PIMA school

February 22, 2021

Contents

These are the notes for the PIMA school 2021.

Chapter 1

Introduction

1.1 Introcuction to Shell terminal

The shell is a program where users can type commands. With the shell, its possible to invoke complicated programs like climate modeling software or simple commands that create an empty directory with only one line of code. The most popular Unix shell is Bash (the Bourne Again SHell so-called because its derived from a shell written by Stephen Bourne). Bash is the default shell on most modern implementations of Unix and in most packages that provide Unix-like tools for Windows.

Using the shell will take some effort and some time to learn. While a GUI presents you with choices to select, CLI choices are not automatically presented to you, so you must learn a few commands like new vocabulary in a language youre studying. However, unlike a spoken language, a small number of words (i.e. commands) gets you a long way, and well cover those essential few today.

The grammar of a shell allows you to combine existing tools into powerful pipelines and handle large volumes of data automatically. Sequences of commands can be written into a script, improving the reproducibility of workflows.

In addition, the command line is often the easiest way to interact with remote machines and supercomputers. Familiarity with the shell is near essential to run a variety of specialized tools and resources including high-performance computing systems. As clusters and cloud computing systems become more popular for scientific data crunching, being able to interact with the shell is becoming a necessary skill. We can build on the command-line skills covered here to tackle a wide range of scientific questions and computational challenges.

Lets get started.

When the shell is first opened, you are presented with a *prompt*, indicating that the shell is waiting for input.

The shell typically uses $ as the prompt, but may use a different symbol. In the examples for this lesson, well show the prompt as $. Most importantly: when typing commands, either from

Figure 1.1: bash prompt

```
Bash
$ ls
```

```
Output

Desktop     Downloads   Movies      Pictures
Documents   Library     Music       Public
```

Figure 1.2: ls command

```
Bash
$ pwd
```

```
Output
/Users/nelle
```

Figure 1.3: pwd command

these lessons or from other sources, do not type the prompt, only the commands that follow it. Also note that after you type a command, you have to press the Enter key to execute it.

The prompt is followed by a text cursor, a character that indicates the position where your typing will appear. The cursor is usually a flashing or solid block, but it can also be an underscore or a pipe. You may have seen it in a text editor program, for example.

So lets try our first command, ls which is short for listing. This command will list the contents of the current directory:

The part of the operating system responsible for managing files and directories is called the file system. It organizes our data into files, which hold information, and directories (also called folders), which hold files or other directories.

Several commands are frequently used to create, inspect, rename, and delete files and directories. To start exploring them, well go to our open shell window.

First lets find out where we are by running a command called *pwd* (which stands for print working directory). Directories are like places - at any time while we are using the shell we are in exactly one place, called our current working directory. Commands mostly read and write files in the current working directory, i.e. here, so knowing where you are before running a command is important. pwd shows you where you are:

Here, the computers response is */Users/nelle*, which is Nelles home directory: The home directory path will look different on different operating systems. On Linux it may look like /home/nelle, and on Windows it will be similar to C:/Documents and Settings/nelle or C:/Users /nelle. (Note that it may look slightly different for different versions of Windows.) In future examples, weve used Mac output as the default - Linux and Windows output may differ slightly, but should be generally similar.

We will also assume that your pwd command returns your users home directory. If pwd returns something different you may need to navigate there using *cd* or some commands in this lesson will not work as written. See Exploring Other Directories for more details on the cd command.

Lets create a new directory called *pimaschool* using the command (which has no output):

```
Bash

$ cd Desktop
$ cd data-shell
$ cd data
```

Figure 1.4: cd command

```
Bash

$ cd ..
```

Figure 1.5: command to go up one directory

```
[(base) Stefanos-MacBook-Pro:~ valenti$ mkdir ~/pimaschool
[(base) Stefanos-MacBook-Pro:~ valenti$ cd pimaschool/
[(base) Stefanos-MacBook-Pro:pimaschool valenti$ conda activate pima
```

