Practical Kinetics

Exercise 0:

Getting Started

Objectives:

1. Install Python and IPython Notebook

2. `print "Hello World!"`

What is Python?

Python is a programming language that is:

1. **Easy to use.** It reads like English:

```
if temperature < 30:
    print "Wear a hat."
```

2. **Free and widely used.** It's the fifth-most popular language in the world!

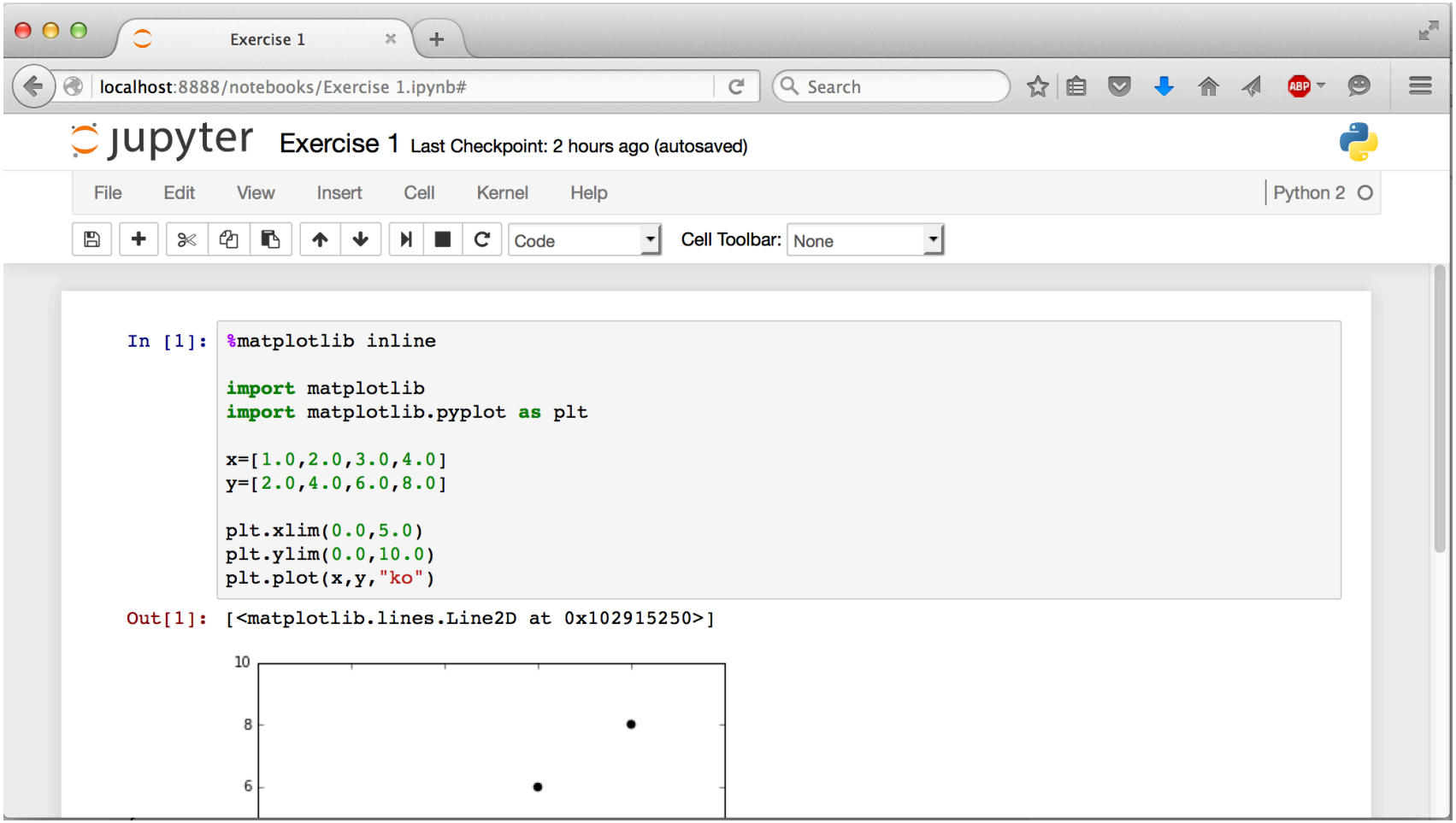
Jan 2016	Jan 2015	Change	Programming Language	Ratings	Change
1	2	^	Java	21.465%	+5.94%
2	1	v	C	16.036%	-0.67%
3	4	^	C++	6.914%	+0.21%
4	5	^	C#	4.707%	-0.34%
5	8	^	Python	3.854%	+1.24%

(Source: tiobe.com)

3. **Great for doing science.** Many common tasks like importing spreadsheet data, curve fitting, and solving differential equations are easy in Python.

What is IPython Notebook?

"I" stands for "interactive." It's a way to run Python in your browser:



You can also annotate your code and share it with others. There is no difference between the Python code in IPython Notebooks and .py files.

How to Run Python

Option 1. Run Locally in IPython Notebook **(recommended)**

Code in your browser. Calculations are performed by your own computer.

You will have to install Python, but you don't have to depend on an Internet connection, files stay on your own computer, and calculations are free.

Option 2: Run on the Web at wakari.io

Code in your browser. Calculations are performed by computers in the cloud.

You won't have to install any software, but you will have to pay if you are doing anything more than a casual calculation.

