

# 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!

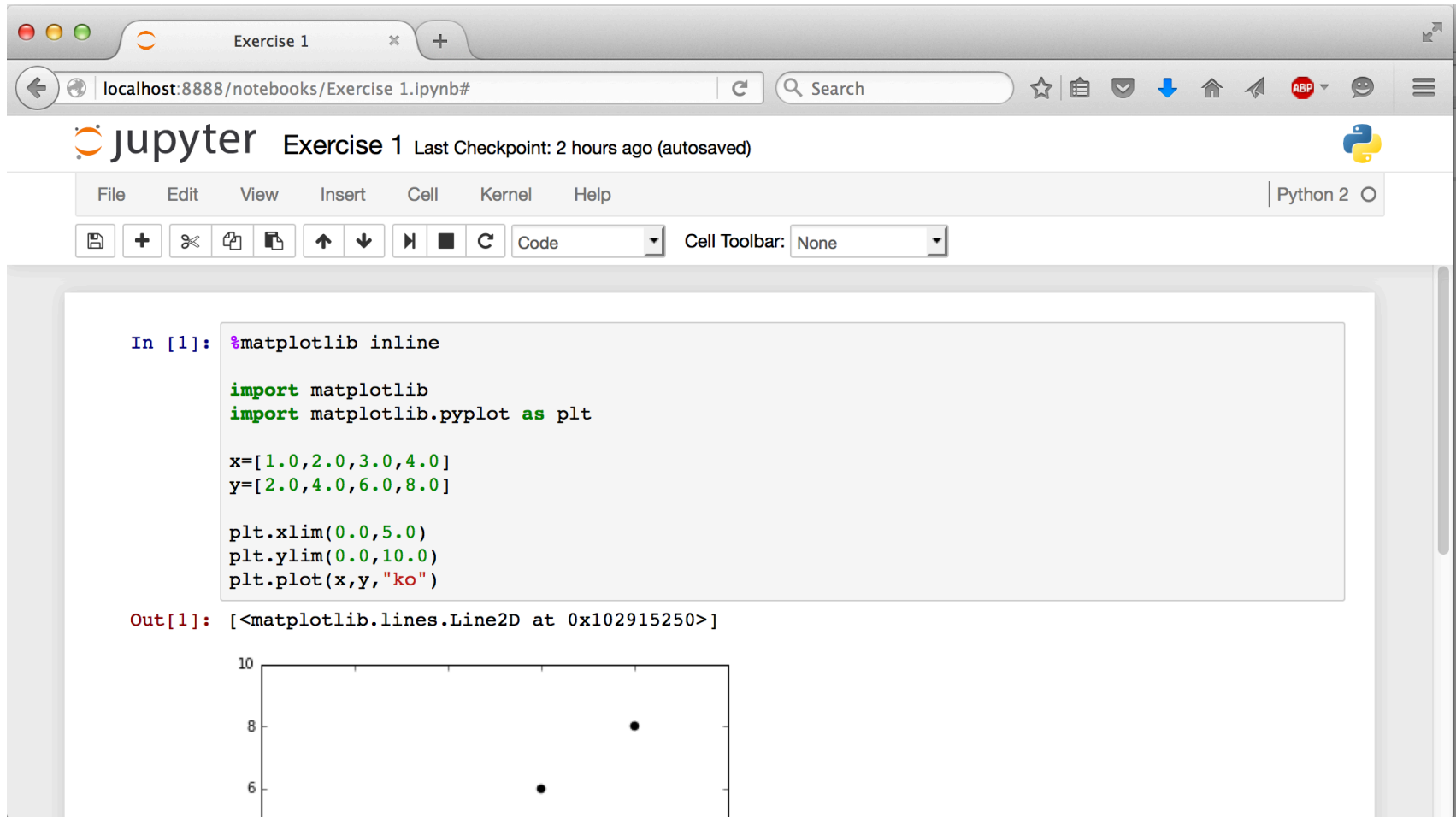
Jan 2016	Jan 2015	Change	Programming Language	Ratings	Change
1	2	▲	Java	21.465%	+5.94%
2	1	▼	C	16.036%	-0.67%
3	4	▲	C++	6.914%	+0.21%
4	5	▲	C#	4.707%	-0.34%
5	8	▲	Python	3.854%	+1.24%

(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](http://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.

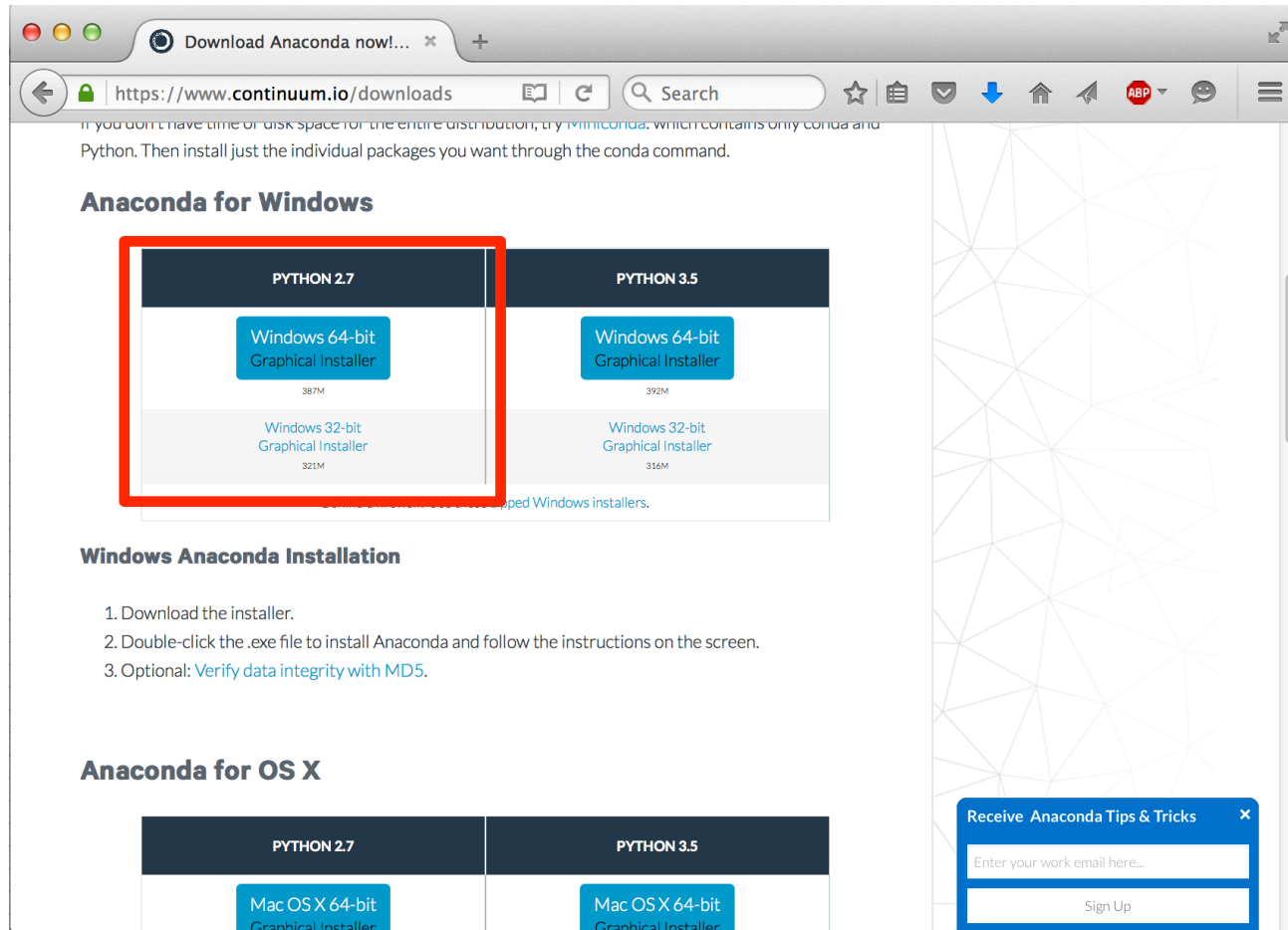
## Option 3: Run Locally with a Text Editor (**advanced**)

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>.

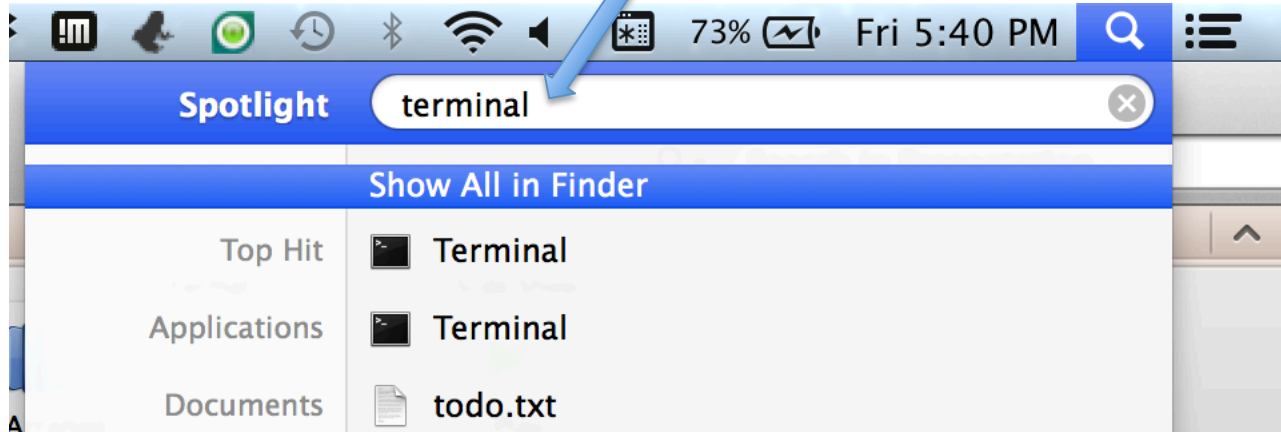


Installers for both Windows and Mac are available. Select Python 2.7.

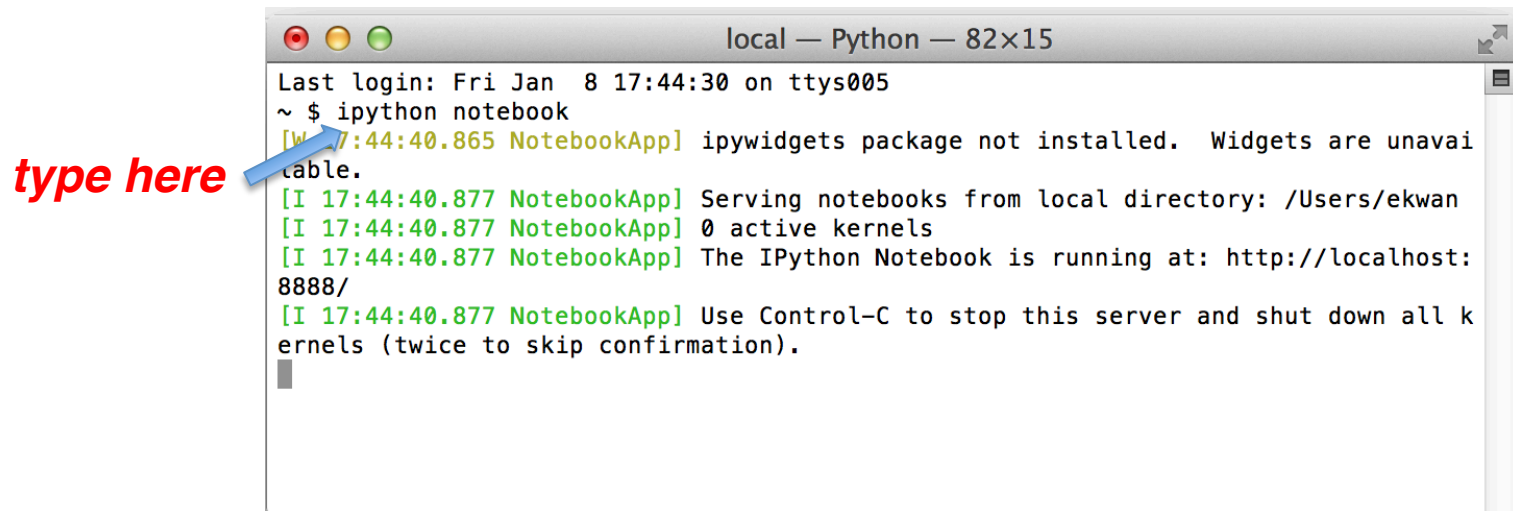
# Option 1: Start Python (Mac)

## To start IPython Notebook:

1. Open spotlight and run Terminal: *type here*



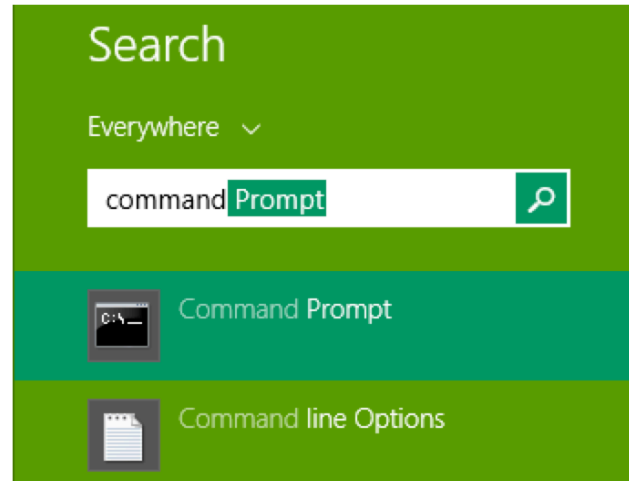
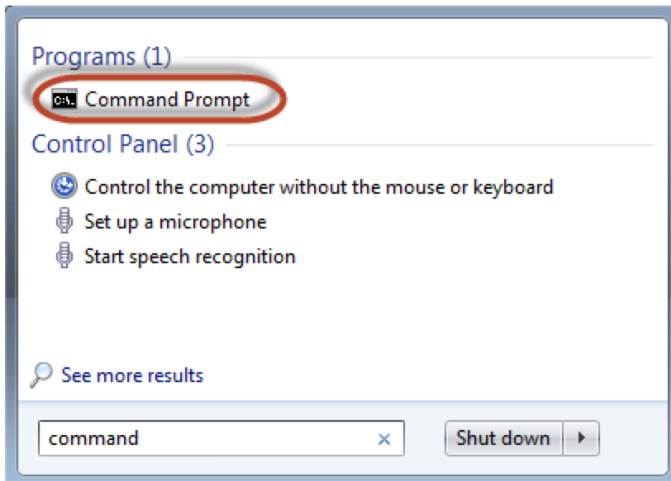
2. Type `ipython notebook` and press **enter**:

A screenshot of a terminal window titled 'local — Python — 82x15'. The terminal shows the output of the command 'ipython notebook'. The output includes the last login time, the command entered, a warning about the ipywidgets package, and the IPython Notebook server starting on localhost:8888. A red text 'type here' with a blue arrow points to the command 'ipython notebook' in the terminal.

```
Last login: Fri Jan 8 17:44:30 on ttys005
~ $ ipython notebook
[W 17:44:40.865 NotebookApp] ipywidgets package not installed. Widgets are unavai
table.
[I 17:44:40.877 NotebookApp] Serving notebooks from local directory: /Users/ekwan
[I 17:44:40.877 NotebookApp] 0 active kernels
[I 17:44:40.877 NotebookApp] The IPython Notebook is running at: http://localhost:
8888/
[I 17:44:40.877 NotebookApp] Use Control-C to stop this server and shut down all k
ernels (twice to skip confirmation).
```

# Option 1: Start Python (PC)

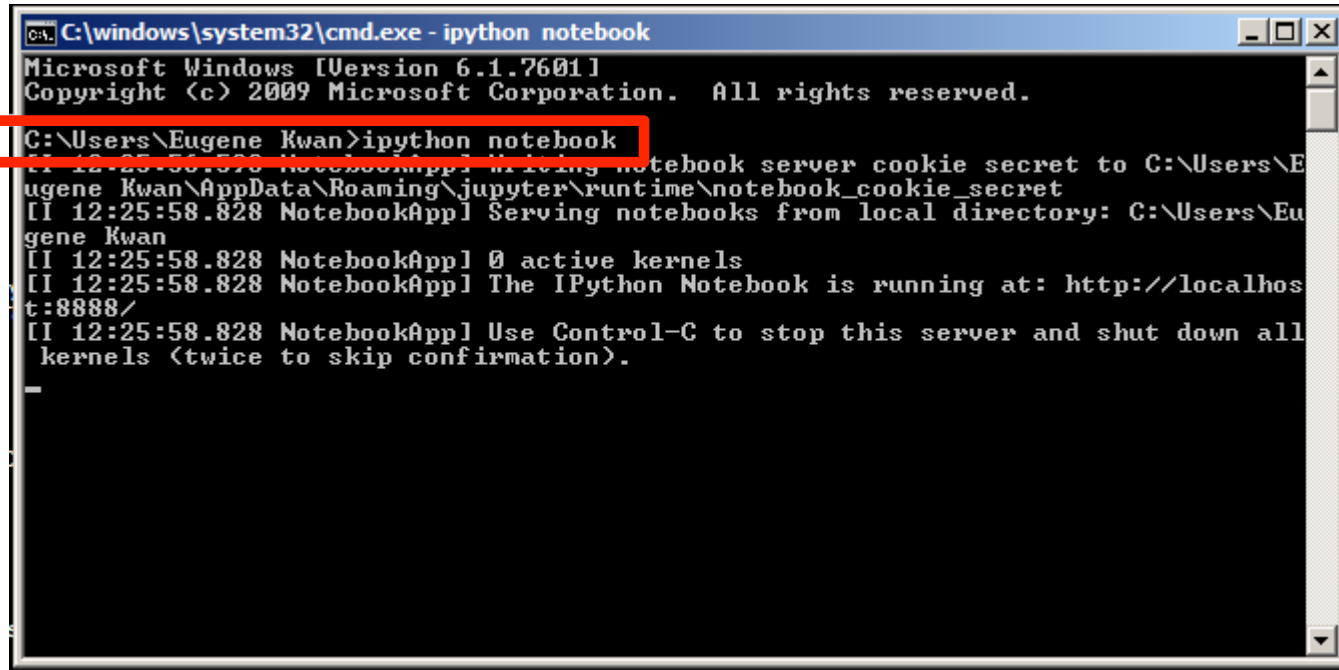
Open the command prompt from the Start menu (various Windows versions shown):



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:



```
C:\windows\system32\cmd.exe - ipython notebook
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.

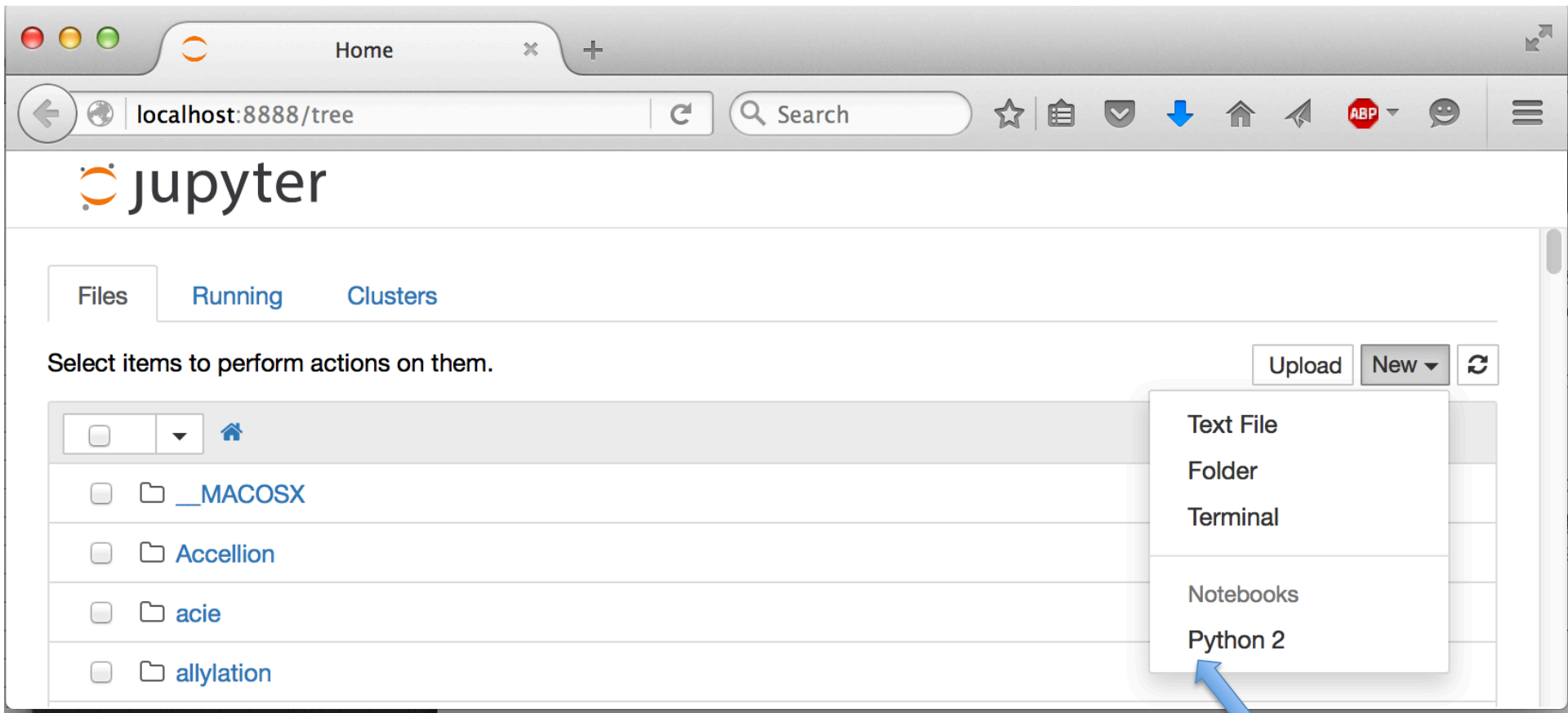
C:\Users\Eugene Kwan>ipython notebook
[I 12:25:58.828 NotebookApp] Writing notebook server cookie secret to C:\Users\Eugene Kwan\AppData\Roaming\jupyter\runtime\notebook_cookie_secret
[I 12:25:58.828 NotebookApp] Serving notebooks from local directory: C:\Users\Eugene Kwan
[I 12:25:58.828 NotebookApp] 0 active kernels
[I 12:25:58.828 NotebookApp] The IPython Notebook is running at: http://localhost:8888/
[I 12:25:58.828 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
```

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)

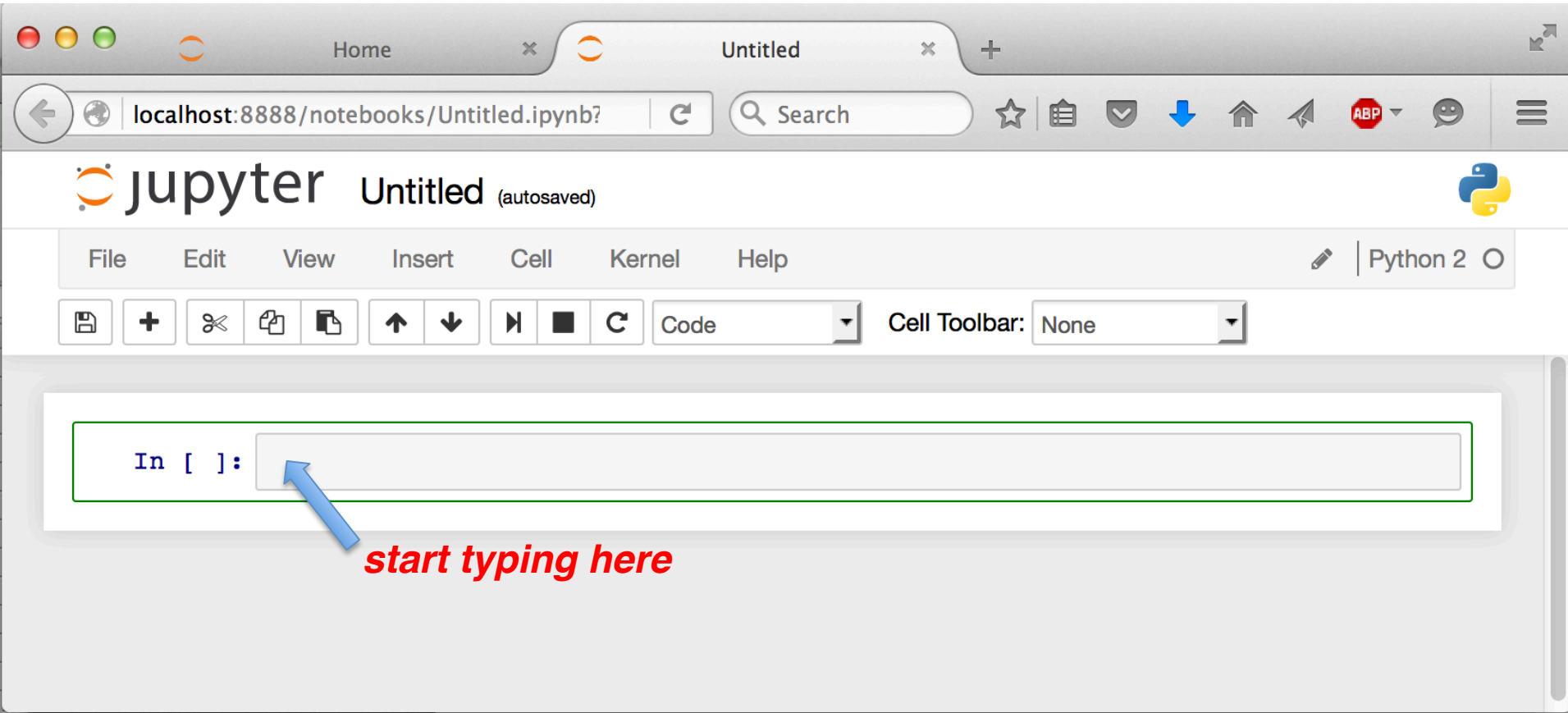
Python will open in your browser:



*click here*

# Option 1: Start a Notebook (Mac and PC)

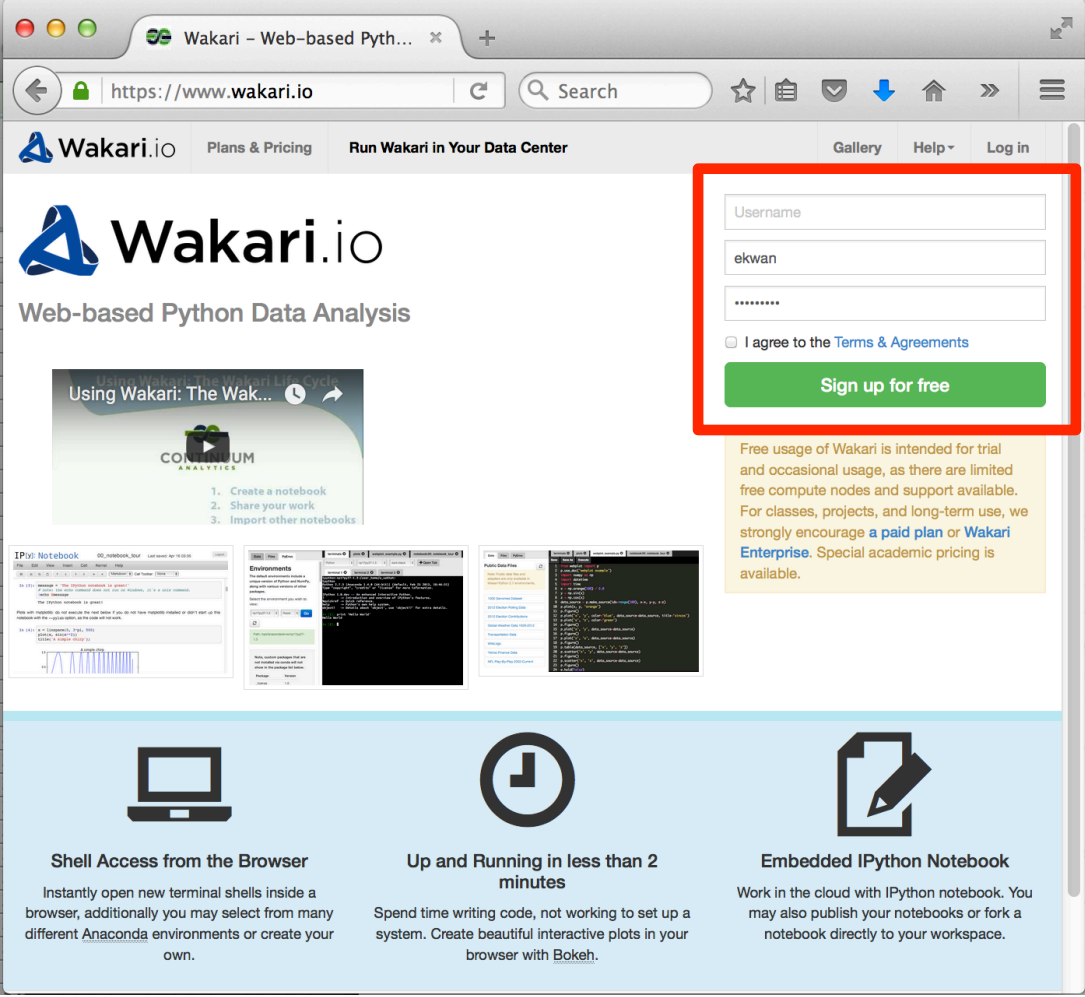
A new tab will open:



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>



The screenshot shows the Wakari.io website in a web browser. The page features the Wakari.io logo, navigation links (Plans & Pricing, Run Wakari in Your Data Center, Gallery, Help, Log in), and a sign-up form. The sign-up form is highlighted with a red rectangle and includes fields for Username (ekwan), Password (\*\*\*\*\*), and a checkbox for agreeing to Terms & Agreements. A green 'Sign up for free' button is located below the form. A blue arrow points from the text 'sign up here' to the button. Below the sign-up form, there is a section titled 'Free usage of Wakari' with details about trial and occasional usage, and links to paid plans and enterprise pricing. At the bottom, there are three icons representing different features: Shell Access from the Browser, Up and Running in less than 2 minutes, and Embedded IPython Notebook.

Wakari.io

Plans & Pricing Run Wakari in Your Data Center Gallery Help Log in

Wakari.io

Web-based Python Data Analysis

Using Wakari: The Wakari Life Cycle

1. Create a notebook  
2. Share your work  
3. Import other notebooks

Username  
ekwan  
\*\*\*\*\*  
☐ I agree to the [Terms & Agreements](#)  
**Sign up for free**

Free usage of Wakari is intended for trial and occasional usage, as there are limited free compute nodes and support available. For classes, projects, and long-term use, we strongly encourage a [paid plan](#) or [Wakari Enterprise](#). Special academic pricing is available.

Shell Access from the Browser  
Instantly open new terminal shells inside a browser, additionally you may select from many different Anaconda environments or create your own.

Up and Running in less than 2 minutes  
Spend time writing code, not working to set up a system. Create beautiful interactive plots in your browser with [Bokeh](#).

Embedded IPython Notebook  
Work in the cloud with IPython notebook. You may also publish your notebooks or fork a notebook directly to your workspace.