Figure 1.6: make a new directory

mkdir pima

```
[(base) Stefanos-MacBook-Pro:~ valenti$ mkdir ~/pimaschool
[(base) Stefanos-MacBook-Pro:~ valenti$ cd pimaschool/
[(base) Stefanos-MacBook-Pro:pimaschool valenti$ conda activate pima
[(pima) Stefanos-MacBook-Pro:pimaschool valenti$ jupyter notebook
 [I 14:12:03.614 NotebookApp] The port 8888 is already in use, trying another port.
 [I 14:12:03.617 NotebookApp] Serving notebooks from local directory: /Users/valenti/pimaschool
 [I 14:12:03.617 NotebookApp] Jupyter Notebook 6.2.0 is running at:
 [I 14:12:03.617 NotebookApp] http://localhost:8889/?token=14751009d3b94da98a2e1d8bbc5ac1ef9b34f6a483789fe8
 [I 14:12:03.617 NotebookApp]  or http://127.0.0.1:8889/?token=14751009d3b94da98a2e1d8bbc5ac1ef9b34f6a483789fe8
 [I 14:12:03.617 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
 [C 14:12:03.634 NotebookApp]

    To access the notebook, open this file in a browser:
        file:///Users/valenti/Library/Jupyter/runtime/nbserver-56655-open.html
    Or copy and paste one of these URLs:
        http://localhost:8889/?token=14751009d3b94da98a2e1d8bbc5ac1ef9b34f6a483789fe8
     or http://127.0.0.1:8889/?token=14751009d3b94da98a2e1d8bbc5ac1ef9b34f6a483789fe8
```
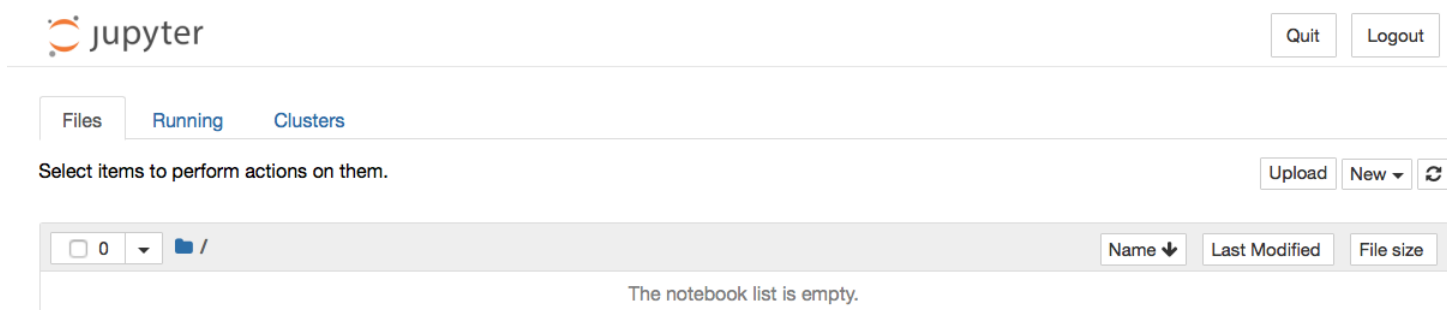
Jupyter

Quit   Logout

Files   Running   Clusters

Select items to perform actions on them.

Upload   New ▾   ⟳

☐ 0 ▾ 📁 /

Name ↓   Last Modified   File size

The notebook list is empty.

Figure 1.7: empty notebook

1.2   Starting a Jupyter notebook

This course will make extensive use of the Jupyter Notebook interface to Scientific Python, which is well suited to academic work (including independent research) because it combines code with output in digestable chunks. Even when the end product is a polished piece of software, much of the development occurs in the sort of interactive sessions that Jupyter Notebooks provide.

After following the software installation instructions on the course website, activate the pima environment with:

```
$ conda activate pima
```

Then, navigate to a working directory for this session, and start the notebook with:

```
$ jupyter notebook
```

This should start the Jupyter Notebook server and open a client in your web browser. An example starting a Jupyter Notebook from Linux is shown in Fig. 1.1.

You should create one new Jupyter Notebook, by choosing the New (Python 3) option in your client. Change the name of your notebook to something that clearly identifies what we are doing. Start each notebook with comments (starting with # symbol) indicating the title of the notebook. See the first cell of Fig. xx for an example. This first cell is also a good place to issue the ipython magic function: % pylab inline which will setup the notebook for inline plots and load the numpy and matplotlib libraries for you.