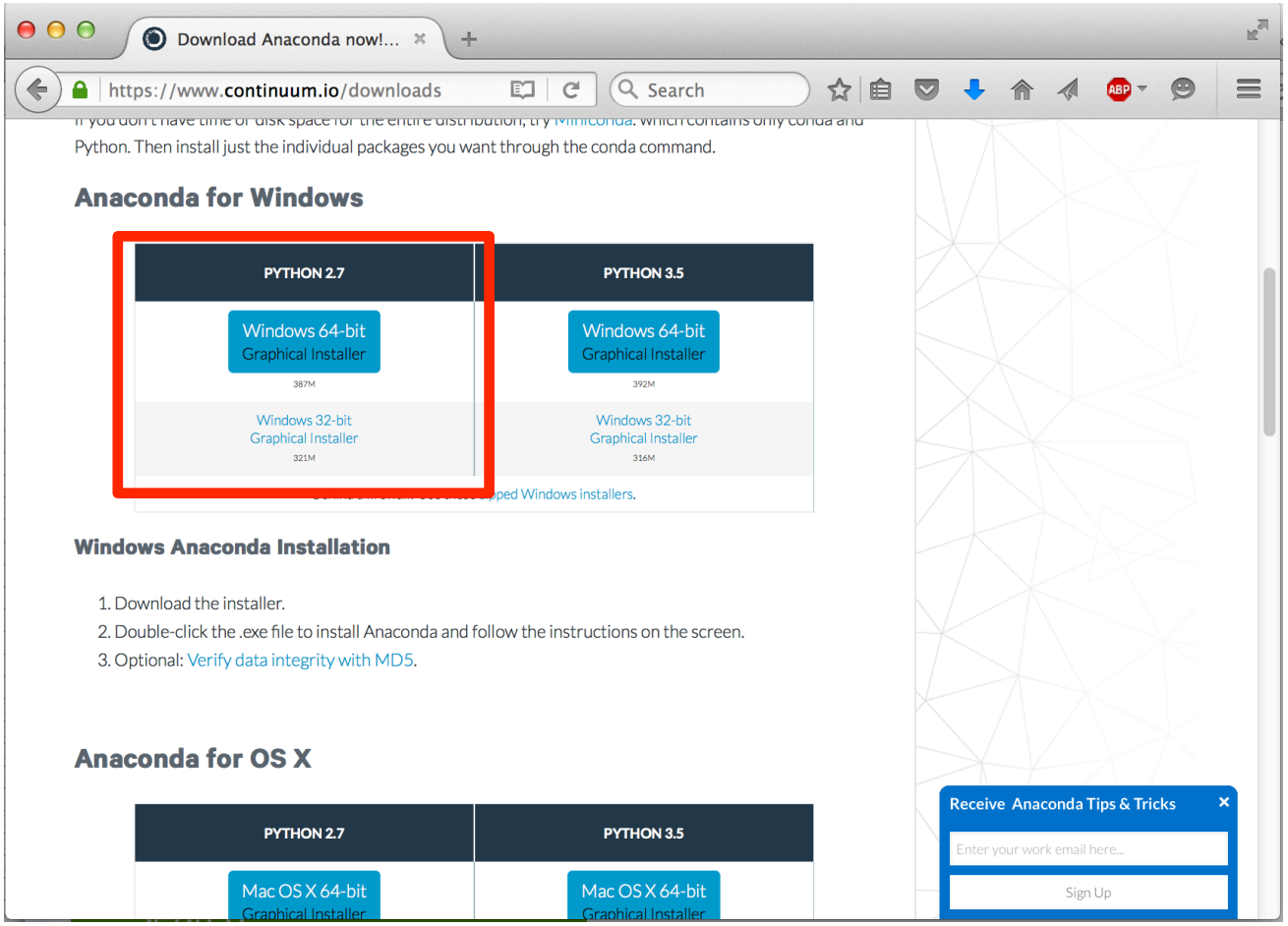
Option 3: Run Locally with a Text Editor (advanced)

Code in a text editor. Calculations are performed by your own computer.

If you already have some programming background, you might prefer to code in `vim`, `emacs`, or another text editor. This option is faster and more versatile, but will not be covered in this tutorial.

Option 1: Install Python Locally

To run Python on your own computer, download the standard Anaconda package from https://www.continuum.io/downloads.

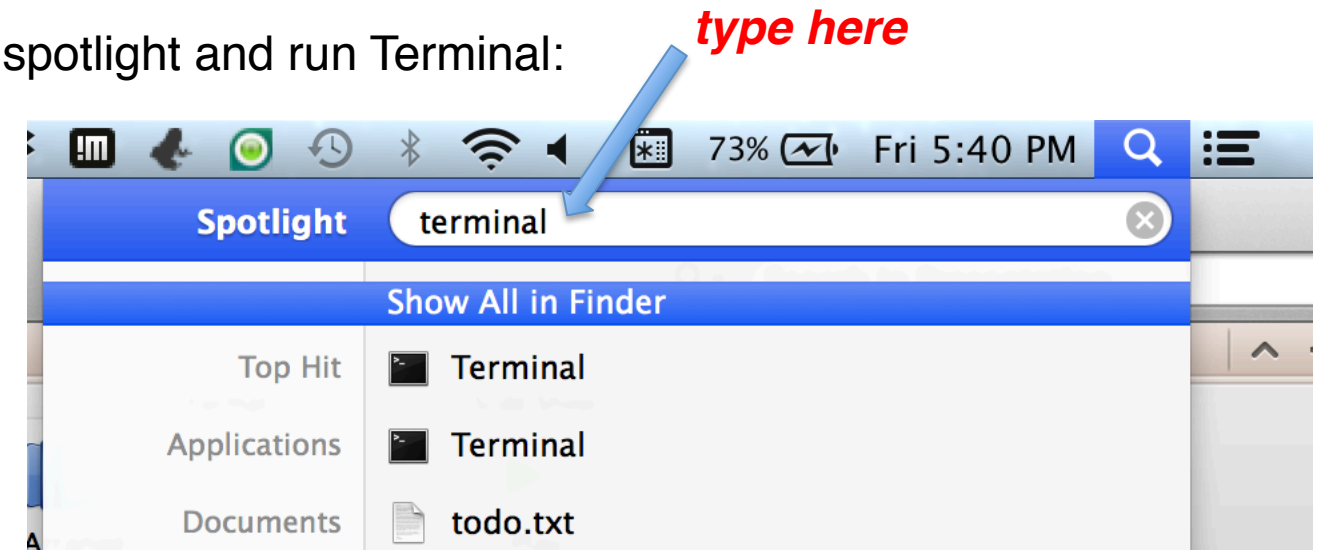


Installers for both Windows and Mac are available. Select Python 2.7.

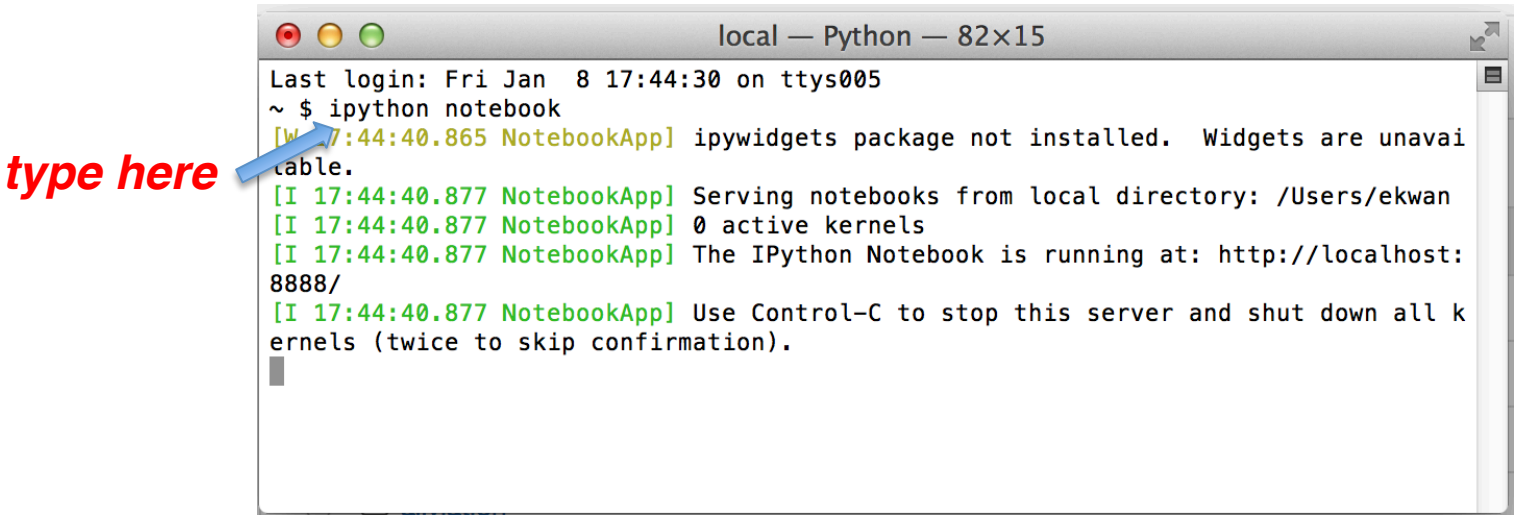
Option 1: Start Python (Mac)

To start IPython Notebook:

1. Open spotlight and run Terminal:

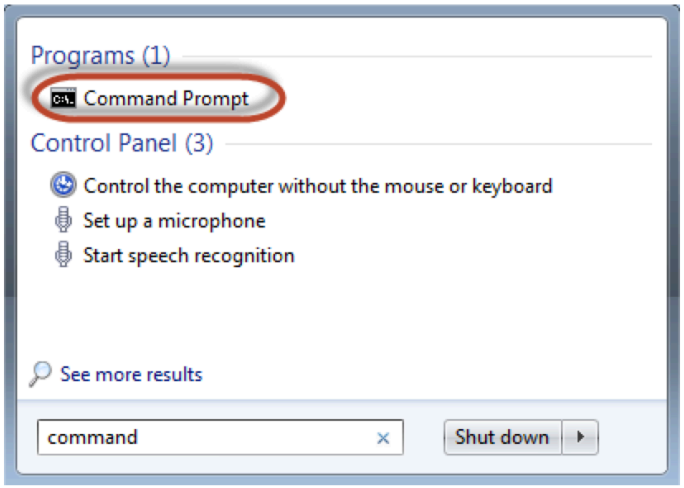


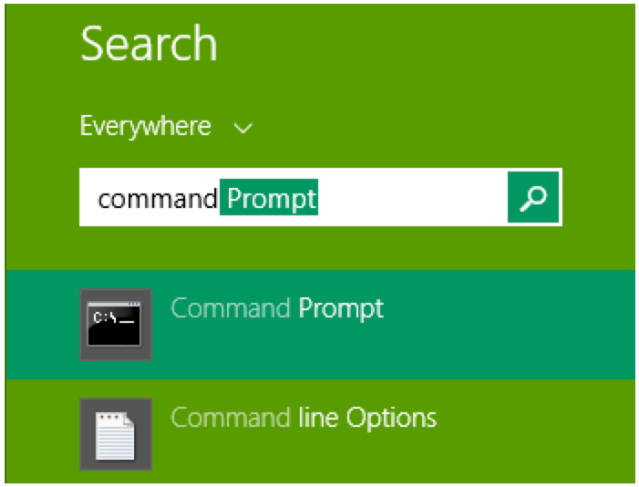
2. Type `ipython notebook` and press **enter**:



Option 1: Start Python (PC)

Open the command prompt from the Start menu (various Windows versions shown):

