Installation of the Anaconda Environment

NB2214 2024 Team

Troubleshooting tips can be found in these boxes.

Tips and general information can be found in these boxes.

Contents

1 Goal

The goal of this manual is to help you install:

- Miniconda, which installs the programming language Python.
- When installing Miniconda, we also install `conda`, a computer program used to manage the Python packages. These Python packages provide extra functionality to Python.
- A number of these packages needed for the course will be installed as well.

Finally, this manual also shows how to open Jupyter Lab, which is program for writing and executing Python code.

2 Windows Installation

2.1 Checklist

Make sure of the following:

1. You are running the latest version of Windows

2.2 Miniconda Install

If you followed the course last year, you should have installed Anaconda already. You can check this by following the steps below:

1. Press the Start button in Windows
2. type `Anaconda Prompt`

If Windows finds an application called "Anaconda Prompt (Anaconda3)", you already have Anaconda installed. This should look like Figure 1. You can skip this section (Section 2.2) and continue with Section 2.3.

1. Download the `.exe` installer via the link.
2. Double click the `.exe` file.
3. Follow the instructions on the screen. If you are unsure about any setting, accept the defaults.

For a full description of the install, check the Anaconda Website.

2.3 Packages Install

1. Download `requirements_windows.txt` from Brightspace. Navigate to Content > Resources > ALPACA Resources > Downloads. The file can be downloaded to any location, for instance to the Downloads folder.
2. Open the Anaconda prompt. Do this by pressing the Start button in Windows and typing `Anaconda Prompt`

Sometimes, if you have PyMOL installed (for example for the course Biomolecular Strucutures and Functions), the console that opens won't be the the Anaconda Prompt, but the PyMOL Anaconda Prompt. You van recognize this because the first line of the prompt looks like:

```
(C:\users\***\PyMOL) C:\Users\***>
```

If this happens, you should not follow the install instruction below. Instead try different applications available in the Start menu. Some options to try are:

- Anaconda Prompt (anaconda3)
- Aanconda Powershell Prompt

Note that there might be multiple Anaconda Prompts. A correct prompt should look something like:

```
(base) C:\Users\***>
```

Once you've found a working prompt, pin it to your task bar by right clicking it in the start menu. This will give you easy access to the correct prompt in the future.

