Setting Up a Sustainable Python Environment

Fall 2025

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Abstract

This document provides guidance for setting up a sustainable and maintainable local research environment in Python. It is intended to be accessible to those with little to no familiarity with Python or programming languages in general while serving as a useful project reference for individuals who regularly utilize Python in their day-to-day life. Only basic familiarity with computers and their operation is assumed of the reader. Moreover, while this document does provide background and motivation for the project setup, it is perfectly acceptable to simply run through the commands as presented in order to get up and running without regard for why the environment works. Functionality is, after all, the primary motivation for this guide. A sequential list of the commands used in this guide can be found in Appendix A to this end.

The Python programming language is ubiquitous in data science research due to its accessibility as a programming language, extensive cross-platform support, and open ecosystem of support libraries. In particular, extensive resources have been invested into optimizing various numerical and scientific computation libraries for Python in no small part due to the recent explosion of academic and commercial interest in machine learning. For these reasons, a Python environment serves as an excellent place to begin exploring data science in a concrete setting.[1] Python's accessibility and ease-of-use does, however, make it quite easy for one to assemble a Python environment, which is a mishmash of the various guides, tutorials, and videos which are widely available. Each of these guides tends to be flavored by the author's particular background, experience, and preferences, and as such, the resulting environment can quickly become difficult to navigate. Although such biases are bound to be present in any guide, the focus of this document is to create an environment which is simple, follows industry best practices, and most importantly may be extended to as many environments as possible. We begin by installing Python.

[1] The reader is of course encouraged to explore other computational languages in addition to Python (such as MATLAB, Julia, R, etc.) to determine which may be best for their particular research.

1 Installation

There is no shortage of "right" ways to install Python [2], and these are of course unique to one's preferred operating system, available computational resources, permissions, etc. This guide is designed to be compatible with any pre-existing Python environments which the reader may already have. To check whether your system already has an existing Python installation (and which Python version is installed), run the following in your terminal: [3]

Listing 1: Python Version (Windows)

```
C:\Users\MathyMcMathFace> python3 --version
Python 3.10.2
```

Listing 2: Python Version (MacOS/Linux)

```
$ python3 --version
Python 3.10.2
```

If the above command for your system fails or reports an version of Python which is older than 3.4, you will need to install a new Python distribution; we recommend the following sources for their ease-of-use and simplicity:

1.1 Windows

We recommend installing Python for Windows through the Windows Store by opening a Command Prompt and typing `python` followed by the `[Enter]` key, which will automatically take you to the correct application page in the Windows Store. Alternatively, the following link will take you directly to the Python application page: `https://www.microsoft.com/store/productId/9PJPW5LDXLZ5`.

Simply click the `Get` button and wait for installation to complete.

1.2 MacOS

The latest Python versions for MacOS may be installed by navigating to `https://www.python.org/downloads/` in your favorite browser, clicking the `Download Python 3.x.x` button (`3.10.2` at the time of writing) on that page, and running the downloaded executable. The installation process is standard fare; accepting the default options during the installation process will result in a perfectly fine research environment.

[2] There is also no shortage of "wrong" ways, however - these are the ways which have you scratching your head wondering what on earth you were thinking when you come back to a dusty project several months later, or which cause the reader to experience great relief upon shutting down their computer.

[3] On Windows, this corresponds to the Command Prompt application, which can be accessed via the Start Menu. On MacOS/Linux, this corresponds to the Terminal application.

1.3 Linux

We recommend that you install Python via your distribution's package manager:[4]

Listing 3: Debian/Ubuntu

```
$ sudo apt install -y python3
```

Listing 4: Fedora

```
$ sudo dnf install -y python3
```

Listing 5: Arch Linux

```
$ sudo pacman -S python
```

The success of your installation can be verified by opening a new terminal and running the above version command.

2 Package Management

While Python itself is certainly useful out of the box, it does not take long for one to realize that there are a great many algorithms and functionalities that would be useful in several areas of research. One might think that it would be quite convenient if there existed a way to write such algorithms once and for all and subsequently share them across multiple projects. As it turns out, Python provides a mechanism for precisely this by way of a package management system called `pip`.[5] `pip` is included in all Python distributions from version `3.4+`, and as such will serve us quite conveniently as we explore specialized Python packages which are particularly useful for mathematical computation. [6]

3 Virtual Environments

One advantage to working with a popular open-source software such as Python is that there exists a rich ecosystem consisting of packages that do much of what one might think of to do with software. Because these packages are typically maintained by someone else, however, one cannot always be sure that code written against a particular package version will always run correctly against every subsequent version of the package that is published. Moreover,

[4]Most modern Linux distributions ship with Python pre-installed; in the event that your system does not have a Python distribution, you probably know more about your Linux installation than we do.

[5]Python is far from unique in this aspect - nearly every programming language in existence today has its own package manager(s) for this purpose.

[6]`pip` is also the industry-standard package management system for managing package dependencies in most professional Python projects. We will soon see its utility in the context of research.

it may be the case that two projects are actually incompatible with different versions of the same package, and that installing a single package version for all projects must necessarily break one or the other.[7] Upon consideration, one might come to the conclusion that it would be convenient if there existed some way to isolate one project's dependencies from another to prevent this sort of thing from happening. A moment's thought will convince the reader that it would additionally be convenient if such a mechanism also were to provide a way to explicitly list the packages upon which the project depends along with the package versions known to work with the project. Python again comes to the rescue with virtual environments.[8] Virtual environments are designed to solve the project dependency management problem, and provide a convenient way to ensure that projects are reproducable across operating systems and machines.[9] When operating the context of a virtual environment (which we refer to as *activating* the virtual environment, for reasons which will be evident in short order), packages installed with `pip` will only be installed into the project directory (folder), and will not affect the environment of any other existing or new Python projects on the system.

We now proceed to set up a single virtual environment for research. The advantage to a single environment is two-fold: First, by installing to a single virtual environment, we only have to install any particular package once in order for all our projects to be able to use the package. Since it's more common that we wish to use one version across multiple projects than it is for a project to require its own specific version, we defer the creation of multiple virtual environments to those projects which require specific package versions. The second advantage is that if we wish to share some aspect of our research, we need only share the project files and the file which contains the project's dependencies and their respective package versions.[10]

We begin by creating a new folder for our research. We use a folder named `research` in the user home[11] directory, though this choice is of course arbitrary.

[7] The ideal solution is naturally to update one or the other projects in order to make them both compatible with the same package version. In practice, however, this tends to involve a cost-benefit analysis that rarely ends in favor of updating the projects.

[8] In contrast to `pip`, it is unfortunately less common for other languages to provide mechanisms out of the box which are analogous to virtual environments.

[9] There is of course sometimes behavior which must necessarily be different across operating systems or hardware, but these differences are usually constrained to packages designed to work with particular hardware.

[10] By convention, this file is named `requirements.txt` and resides in the project's root folder.

[11] The user home directory is where any terminal - Windows or UNIX - will open to by default and hence serves as a convenient location for frequently-used files.

Except where commands differ between Linux and Windows, we will omit Linux command(s) for the sake of brevity.[12]

Listing 6: Create Research Directory (Windows)

```
C:\Users\MathyMcMathFace> mkdir research
C:\Users\MathyMcMathFace> cd research
```

We now create our virtual environment in a new (also arbitrarily named) `python-projects` directory:

Listing 7: Create Virtual Environment (Windows)

```
C:\Users\MathyMcMathFace\research> python3 -m venv python-projects/venv
C:\Users\MathyMcMathFace\research> cd python-projects
```

The last step is to *activate* our virtual environment. This informs your terminal that it should now look in the virtual environment for installed packages and commands, and must be done each time you wish to run a command in the context of your virtual environment.[13] Only a single virtual environment may be activated at a time in any given terminal window.

Listing 8: Activate Virtual Environment (Windows)

```
C:\Users\MathyMcMathFace\research\python-projects> .\venv\Scripts\activate
```

Listing 9: Activate Virtual Environment (MacOS/Linux)

```
[~/research/python-projects]$ source ./venv/bin/activate
```

At this point, we are ready to install any package we may wish via `pip`. For the sake of clarity, whenever a command is to be executed within the context of a virtual environment it will be preceded by `(venv)`. It should be understood that such commands execute in a terminal from the `python-projects` directory[14] created in this guide.

4 Jupyter Notebooks

It is at this juncture that we finally utilize the virtual environment we have created for applications specific to data science and computational mathematics. We do this by working within the context of a Jupyter Notebook, which is a web-based development environment which intersperses Python code blocks, Markdown, TeX in order to provide a cohesive workflow for data science and exploratory computation.

[12] A full list of the commands used for each operating system is included in Appendix A.

[13] For instance, if you restart your computer, open a new terminal, etc.

[14] Or equivalent, if the virtual environment was installed to a directory other than the one suggested in this guide.

4.1 Installing Dependencies

We begin by installing Jupyter itself alongside several useful computational packages which are ubiquitous in computational Python:

Listing 10: Computational Python Libraries (Windows)

```
(venv) pip install jupyterlab scipy numpy matplotlib scikit-learn pandas ipywidgets
```

4.2 Saving Dependencies

To lock our project dependencies and their versions into place, we save them to `requirements.txt`;[15] This should be done any time `pip` is used to install or update a package in this virtual environment:

Listing 11: Save Project Dependencies (Windows)

```
(venv) pip freeze > requirements.txt
```

4.3 Starting Jupyter

The last step is to start the Jupyter server:

Listing 12: Starting Jupyter (Windows)

```
(venv) jupyter notebook
```

[15] To install dependencies from a `requirements.txt` file in another project or virtual environment, simply run `pip install -r requirements.txt`.

Once your Jupyter server has started, navigate to `http://localhost:8888/lab` in your browser. To verify everything is running correctly, create a new notebook:

In your new notebook, paste the following into the empty code cell and click the `Run` button:

Listing 13: Simple Sine Wave

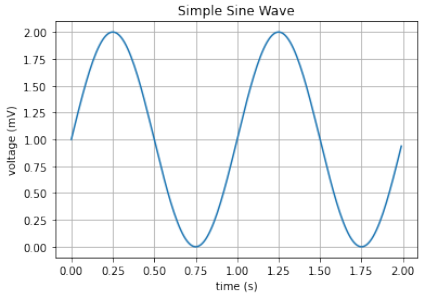
```
# Import newly-installed libraries
import matplotlib.pyplot as plt
import numpy as np

# Data for plotting
t = np.arange(0.0, 2.0, 0.01)
s = 1 + np.sin(2 * np.pi * t)

fig, ax = plt.subplots()
ax.plot(t, s)

ax.set(xlabel='time (s)', ylabel='voltage (mV)', title='Simple Sine Wave')
ax.grid()
```

You should see the following output:



4.4 Returning to Your Virtual Environment

Whenever you have exited your virtual environment (e.g., by running the above `deactivate` command in a virtual environment, rebooting, or closing all activated terminals), you must re-activate your virtual environment in order to run Python commands (e.g., `jupyter notebook`) by navigating to the directory your virtual environment was created in (`python-projects`, in our case), and execute whichever of the following commands pertains to your operating system:

Listing 14: Activate Virtual Environment (Windows)

```
C:\Users\MathyMcMathFace\research\python-projects> .\venv\Scripts\activate
```

Listing 15: Activate Virtual Environment (MacOS/Linux)

```
[~/research/python-projects]$ source ./venv/bin/activate
```

You will likely want to start your Jupyter server at this point if it's not already running elsewhere:

Listing 16: Starting Jupyter (Windows)

```
(venv) jupyter notebook
```

5 Appendix A - Command Reference

This section contains a brief listing of the commands used to create and activate virtual environments.

5.1 Windows

To create a new virtual environment:

Listing 17: Create a Virtual Environment (Windows)

```
C:\Users\MathyMcMathFace> mkdir research
C:\Users\MathyMcMathFace> cd research
C:\Users\MathyMcMathFace\research> python3 -m venv python-projects/venv
C:\Users\MathyMcMathFace\research> cd python-projects
```

To begin working in the virtual environment created by the above commands, navigate to the created virtual environment directory (`python-projects` in our example) and run:

Listing 18: Activate a Virtual Environment (Windows)

```
C:\Users\MathyMcMathFace\research\python-projects> .\venv\Scripts\activate
```

Once your virtual environment has been activated, install Jupyter Notebook along with some other Python libraries which are useful for scientific computation (this need only be done once per virtual environment):

Listing 19: Computational Python Libraries (Windows)

```
(venv) pip install jupyterlab scipy numpy matplotlib scikit-learn pandas ipywidgets
```

Lastly, to start a Jupyter Notebook server inside an activated virtual environment, simply run:

Listing 20: Start Jupyter Server (Windows)

```
(venv) jupyter notebook
```

5.2 MacOS/Linux

To create a new virtual environment:

Listing 21: Create a Virtual Environment (MacOS/Linux)

```
[~]$ mkdir research
[~]$ cd research
[~/research]$ python3 -m venv python-projects/venv
[~/research]$ cd python-projects
```

To begin working in the virtual environment created by the above commands, navigate to the created virtual environment directory (`python-projects` in our example) and run:

Listing 22: Activate a Virtual Environment (MacOS/Linux)

```
[~/research/python-projects]$ source ./venv/bin/activate
```

Once your virtual environment has been activated, install Jupyter Notebook along with some other Python libraries which are useful for scientific computation (this need only be done once per virtual environment):

Listing 23: Computational Python Libraries (MacOS/Linux)

```
(venv) pip install jupyterlab scipy numpy matplotlib scikit-learn pandas ipywidgets
```

Lastly, to start a Jupyter Notebook server inside an activated virtual environment, simply run:

Listing 24: Start Jupyter Server (MacOS/Linux)

```
(venv) jupyter notebook
```