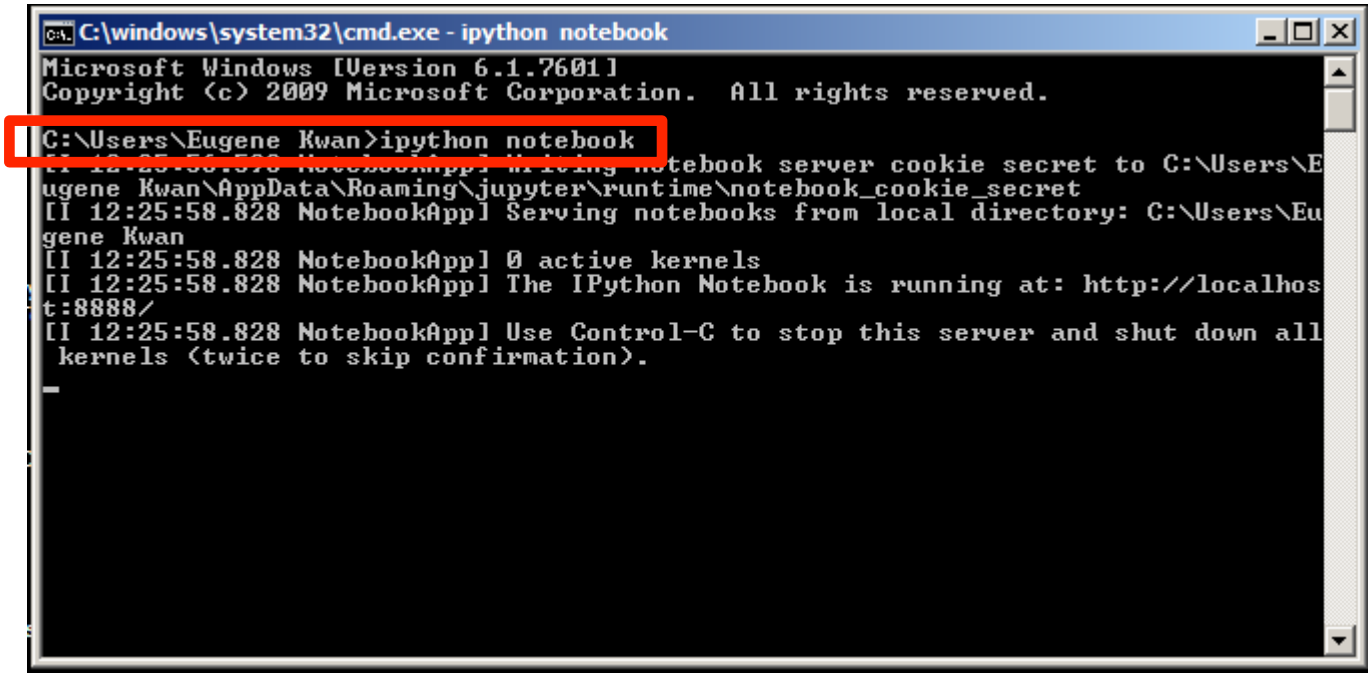




1. Click on the Start button (or its equivalent).
2. Search for “command prompt.” Alternatively, run `cmd`.
3. Start the prompt. A black console will open.

Option 1: Run Python (PC)

This is the command prompt console:



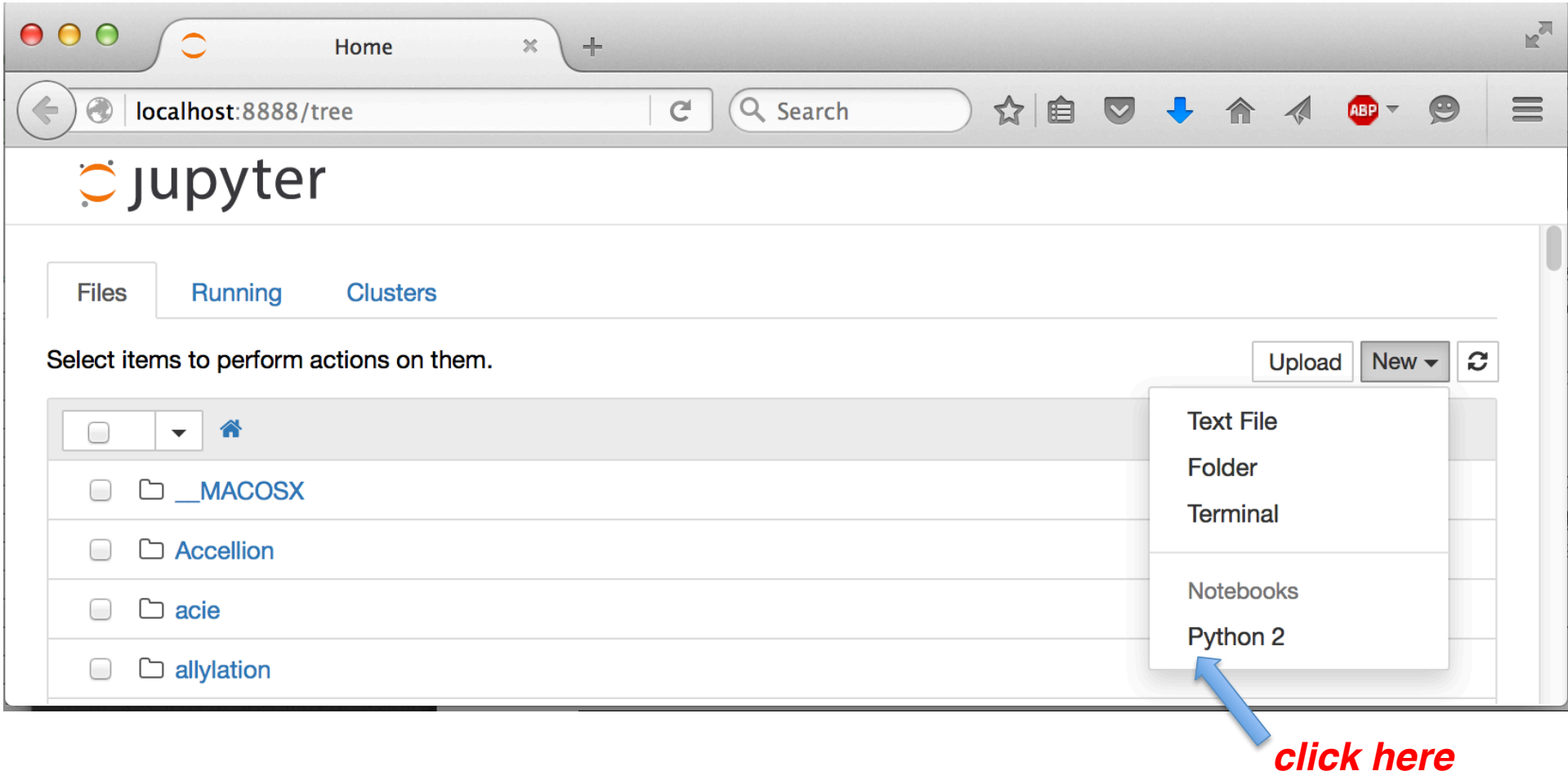
1. Type `ipython notebook` and press **enter**.

2. The Python kernel will start in the console. That's all the text under the red box above.

3. IPython Notebook will start in your browser. If it doesn't, navigate to http://localhost:8888/

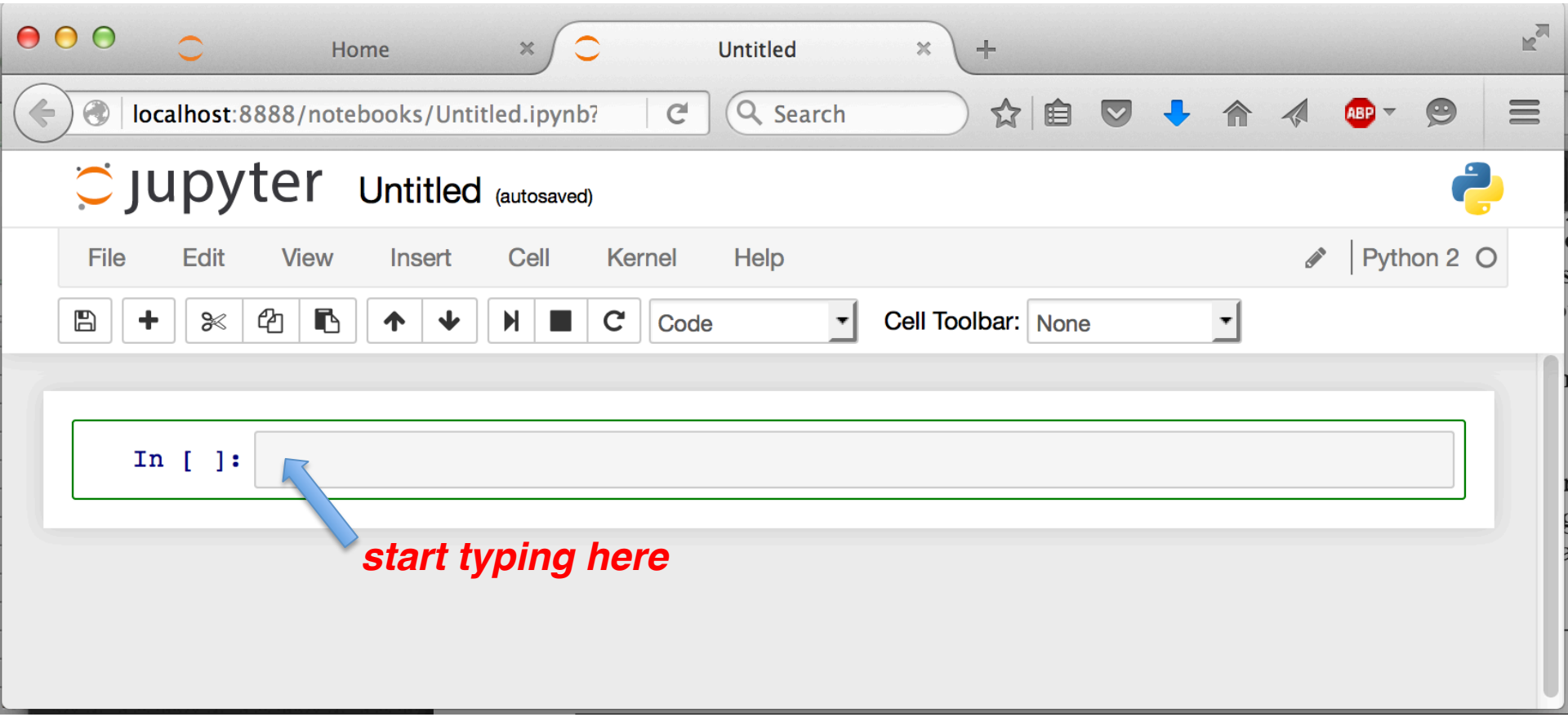
Option 1: Start a Notebook (Mac and PC)

Python will open in your browser:



Option 1: Start a Notebook (Mac and PC)

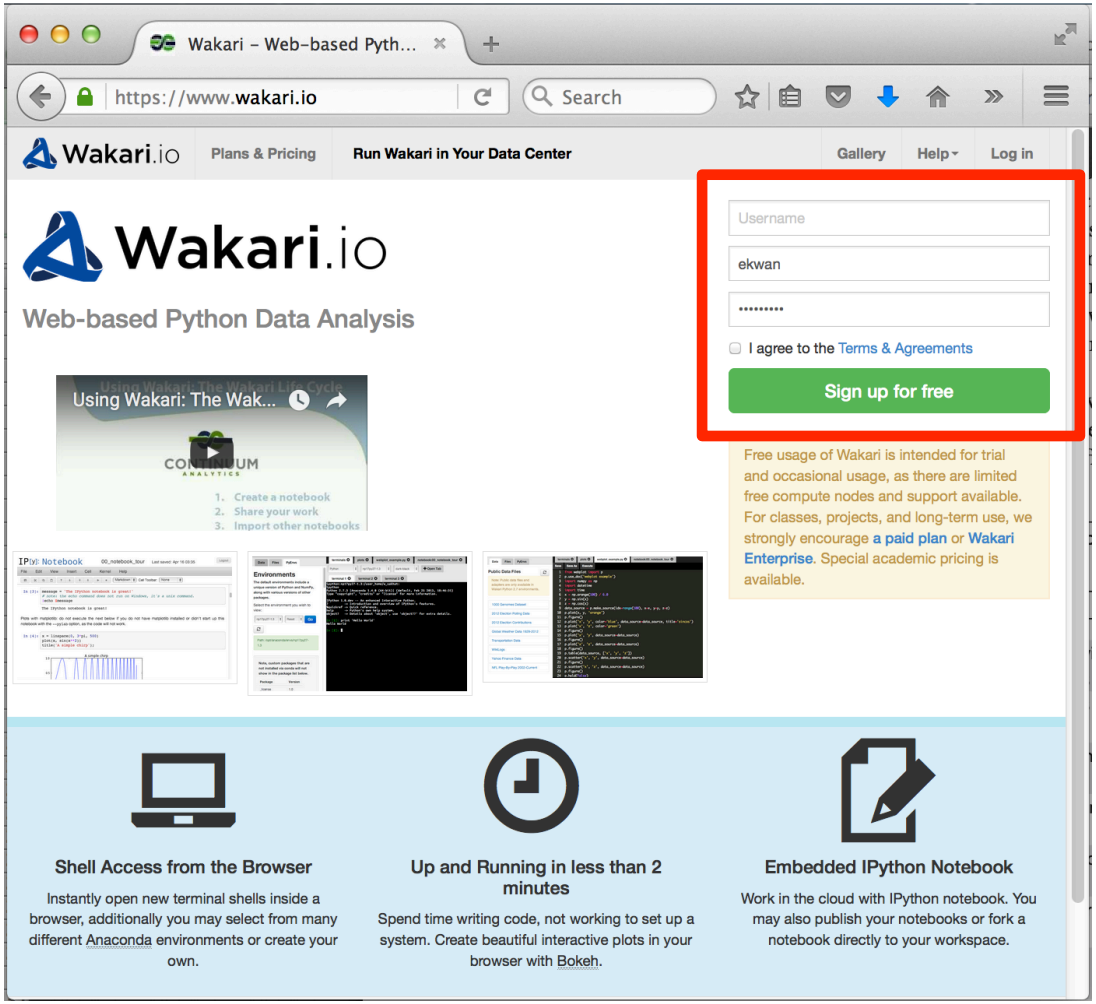
A new tab will open:



You can start typing Python commands where indicated.

Option 2: Running on the Web

You can also run Python on the web at https://www.wakari.io

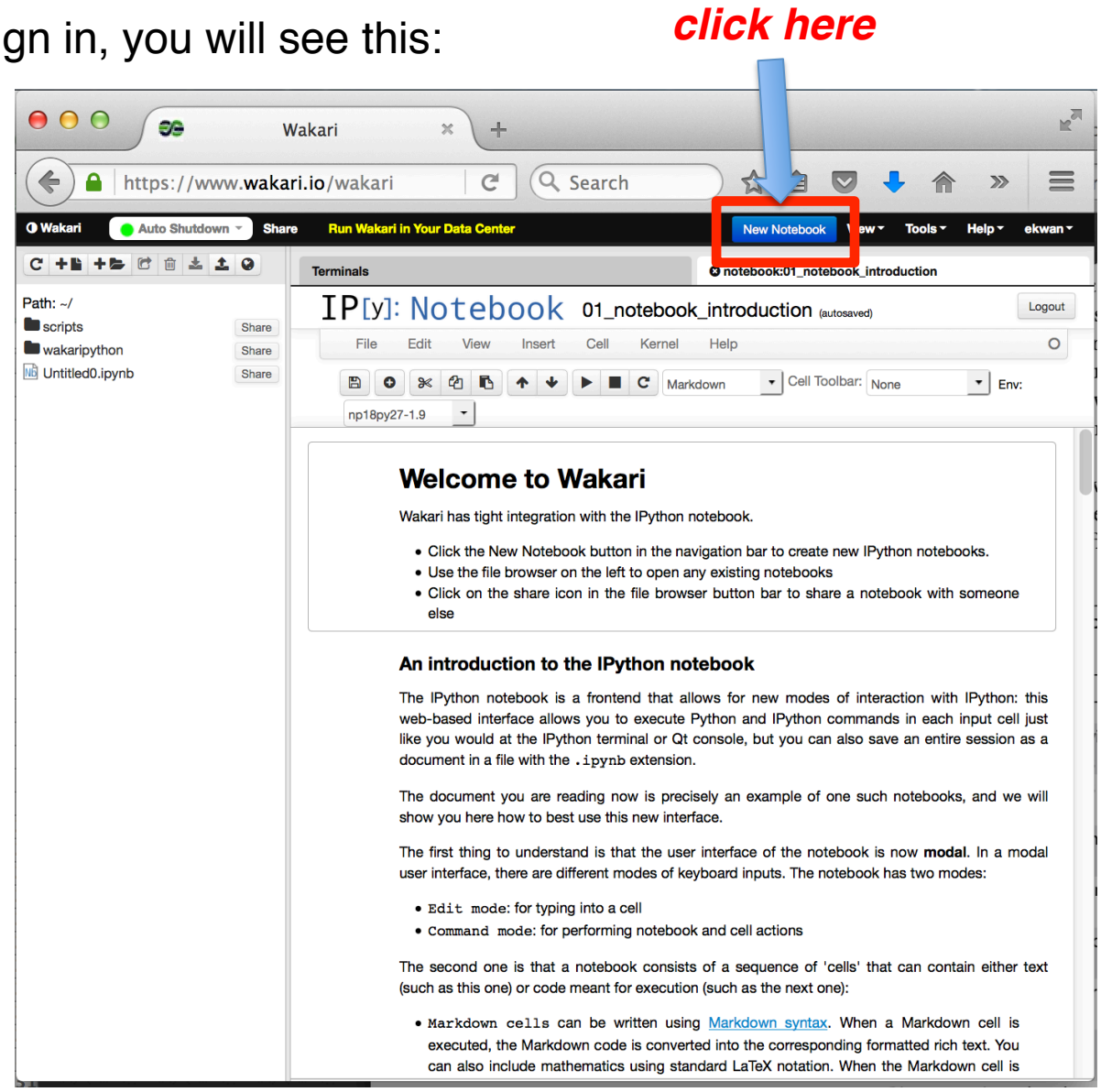


sign up here

You will need to make an account before you can sign in. It's free.

Option 2: Running on the Web

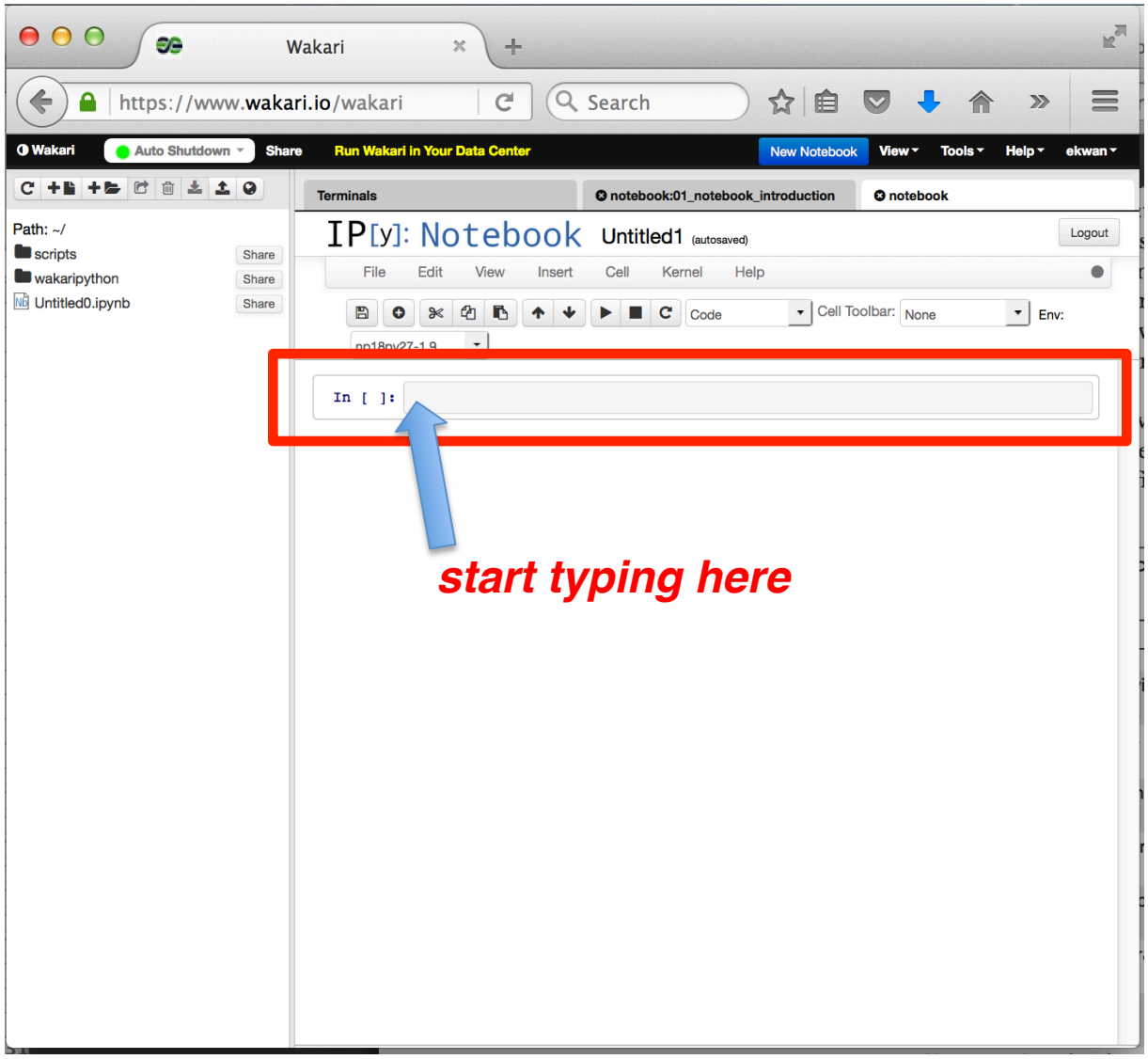
When you sign in, you will see this:



Click “New Notebook” to get started.

Option 2: Running on the Web

When you sign in, you will see this:



You can start typing in the indicated cell.

Hello World!

To verify everything is working correctly, type the following code in:

```
import numpy as np
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt

print "Hello world!"

x = np.linspace(0,2*np.pi,100)
y = np.sin(x)

plt.plot(x,y,"k")
plt.savefig("plot.png")
```

Notice that when you press **enter**, your cursor will go to the next line.

To run the code, press **shift-enter**.

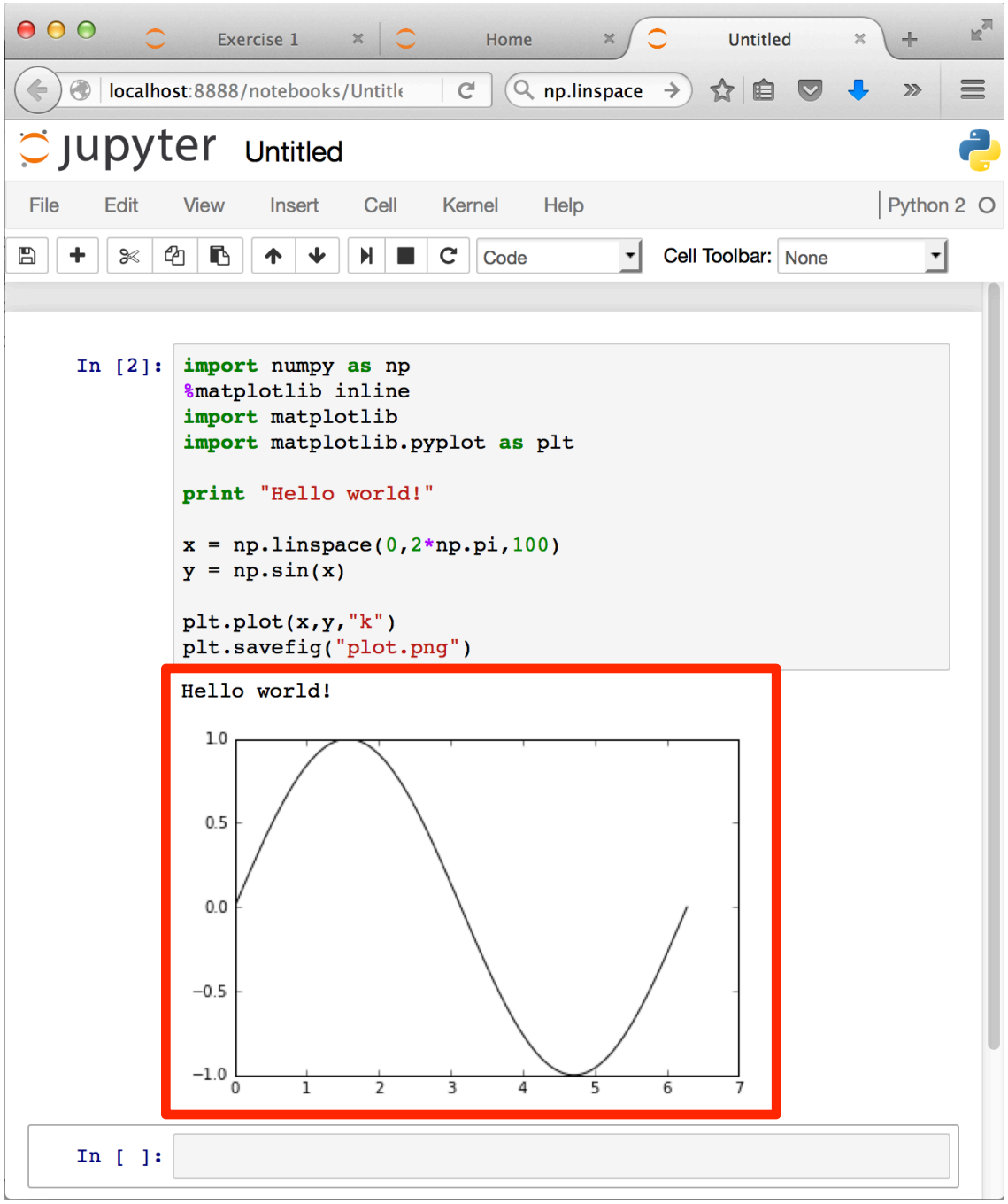
Hello World!

You should see it print out “Hello world!” and a simple graph. I highlighted the expected output in red.

Note that copying and pasting the code may not work because of carriage return issues. Typing it directly should work.

A new cell appears after execution. You can type more code in there, or change the code you just wrote and run it again.

Congratulations! You just ran your first Python program!



The Working Directory (Local)

When you run Python locally, notebooks will be saved into the current directory. This is determined by the directory that Python is started from. To change it:

Mac: type `cd some_directory` before typing `ipython notebook`.

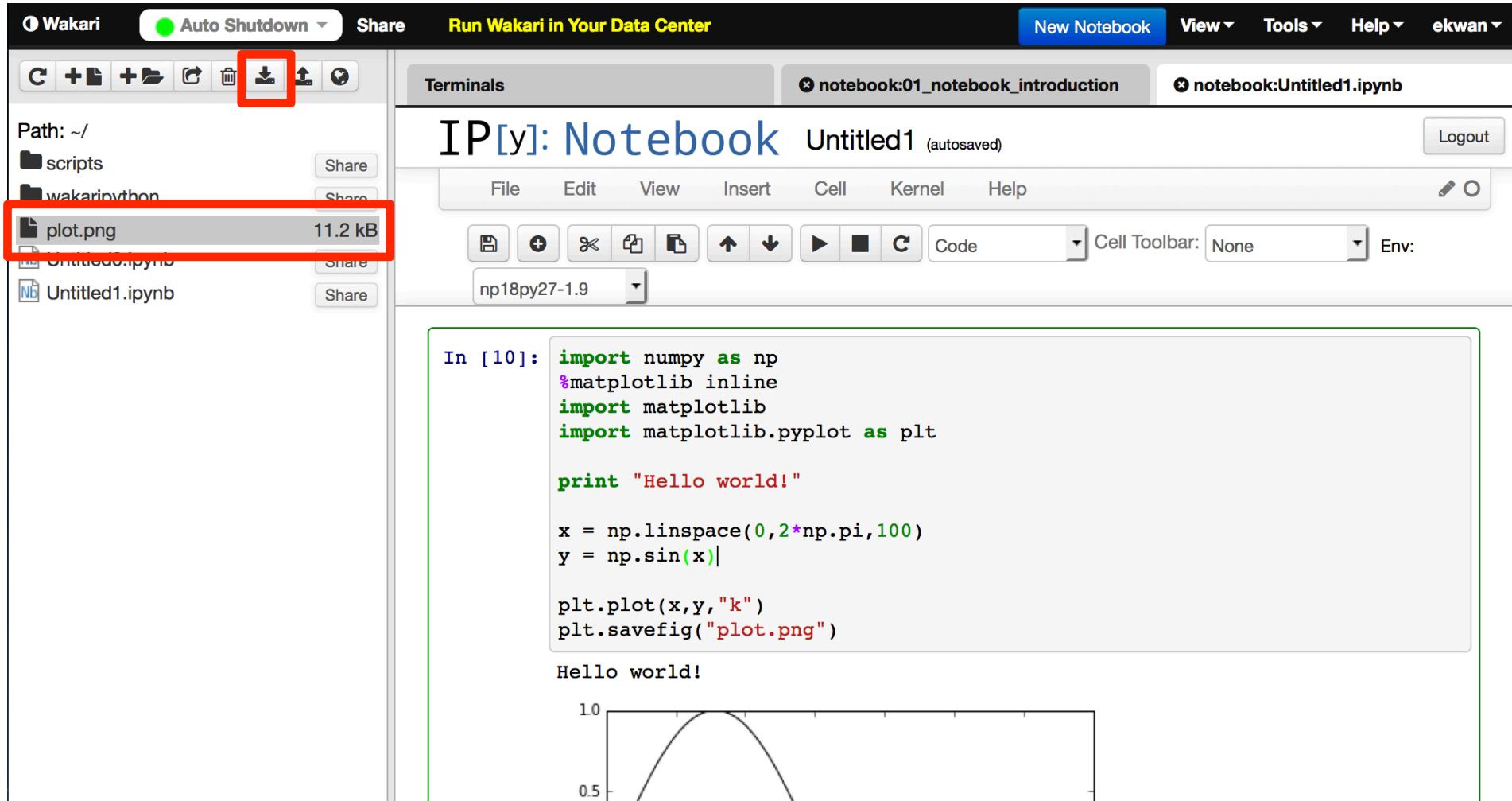
PC: type `cd C:\mypath\` before typing `ipython notebook`.

```
Last login: Sat Jan  9 23:41:36 on ttys006
~ $ cd kinetics_tutorial/
~/kinetics_tutorial $ ipython notebook
[W 13:04:06.148 NotebookApp] ipywidgets package not installed.  Widgets are unavailable.
[I 13:04:06.155 NotebookApp] The port 8888 is already in use, trying another random port.
[I 13:04:06.252 NotebookApp] Serving notebooks from local directory: /Users/ekwan/kinetics_tutorial
[I 13:04:06.252 NotebookApp] 0 active kernels
[I 13:04:06.252 NotebookApp] The IPython Notebook is running at: http://localhost:8889/
[I 13:04:06.252 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
```

In the “Hello world!” script, the line `plt.savefig("plot.png”)` should have saved a PNG of the graph to your working directory.

The Working Directory (Wakari)

When you run Python on Wakari, notebooks will be saved into a cloud directory, which is shown on the left hand side. Running the "Hello world!" script should create `plot.png`. Press the download button to copy it to your own computer.



Summary

1. Python is a free, popular, and versatile programming language for doing science. IPython Notebook lets you code in your browser.

2. You can run Python locally or on the cloud.

3. Enter code in cells. Pressing **enter** goes to the next line. Pressing **shift-enter** executes the code in the current cell.

4. Files will be written to the working directory. Set it before starting Python.