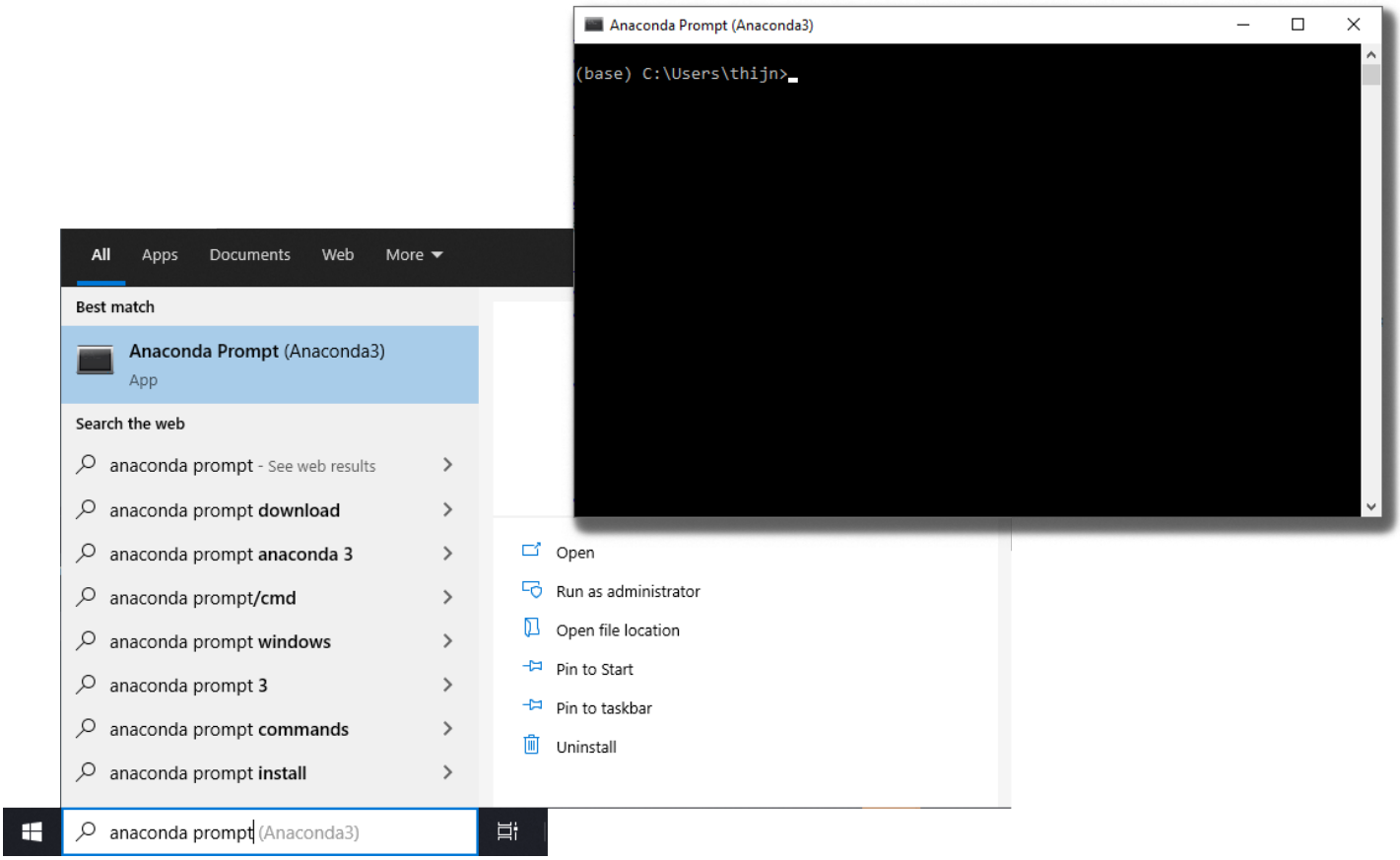

Figure 1: Opening the Anaconda Prompt

3. Add conda-forge to the available channels. In Terminal, type the following commands. Each command is followed pressing `Enter`.

```
conda config --add channels conda-forge
```

```
conda config --set channel_priority strict
```

4. Type the following onto the command line.

Do not press `Enter` yet. A path to the requirements file still needs to be appended to the command.

```
conda create -y --name=nb2214-2024 python=3.10 --channel twh --file=
```

5. Open File Explorer and navigate to the `requirements_windows.txt`. Drag and drop the `requirements_windows.txt` file onto Anaconda Prompt.