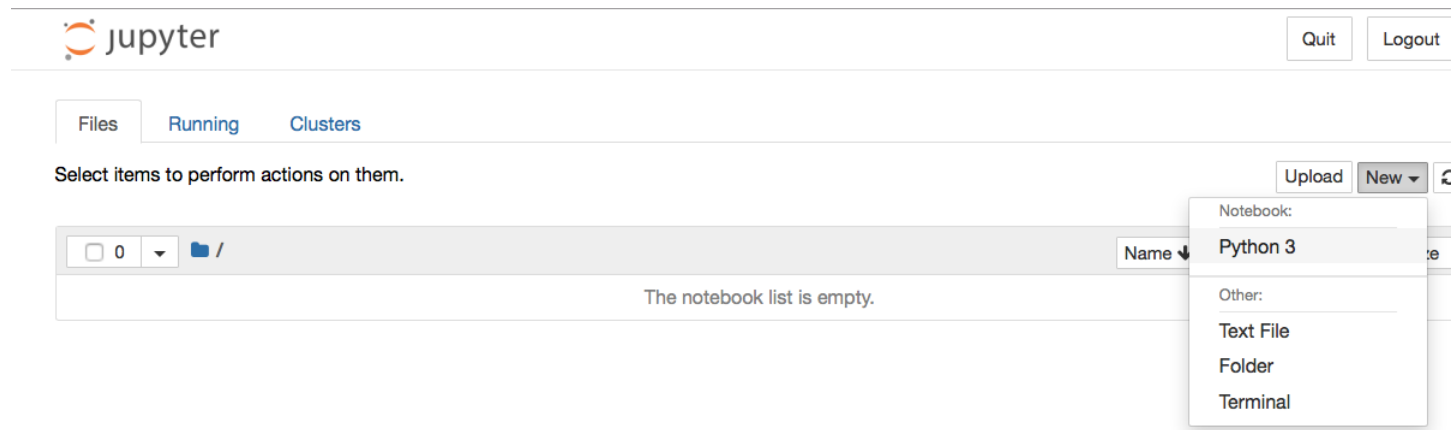Now that we have made our first notebook we can save it and it will have ipynb extension.
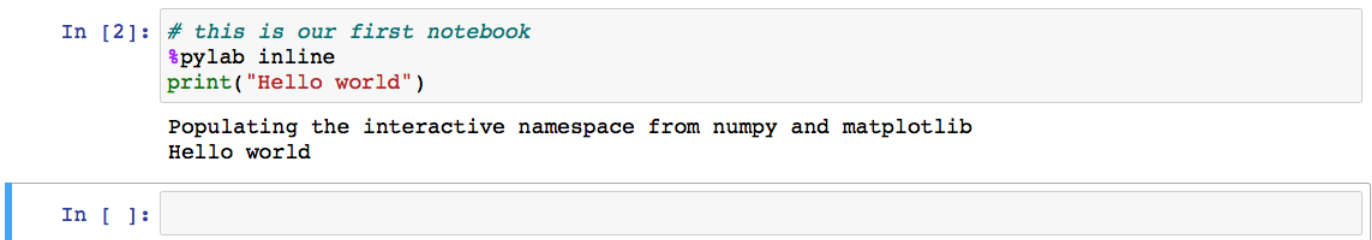
Figure 1.8: make new python 3 file in notebook

```
In [2]: # this is our first notebook
        %pylab inline
        print("Hello world")

        Populating the interactive namespace from numpy and matplotlib
        Hello world

In [ ]:
```

Figure 1.9: notebook "hello world"

1.2.1 notebook fast command

Here we report some short command for notebook:

Control vs Edit modes

- esc for control mode

- a : insert a new cell above current cell

- b : insert a new cell below current cell

- d+d : delete current cell

- m : convert cell to markdown

- y : convert cell to code

- enter for edit mode

- shift+enter : execute cell

Code vs Markdown Cells

- Markdown:

    bullets

    headings

equations

links

very simiar to HTML

Navigating the notebook

- plus : add a new cell

- File - Save and Checkpoint or picture of floppy drive: save

- Close browser window and type ctl+c twice in command line : Exit

Chapter 2

lecture 2

In order to run lecture 2 we need to donwload a notebook from here: