device_put, numpy as jnp

x = device_put(jnp.arange(10), device=devices("cpu")[0]) # NOTE: put '[0]'

x = device_put(jnp.arange(10), device=devices("gpu")[0]) # NOTE: put
    '[0]'
print(f"Device: {x.device_buffer.device()}")
```

Listing 6: Device specification in Jax

• Specifying the dtype of an array:

```
x = jnp.array([1, 2, 3], dtype=jnp.float32)
print(f"Dtype: {x.dtype}")
```

Listing 7: Jax device retrieval

• To find out the device of a Jax array, use this:

```
x.device_buffer.device() # x: Jay array
```

Listing 8: Jax device retrieval

• To make a Jax array out of a Python list or a Numpy array (do not use for tensors):

```
from jax import numpy as jnp

a = jnp.array([1., 2., 3.])
b = jnp.array(np.array([1., 2., 3.]))
```

Listing 9: Jax array creation

• jit (just-in-time compilation): sets up a function with XLA (extended linear algebra): check out the NB test__jit-compil.ipynb. To use jit, do this:

```
import jax
from jax import numpy as jnp

@jax.jit
def selu(x: jnp.array, lamb: float = 1., alpha: float = 0.):
return lamb * jnp.where(x > 0, x, alpha * (jnp.exp(x) - 1.0))
```

Listing 10: Jax array

${f A}$.bashrc

```
ca() {
     local conda_out="$(conda env list | grep -E "$env_name" | head -n 1 | awk '{
        print $1}')"
     # check non-emptiness
     if [ -z "$1" ]; then
      echo "Usage: ca <env_name>"
6
      return 1
     fi
     # check env existence
     if [ ! -z "$conda_out" ]; then
      conda activate "$1"
12
     else
13
      echo "Conda environment '$env_name' does not exist." # single quotes (')
14
         only for display
      return 1
     fi
17
    }
18
19
    # ----- CONDA -----
20
    # activate conda environment
    # usage: 'ca custom-env-name'
    ca() {
     conda activate "$0"
    }
26
27
    # deactivate currently activated conda environment
    cod() {
     conda deactivate
    }
31
32
    # List all available conda envs:
33
    cel() {
     conda env list
37
    # remove conda environment
    # usage: 'crme ant-migrate-dev'
39
    crme() {
40
41
     # check number of passed arguments via '$#'
     if [[ $# -ne 1 ]]; then
      echo "NOTE: Exactly one argument needs to be provided"
     else
45
      conda deactivate && conda remove -n "$1" --all -y
     fi
47
48
```

```
}
49
    # alias for 'conda__remove_packages'
51
    # usage (e.g.): 'crm myenv pkg1 pkg2'
    crm() {
53
     conda__remove_packages "$0"
54
    # remove conda packages from environment
    # usage (e.g.): 'conda__remove_packages myenv pkg1 pkg2'
58
    conda__remove_packages() {
59
60
     # define local variables first
61
     local env_name="$1"
62
     local conda_out="$(conda env list | grep -E "$env_name" | head -n 1 | awk '{
         print $1}')"
64
     # forget first argument (which is saved in 'env_name')
65
     shift
66
     # check non-emptiness
     if [ -z "$env_name" ]; then
      echo "Usage: conda_remove_packages <env_name> [package1] [package2] ... [
70
         packageN]"
      return 1
71
     fi
72
     # check env existence
     if [ ! -z "$conda_out" ]; then
      conda remove -n "$env_name" "$0" -y
      echo "Package(s) '$0' removed from environment '$env_name'"
77
     else
78
      echo "Conda environment '$env_name' does not exist." # single quotes (')
79
          only for display
      return 1
     fi
81
82
    }
83
84
    # ----- AWS ------
85
    # helper function
    get__profile_endpoint_url() {
88
89
     # check if the first argument contains "https://"
90
     if [[ "$1" == https://* ]]; then
91
      local endpoint_url="$1"
93
      # if there's a second argument, it's the profile
      if [ -n "$2" ]; then
       local profile="$2"
96
      fi
97
```

```
elif [ -n "$1" ]; then
100
       # if the first argument doesn't contain "https://", it's the profile
       local profile="$1"
      fi
104
       echo "$1 $2"
106
     }
107
     # define default vals and update based on provided args
109
     update__profile_url() {
110
      local endpoint_url="https://kalousis.s3.unige.ch"
      local profile="default"
112
113
      # update 'endpoint_url' and 'profile' if provided
114
      if [[ "$2" == https://* ]]; then
115
       read endpoint_url profile <<< $(get__profile_endpoint_url "$2" "$3")</pre>
      else
117
       read profile <<< $(get__profile_endpoint_url "$2" "$3") # for 'endpoint_url</pre>
           ', default val will be taken
      fi
119
120
      echo "$endpoint_url $profile"
122
     # listing
124
     # example usages (only bucket name provided):
     # 'lal path'
     # 'lal path default'
127
     # 'lal path https://kalousis.s3.unige.ch'
128
     # 'lal path https://kalousis.s3.unige.ch default'
129
     lal() {
130
      local path="$1"
      read endpoint_url profile <<< $(update__profile_url "$2" "$3")</pre>
      $(which aws) s3 ls s3://"$path" --recursive --endpoint-url "$endpoint_url" --
135
         profile "$profile"
136
     # removing prefixes/files
138
     # example usages (only bucket name provided):
139
     # 'larm path'
140
     # 'larm path default'
141
     # 'larm path https://kalousis.s3.unige.ch'
142
     # 'larm path https://kalousis.s3.unige.ch default'
143
     larm() {
      local path="$1"
145
146
      read endpoint_url profile <<< $(update__profile_url "$2" "$3")</pre>
147
```

```
148
      command_output=$($(which aws) s3 rm s3://"$path" --recursive --endpoint-url "
149
         $endpoint_url" --profile "$profile")
      if [[ -z "$command_output" ]]; then
      # no use of '--recursive', which shouldn't be used for single file deletion
152
       $(which aws) s3 rm s3://"$path" --endpoint-url "$endpoint_url" --profile "
153
           $profile"
      fi
     }
155
156
                           ----- GIT -----
158
     # list all local and remote branches
159
     1b() {
160
      git branch -a
161
     # delete remote branch
164
     1bd() {
165
      git push origin --delete "$0"
168
     # cloning
169
     lcl() {
170
      git clone "$0"
171
172
     # switch branches and create if non-existent
     lsw() {
      if git rev-parse --verify "$1" >/dev/null 2>&1; then
        git switch "$1"
177
      else
178
        git switch -c "$1"
179
      fi
181
182
     # example usage: 'lsta 2' or 'lsta'
183
     lsta() {
184
      local stash_index=${1:-0} # Default to 0 if no argument provided
185
      # Check if the provided argument is an integer
      if ! [[ \$stash_index =\sim ^[0-9]+\$ ]]; then
188
       echo "The provided index is not a valid integer."
189
       return 1
190
      fi
191
192
      # Check if the stash index exists
193
      if ! git rev-parse --verify stash0{$stash_index} >/dev/null 2>&1; then
       echo "No stash found at index $stash_index"
195
       return 1
196
      fi
197
```

```
198
      # If all checks pass, apply the stash
199
      git stash apply "stash@{$stash_index}" --index
200
201
202
     # Forward commands to 'git stash'
203
     1st() {
204
      git stash "$0"
     }
206
207
     # Stash files, if arguments are provided, they are ignored
208
     lstf() {
209
      git stash --include-untracked
210
211
212
     # https://stackoverflow.com/questions/19595067/git-add-commit-and-push-
213
         commands-in-one
     # https://stackoverflow.com/questions/14763608/use-conditional-in-bash-script-
214
         to-check-string-argument
     # if-else statements in bash: https://linuxhandbook.com/if-else-bash/
215
     # example usage: lgit "bit" "add ..."
216
     lpush() {
217
      git add . && git commit -a -m "$1" && git push origin $(bname) && llog
218
219
220
     # https://stackoverflow.com/questions/3236871/how-to-return-a-string-value-
221
         from-a-bash-function
     bname() {
222
      branch=$(git branch --show-current)
      echo $branch
224
225
226
     lupd() {
227
      git fetch origin $(bname) && git log HEAD..origin/$(bname) --oneline
228
229
230
     lpull() {
231
      git pull origin $(bname)
232
234
     ldiff() {
235
      git status "$0" && git diff --color "$0"
237
238
     lforce() {
239
      git push origin $(bname) --force
240
     }
241
242
     llog() {
      git log
244
245
246
```

```
1rm() {
247
      git rm -r "$0"
249
     lreb() {
251
      # Set default value to 5:
252
      num1=$\{1:-5\}
253
      git rebase -i HEAD∼$num1
256
     # Reset entire repo to state of 'HEAD', or reset specific file to a specific
         commit hash.
     lres() {
258
      if [[ $# -eq 0 ]] || [[ $# -eq 1 ]]; then
259
       local commit_hash=${1:-HEAD}
260
       git reset --hard "$commit_hash"
261
      elif [ $# -eq 2 ]; then
262
       local commit_hash="$1"
263
       local file_path="$2"
264
       git restore --source="$commit_hash" "$file_path"
265
      else
       echo "Usage: lres [commit_hash file_path]"
268
     }
269
270
     lsh(){
271
      git show "$0"
272
     # Usage: lmv /path/to/directory file1 file2 file3 ...
275
     lmv() {
276
      local target_dir=$1 # The first argument is the directory path
277
      if [[ ! -d "$target_dir" ]]; then
278
       echo "Target directory does not exist: $target_dir" >&2
       return 1
      fi
281
282
      # Shift the arguments so that $@ contains only the files to move
283
      shift
284
285
      # Now, loop through all the remaining arguments
      for file in "$0"; do
       if [[ -e $file ]]; then
288
        git mv "$file" "$target_dir"
289
290
        echo "File does not exist: $file" >&2
291
       fi
292
      done
293
294
295
       ----- PROTONVPN -----
296
297
```

```
p() {
298
      protonvpn-cli "$0"
299
300
301
                     ----- MISCELLANEOUS ------
302
303
     # pdflatex
304
     pd() {
      /usr/bin/pdflatex "$0"
307
308
     # convert input notebook to PDF
309
     jconv() {
310
      jupyter nbconvert --to pdf "$1"
311
312
313
     # 'less' with ANSI escape characters
314
     less() {
315
      /usr/bin/less -R "$0"
316
317
     diff() {
319
      /usr/bin/diff --color "$0"
320
321
322
     # overload 'shred' func, allow (recursive) shredding of dirs/files
323
     # multiple files/dirs can be provided, mixing allowed
324
     # usage (e.g.): 'shred 10 <file_name>'
325
     # shred <file_name>
     # shred <dir_path>
327
     # shred <file_name> <dir_path>
328
     shred() {
329
330
      # check whether first argument is a number
331
      if [[ "$1" =\sim ^[0-9]+$ ]]; then
       local iterations="$1"
333
       shift
334
      else
335
       iterations=5 # default
336
      fi
337
338
      # check file/dir existences
      for path in "$0"; do
340
       if check_existence "$path"; then
341
       # check whether passed input is directory or not
342
        if [[ -d "$path" ]]; then
343
         echo "Files to be shredded in $path:"
         find "$path" -type f -print0 | xargs -0 ls -ld
345
        fi
347
        echo "Error occurred in check_existence for file/dir: $path"
348
        return 1
349
```

```
fi
350
      done
352
      # prompt user for confirmation
353
      read -rp "Do you wish to proceed with shredding all files in $@ for
354
          $iterations iterations? (yes/no): " confirmation
355
      if [[ $confirmation = [yY] || $confirmation = [yY][eE][sS] ]]; then
       for path in "$0"; do
        if [[ -d "$path" ]]; then
358
         # shred all files within the directory
359
         find "$path" -type f -exec /usr/bin/shred -uz -n "$iterations" {} \;
360
         rm -rf "$path"
361
         echo "All files in '$path' have been shredded for $iterations iterations."
362
        elif [[ -f "$path" ]]; then
         # shred the individual file
364
         /usr/bin/shred -uz -n "$iterations" "$path"
365
         echo "File '$path' has been shredded for $iterations iterations."
366
        fi
367
       done
368
      else
369
       echo "Shredding aborted."
      fi
371
     }
372
373
     # shortcut for clearing terminal output
374
     c() {
375
      clear
     }
377
378
     # shortcuts for exiting terminal
379
     q() {
380
      exit
381
     }
382
383
     e() {
      q
385
     }
386
387
     # tailscale
388
     ts() {
389
      tailscale status "$0"
     }
391
392
     # xournalpp (https://github.com/xournalpp/xournalpp)
393
     xopp() {
394
      xournalpp "$0"
395
396
397
     # strings comparison
398
     # usage (e.g.): 'str_diff "blub1" "blub1" or 'str_diff blub1 blub1'
     # or 'str_diff $(echo "hey") $(echo "hey")'
400
```

```
# NOTE: exactly two arguments need to be provided
401
    str_diff() {
402
403
     # check number of passed arguments via '$#'
404
     if [[ $# -ne 2 ]]; then
405
      echo "NOTE: Exactly two arguments need to be provided"
406
      return 1 # return non-zero exit code to indicate error
407
     else
      # compare strings
410
      if [[ $1 == $2 ]]; then
411
       echo -e "Strings '$1' and '$2' \033[92mmatch\033[0m"
412
      else
413
       echo -e "Strings '$1' and '$2' do \033[91mNOT\033[0m match"
414
      fi
415
     fi
416
417
418
419
420
    # ----- DOCKER -----
421
    d() {
     docker "$@"
423
    }
424
425
    # ----- CHATGPT ------
426
427
    # https://github.com/kardolus/chatgpt-cli/tree/main
428
    gpt(){
     chatgpt -i
430
    }
431
432
    export OPENAI_KEY=[...]
433
434
    # ----- ALWAYS EXECUTE ------
435
436
    add_bit
437
```

Listing 11: Contents of .bashrc file

B Amazing Programs, Extensions, Plugins & Packages

- https://github.com/charmbracelet/glow
- https://github.com/0xacx/chatGPT-shell-cli
- https://github.com/kardolus/chatgpt-cli/tree/main
 - For setting the right model (cf. here for all available models),

```
chatgpt --set-model gpt-4-1106-preview --set-max-tokens 128000
```

- Usage:

```
chatgpt -i
```

- https://tailscale.com/download/
 - Once installation is complete, the command

```
sudo tailscale up
```

should be run to login, though this command will also display after installation in the CLI. The signing in should happen via GitHub. To be able to use Tailscale from a new device, it must be added as a device under https://login.tailscale.com/admin/machines. Once this is done, open a CLI and type

```
ssh name@ip_address # find out <name> and <ip_address> via tailscale console # ssh ellie@100.xx.xxx.xx
```

NOTE that if the file already exists locally, it will be overwritten.

- For file copying (e.g. from the host machine to the currently used machine), do this

```
scp name@ip_address:/path/to/remote_file.ext /local/path # find out < name> and <ip_address> via tailscale console # ssh ellie@100.xx.xxx.xx
```

For directory copying,

```
scp -r name@ip_address:/path/to/remote_dir /local/path # find out < name> and <ip_address> via tailscale console
# ssh ellie@100.xx.xxx.xx
```

- https://tailscale.com/kb/1080/cli/ (no separate installation necessary, only tailscale needs to be installed)
 - Finding out the IPv4 address of the currently active machine,

```
tailscale ip -4
```

- Finding out the IPv4 address of another machine connected via the Tailscale network,

```
tailscale ip -4 custom-name
# tailscale ip -4 ellie
```

- https://github.com/aws/aws-cli
- https://github.com/termcolor/termcolor

C VSCode

C.1 Recommended Extensions

- https://marketplace.visualstudio.com/items?itemName=ms-vscode-remote.vscode-remote-ex
- https://marketplace.visualstudio.com/items?itemName=Gruntfuggly.todo-tree

C.2 settings.json

Opening the file,

- 1. press Ctrl + Shift + P to the Command Palette,
- 2. type Open User Settings (JSON) and select it to open the settings.json file.

C.3 Fix Unresolved Python Imports

• If you run a docker container where a conda environment is installed (with packages that you do not have locally), then VSCode will show those imports as unresolved. To fix this, open the settings.json file, cf. App. C.2, and add the following setting:

Incorporating this into the settings. json file is shown in App. C.5.

• Note that if you have an SSH connection to another machine going on, e.g. in the Remote Development extension, putting the above lines into the settings.json file will not have an immediate effect, for this the SSH connection needs to be restarted.

C.4 Opening a Duplicate Workspace

- 1. press Ctrl + Shift + P to the Command Palette,
- 2. then type Workspaces: Duplicate As Workspace is New Window

C.5 settings.json

Contents of settings.json,

```
"workbench.colorTheme": "Default Dark Modern",
"telemetry.telemetryLevel": "off",
"editor.wordWrap": "wordWrapColumn",
"editor.wordWrapColumn": 79,
"workbench.editor.enablePreview": false,
"gitlens.telemetry.enabled": false,
"notebook.lineNumbers": "on",
"explorer.confirmDragAndDrop": false,
"window.zoomLevel": 1,
"python.analysis.diagnosticSeverityOverrides": {
    "reportMissingImports": "none"
},
```

```
"todo-tree.general.tags": [
14
           "BUG",
15
           "HACK",
16
           "FIXME",
17
           "TODO",
18
           "NOTE",
19
           "XXX",
20
           "[]",
           "[x]"
       ],
23
24
       "files.associations": {"*.log": "plaintext"},
25
       "[plaintext]": {"editor.wordWrap": "off"},
26
       "[shellscript]": {"editor.wordWrap": "off"},
       "workbench.editor.tabSizing": "shrink"
      }
```

D LibreOffice

D.1 Dark Theme

Go to $Tools \to Options \to LibreOffice \to Application\ Colors \to Custom\ Colors \to General \to Document\ Background\ and\ choose\ a\ dark\ color.$

E UNIGE-specific

• Setting up UNIGE e-mail in TB: https://plone.unige.ch/distic/pub/messagerie/configuration/comment-configurer-compte-