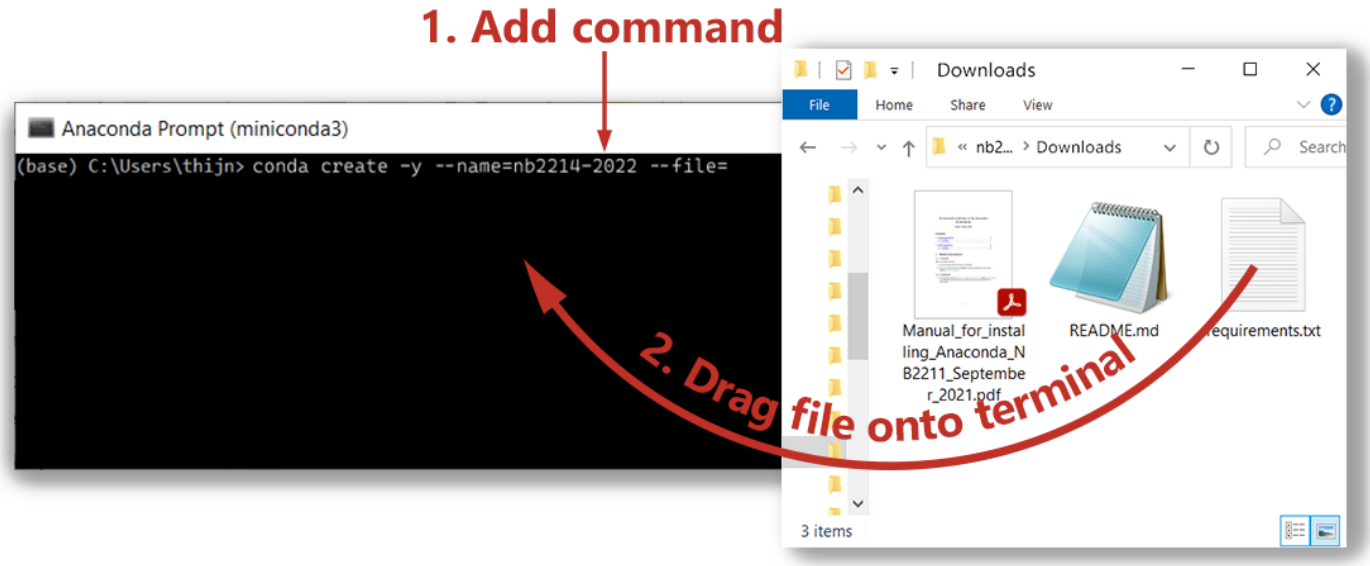

Figure 2: Drag and drop process on Windows. Note that the specific command seen in the image may be outdated. For the actual commands in the terminal, please refer to the text below.

The terminal should look something like the text below.

Your command will look different, do not copy the command below.

```
conda create -y --name=nb2214-2024 python=3.10 --channel twh
--file=C:/.../requirements_windows.txt
```

6. Press Enter. Wait for the install to complete.

During the installation, the command line might give the following prompt:

```
Proceed ([y]/n)?
```

Press Y, then press Enter.

You might encounter the following warning. Please note that it can be ignored:

```
==> WARNING: A newer version of conda exists. <==
```

7. Activate the `nb2211-2024` environment. In Terminal, type the following command and press `Enter`.

```
conda activate nb2214-2024
```

8. Install the ALPACA kernel into Juptyer Notebook

```
python -m alpaca_kernel install
```

If you have used Anaconda before, you might encounter the following error:

```
Error while finding module specification for 'alpaca_kernel.install'
↪  (ModuleNotFoundError: No module named 'alpaca_kernel')
```

If this is the case, run the command:

```
jupyter kernelspec list
```

This will generate a list of *Available kernels*. If `alpaca` shows up in this list, you can skip step 8.

9. You can now use Anaconda to use Jupyter Lab on your device!

If you are having issues when installing, please check the following:

- Check whether no steps were skipped.
- Check that you are using the Anaconda Prompt, not Windows Powershell or the Command Prompt.

2.4 Usage

Instructions for using Jupyter Lab:

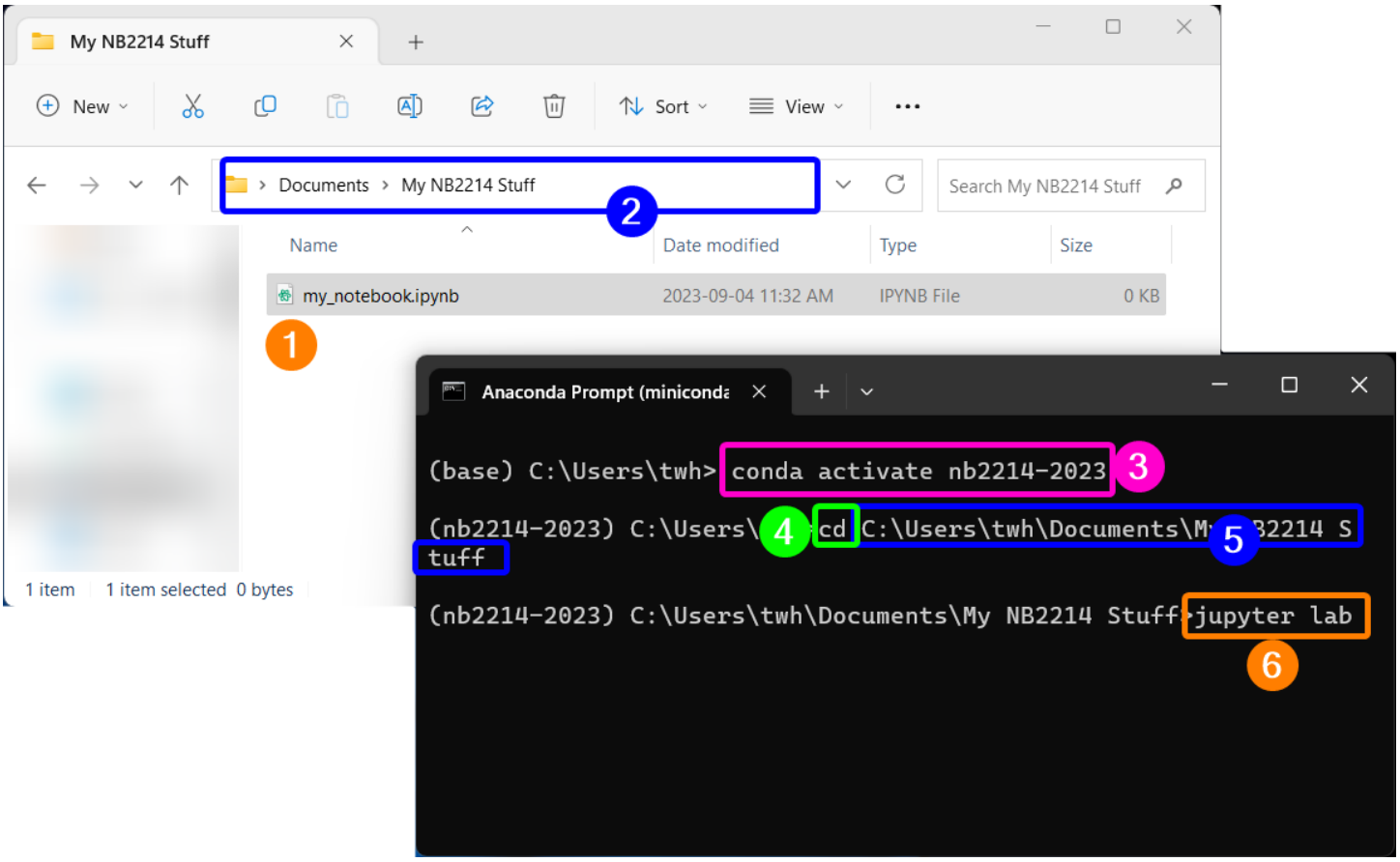

Figure 3: Method for opening Jupyter Lab in the location of your choosing. For the actual commands in the terminal, please refer to the text below.

1. Using File Explorer, navigate to the folder in which you want to use Jupyter Lab.

2. Move the mouse over the path. Click it once to highlight it. Copy this path to your clipboard.
3. Open the Anaconda prompt. Do this by pressing the Start button in Windows and typing `Anaconda Prompt`. If not the case yet, activate the `nb2214-23` environment by using the command below. Do not forget to press `Enter` to run the command.

```
conda activate nb2214-2024
```

4. Next, use the *change directory* command or `cd` to change the directory. Type the following onto the command line.

Do not press `Enter` yet. The path still needs to be appended to the command.

```
cd
```

5. Add a space and paste the path you copied earlier The terminal should look something like the text below. Press `Enter` to run the command.

Your command will look different, do not copy the command below.

```
cd "C:\Users\...\Folder Name"
```

If you are having issues with changing directory, that might be because there are spaces or other characters in your path. Try enclosing the path in parentheses as seen in the example above.

Sometimes, you might want to switch to a folder on a different drive on your computer. This is often necessary on the TU Delft computers as your personal files are on a different drive. To do this, add `/d` between `cd` and the path, e.g.:

```
cd /d "C:\Users\...\Folder Name"
```

6. The path to the left of the `>` symbol should now be where your notebooks are. Now you can open Jupyter Lab by running:

```
jupyter lab
```

To run Jupyter Notebook, an older version of Jupyter Lab instead (not recommended), use:

```
jupyter notebook
```

You can also skip step 4 and 5 and open Jupyter directly after activating the `nb2214-2024` environment.

3 MacOS Installation

3.1 Checklist

Make sure of the following:

1. You are running the latest version of MacOS

3.2 Miniconda Install

If you followed the course last year, you should have installed Anaconda already. You can check this by following the steps below:

1. Simultaneously press the ⌘ (command) and the `space` key on the keyboard.
2. A search bar will appear
3. Type: `Terminal`
4. Press enter.

This will have opened up the Terminal application. The first line contains time and date information. If the second line starts with `base`, the Anaconda has already been installed. This should look like Figure 4. You can skip this section (Section 3.2) and continue with Section 3.3.

1. Download the `.pkg` installer. via the link.

If you are unsure which file to download, use the table below:

Intel Mac	`Miniconda3 macOS Intel x86 64-bit pkg`
Apple Silicon Mac	`Miniconda3 macOS Apple M1 64-bit pkg`

To find whether you have an Apple Silicon Mac, check the instructions at Apple Website.

2. Double click the `.pkg` file.
3. Follow the instructions on the screen. If you are unsure about any setting, accept the defaults.

For a full description of the install, check the Anaconda Website.

3.3 Packages Install

1. Download `requirements_macos.txt` from Brightspace. Navigate to Content › Resources › ALPACA Resources › Downloads. The file can be downloaded to any location, for instance to the Downloads folder.
2. Open Terminal. Do this by simultaneously pressing the ⌘ (command) and the `space` key on the keyboard. A search bar will appear. Type: `Terminal` and press enter.

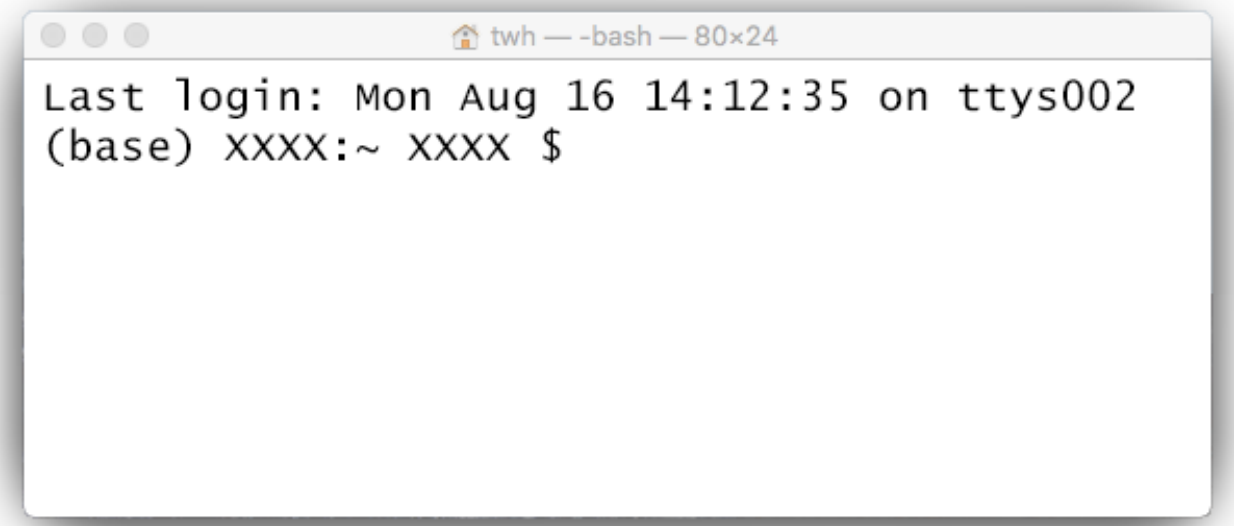

Figure 4: Terminal in macOS.

3. Add conda-forge to the available channels. In Terminal, type the following commands. Each command is followed pressing `Enter`.

```
conda config --add channels conda-forge
```

```
conda config --set channel_priority strict
```

4. Type the following onto the command line.

> Do not press `Enter` yet. A path to the requirements file still needs to be appended to the command.

```
conda create -y --name=nb2214-2024 python=3.10 --file=
```

5. Open Finder and navigate to the `requirements_macos.txt`. Drag the file onto the Terminal window.

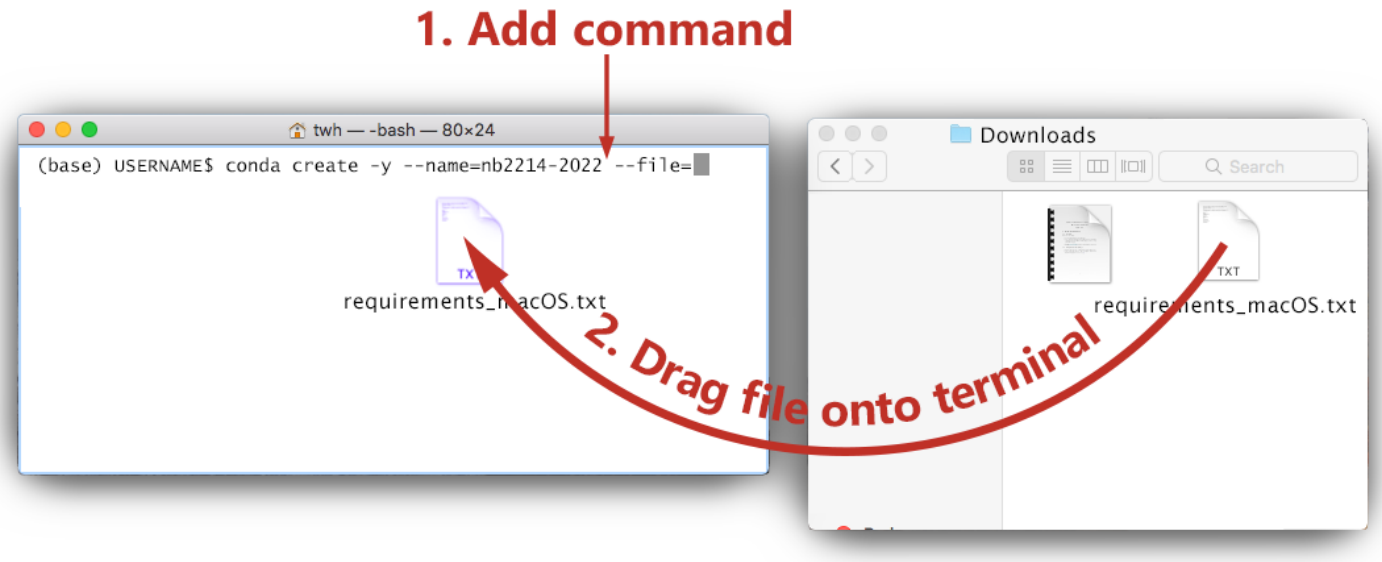

Figure 5: Drag and drop process on macOS. Note that the specific command seen in the image may be outdated. For the actual commands in the terminal, please refer to the text below.

The terminal should look something like the text below.

Your command will look different, do not copy the command below.

```
conda create -y --name=nb2214-2024 python=3.10
--file=.../requirements_macos.txt
```

6. Press Enter. Wait for the install to complete.

During the installation, the command line might give the following prompt:

```
Proceed ([y]/n)?
```

Press Y, then press Enter.

You might encounter the following warning. Please note that it can be ignored:

```
==> WARNING: A newer version of conda exists. <==
```

7. Activate the `nb2211-2024` environment. In Terminal, type the following command and press `Enter`.

```
conda activate nb2214-2024
```

8. Download the ALPACA kernel

```
pip install 'alpaca_kernel_2 @ git+https://github.com/twhoekstra/alpaca_kernel_2.git'
```

You might encounter the following warning.

```
xcrun: error: invalid active developer path
↪  (/Library/Developer/CommandLineTools), missing xcrun at:
↪  /Library/Developer/CommandLineTools/usr/bin/xcrun
```

Open Terminal, and run the following:

```
xcode-select --install
```

This will pop a dialogue box, Select "Install", and it will download and install the Command Line Tools package and fix the problem. (The popped Window may be behind other windows.)

9. Install the ALPACA kernel into Jupyer Notebook. Note that you will be prompted to input your password.

```
sudo python -m alpaca_kernel install
```

10. Install the Python kernel into Juptyer Notebook

```
sudo python -m ipykernel install
```

If you have used Anaconda before, you might encounter the following error:

```
Error while finding module specification for 'alpaca_kernel.install'
↪  (ModuleNotFoundError: No module named 'alpaca_kernel')
```

If this is the case, run the command:

```
jupyter kernelspec list
```

This will generate a list of *Available kernels*. If `alpaca` shows up in this list, you can skip step 8.

11. You can now use Anaconda to use Jupyter Lab on your device!

If you are having issues when installing, please check the following:

- Check whether no steps were skipped.
- Check that you are using `requirements_macos.txt`, not the one intended for Windows.
- Check that you installed the ALPACA kernel.

3.4 Usage

Instructions for using Jupyter Lab:

1. Click the Finder icon in the Dock to open a Finder window. Using Finder, navigate to the folder in which you want to use Jupyter Lab.
2. Choose View > Show Path Bar, or press ⌥ (option) to show the path bar momentarily. The location and nested folders that contain your file or folder are displayed near the bottom of the Finder window.
3. Control-click the folder in the path bar, then choose Copy "folder" as pathname.
4. Open Terminal. Do this by simultaneously pressing the ⌘ (command) and the `space` key on the keyboard. A search bar will appear. Type: `Terminal` and press enter.

5. If not the case yet, activate the `nb2214-23` environment by using the command below. Do not forget to press `Enter` to run the command.

```
conda activate nb2214-2024
```

6. Next, use the *change directory* command or `cd` to change the directory. Type the following onto the command line.

Do not press `Enter` yet. The path still needs to be appended to the command.

```
cd
```

7. Add a space and paste the path you copied earlier The terminal should look something like the text below. Press `Enter` to run the command.

Your command will look different, do not copy the command below.

```
cd "/Users/.../Folder Name"
```

If you are having issues with changing directory, that might be because there are spaces or other characters in your path. Try enclosing the path in parentheses as seen in the example above.

8. The path to the left of the > symbol should now be where your notebooks are. Now you can open Jupyter Lab by running:

```
jupyter lab
```

To run Jupyter Notebook, an older version of Jupyter Lab instead (not recommended), use:

```
jupyter notebook
```

You can also skip step 4 and 5 and open Jupyter directly after activating the `nb2214-2024` environment.

4 Linux Installation

4.1 Checklist

Make sure of the following:

1. You are running the latest version of Ubuntu.

4.2 Miniconda Install

For a full description of the install, check the Anaconda Website.

1. These four commands quickly and quietly install the latest 64-bit version of the installer and then clean up after themselves. To install a different version or architecture of Miniconda for Linux, change the name of the `.sh` installer in the wget command.

```
mkdir -p ~/miniconda3
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh -O ~/miniconda3/miniconda.sh
bash ~/miniconda3/miniconda.sh -b -u -p ~/miniconda3
rm ~/miniconda3/miniconda.sh
```

2. After installing, initialize your newly-installed Miniconda. The following commands initialize for bash and zsh shells:

```
~/miniconda3/bin/conda init bash
~/miniconda3/bin/conda init zsh
```

4.3 Packages Install

Follow the same steps as for in Section 3. Note that the user interface will look similar but might have differences.

4.4 Usage

Follow the same steps as for in Section 3. Once again, note that the user interface will look similar but might have differences.

5 Troubleshooting

`Python was not found`
Description of the problem: Whilst trying to run `python -m alpaca_kernel install`, you get an error message saying Python could not be found.
Complete error message: `Python was not found; run without arguments to install from the Microsoft Store`
Troubleshooting steps:

- Reinstall Miniconda.
    1. Remove Miniconda. Follow the steps noted in the Anaconda documentation.
    2. Restart computer.
    3. Download Miniconda
    4. Reinstall the environment using the instructions above.