

Software Setup — Assignment 2

CS 279, BIOE 279, BMDS 245, BIOPHYS 279, and CME 279

Where to work

We strongly recommend working on the Learning Technology & Spaces (LTS) machines. All the software for this assignment is already installed on the LTS machines.

You can also work on your own computer, but course staff can give only limited help with installation problems. If you run into problems, switch to the LTS machines rather than spending time debugging. Post on Ed or come to office hours if you get stuck.

To work on your own computer, you need:

- PyMOL 3.1, which was used in assignment 1. Installation instructions are in the [Assignment 1 Software Guide](#).
- conda, with a Python 3.9 environment that has matplotlib installed.
- PyRosetta 4, only if you attempt the challenge question (see the last section of this guide).

The steps below set these up in order.

Step 1: Check whether you already have conda

Open a terminal (Windows users: see the Windows section in Step 2 first) and run:

```
conda --version
```

Then find your result below:

- **You see conda 24 or higher** (for example, conda 24.9.2 or 26.5.3): you are all set. Skip to Step 3. It does not matter whether you have Anaconda or Miniconda; both work.
- **You see a version below 24** (for example, conda 4.12.0 or conda 23.7.4): update conda with the command below, then skip to Step 3. You do not need to uninstall it.

```
conda update -n base conda
```

- **The update fails with an error:** uninstall conda by following [Anaconda's uninstall guide](#), then go to Step 2.
- **You see “command not found”:** close the terminal **completely**, open a new one, and try again. If you still see “command not found”, go to Step 2.

Do not install a second copy of conda. Two copies on one computer cause errors that are hard to fix.

Step 2: Install Miniconda (only if Step 1 sent you here)

Go to anaconda.com/download/success and scroll down to the **Miniconda Installers** section. Don't use the Anaconda installers. Miniconda is much smaller and includes everything you need.

macOS

First, check which kind of Mac you have: open the Apple menu and click **About This Mac**.

- **Chip: Apple M1, M2, M3, or M4** (Apple Silicon): download the **64-Bit (Apple Silicon) Graphical Installer** from the Miniconda section. It needs macOS 12.1 or newer, which is also shown in About This Mac. If your macOS is older, update it or use the LTS machines.
- **Processor: Intel:** the download page no longer lists an Intel installer. Instead, download [Miniconda3-latest-MacOSX-x86_64.pkg](#), the last Intel version, from Anaconda's installer archive. We have not tested this; if you run into problems, please use the LTS machines.

Then:

1. Open the downloaded .pkg file and follow the prompts, accepting the defaults.
2. Open a new terminal window.
3. Run `conda --version`. You should see a version number.

Linux

Not tested by course staff. These steps may be helpful, but we have not tested them on Linux. If you run into problems, please use the LTS machines.

1. Download the Linux installer (a .sh file).
2. In a terminal, run the installer and accept the defaults. Replace the filename with the one you downloaded:

```
bash ~/Downloads/Miniconda3-latest-Linux-x86_64.sh
```

3. Close the terminal, open a new one, and run `conda --version`. You should see a version number.

Windows

Not tested by course staff. We strongly recommend using the LTS machines. If you would still like to work on Windows, these steps may be helpful:

1. Open PowerShell as Administrator, run `wsl --install`, and restart your computer.
2. Open **Ubuntu** from the Start menu. Do all of Steps 1 to 3 inside this Ubuntu terminal, using the Linux instructions above.

Install conda inside Ubuntu only. Do not also install the Windows version of Miniconda or Anaconda.

Note: When installing PyMOL with the Windows .exe installer (see the [Assignment 1 Software Guide](#)), install directly on Windows, not inside Ubuntu.

Step 3: Create the course environment

A conda environment is a separate set of packages for this course, so nothing here interferes with other Python work on your computer. Create one called `cs279`:

```
conda create -n cs279 python=3.9
```

If conda asks you to accept the Terms of Service, type `a` and press Enter. Then activate the environment:

```
conda activate cs279
```

Your prompt should now start with `(cs279)`. Install `matplotlib`:

```
conda install matplotlib
```

Important: run `conda activate cs279` every time you open a new terminal, before running any assignment code.

Step 4: Check your setup

Open a new terminal and run these three commands:

```
conda activate cs279
```

```
python --version
```

```
python -c "import matplotlib; print(matplotlib.__version__)"
```

You should see Python 3.9.x and then a matplotlib version number. Finally, open PyMOL and check that it starts. If all of this works, you are ready to begin.

Common problems

“conda: command not found”: open a new terminal window. Installing conda only affects terminals opened afterwards.

“ModuleNotFoundError: No module named ‘matplotlib’” in the terminal: you have not activated the environment. Run `conda activate cs279` and try again.

“No module named ‘pymol’”: you ran a PyMOL script from the terminal. Run it inside PyMOL instead.

The python command does not exist: try `python3` instead. On the LTS machines, use `python3.9`.

If none of these help, post on Ed with the exact command you ran and the full error message, or come to office hours.

Challenge question: PyRosetta setup

You only need this section if you attempt the optional challenge question, which uses PyMOL and PyRosetta 4.

We strongly recommend using the LTS Macs for the challenge question. PyRosetta is already installed there. It is difficult to install on your own computer, and because the challenge question is optional, course staff can give only limited help with installing it.

On an LTS Mac (recommended)

Download the challenge problem from the course website and unzip it. Then, in every new Terminal window, run these two commands. If you unzipped the folder somewhere other than Downloads, change the first command to match.

```
cd ~/Downloads/challenge_problem
```

```
source /Applications/PyRosetta/SetPyRosettaEnvironment.sh
```

The second command should print a line that starts with Setting PyRosetta root as: `/Applications/PyRosetta`.

Files on the LTS Macs are deleted when you log out, so save your work to Google Drive or a USB drive before you leave.

On your own Mac

First, complete Steps 1 to 3 above, so that you have the cs279 environment. Then:

1. Open a new Terminal window and activate the environment:

```
conda activate cs279
```

2. Install PyRosetta. This is a large download (about 1.5 GB) and can take 10 minutes or more. PyRosetta is free for academic use.

```
pip install pyrosetta --find-links https://west.rosettacommons.org/pyrosetta/quarterly/release
```

3. Check that PyRosetta works:

```
python -c "import pyrosetta; pyrosetta.init()"
```

If this prints some PyRosetta information and no error, the installation worked.

In every new Terminal window, run `conda activate cs279` and then `cd` into your `challenge_problem` folder.

Linux (not tested by course staff): the same steps may work, but we have not tested them. **Windows:** please use the LTS Macs for the challenge question.

Connecting PyMOL to PyRosetta

To watch the predictions as they run, open PyMOL, use `cd` to go to your `challenge_problem` folder, and run:

```
run PyMOLRosettaServer.py
```

Then run the `predict.py` commands from the assignment in your **Terminal** window, not in PyMOL.