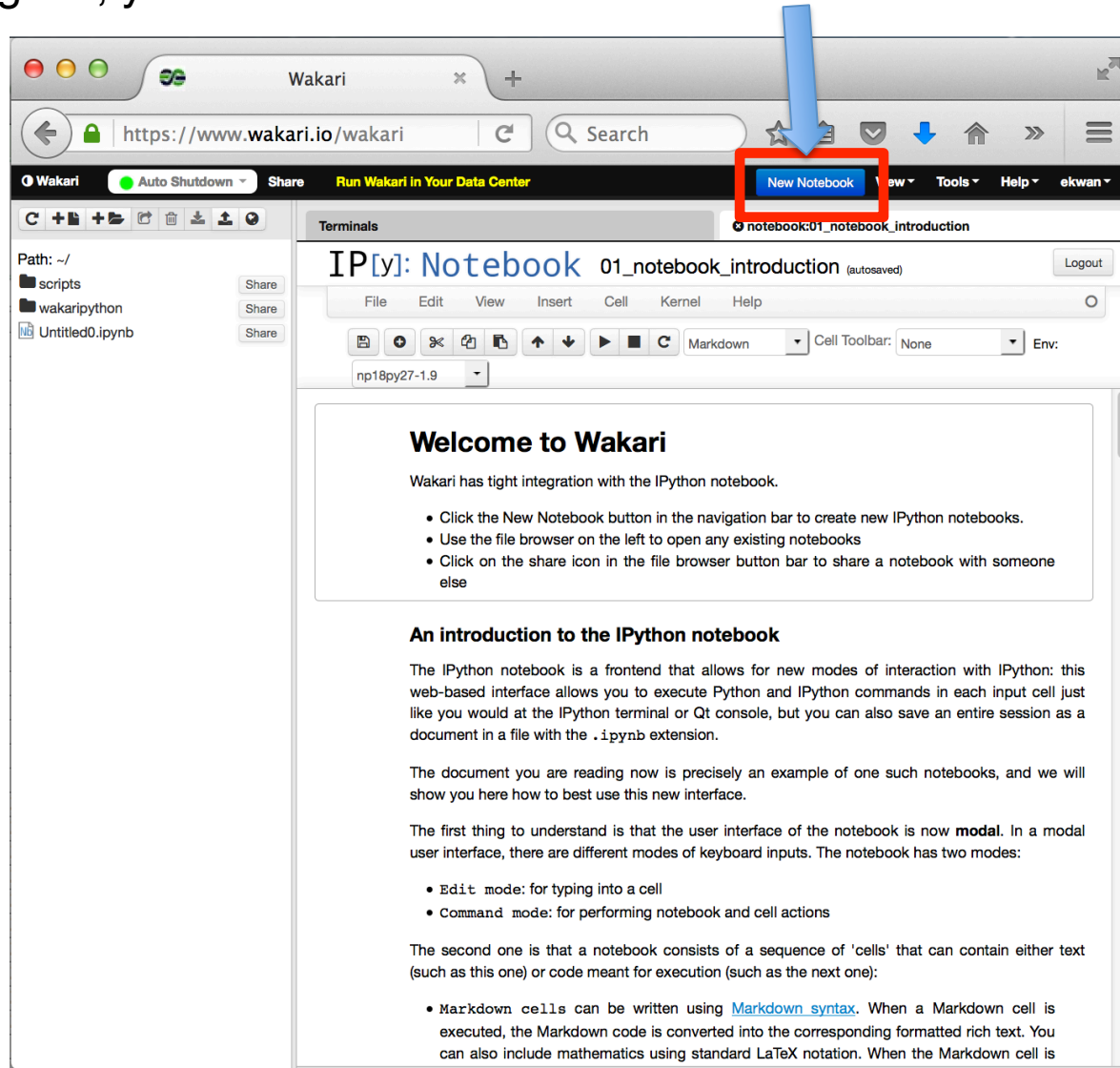
*sign up  
here*

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:

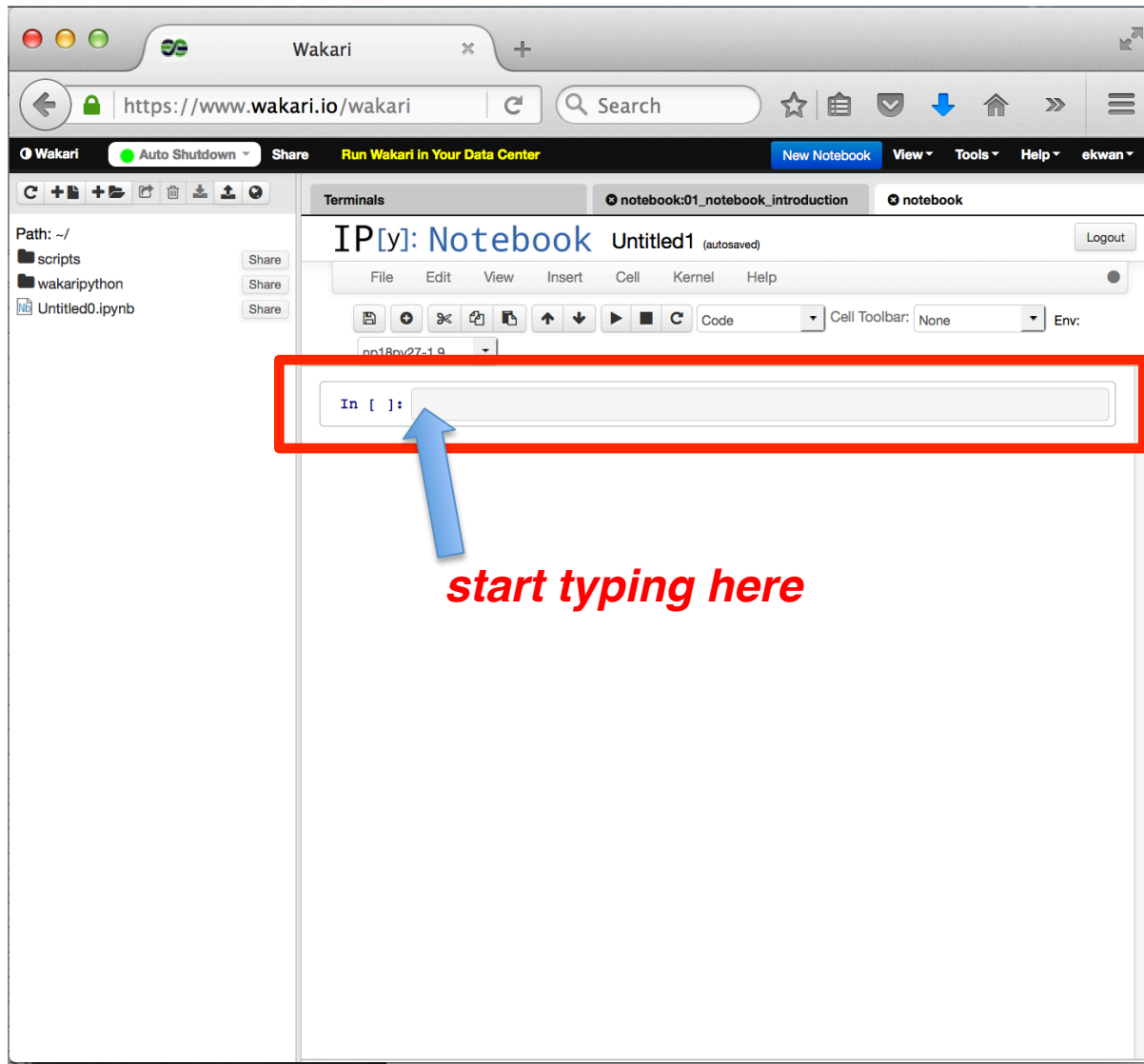
*click here*



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**.

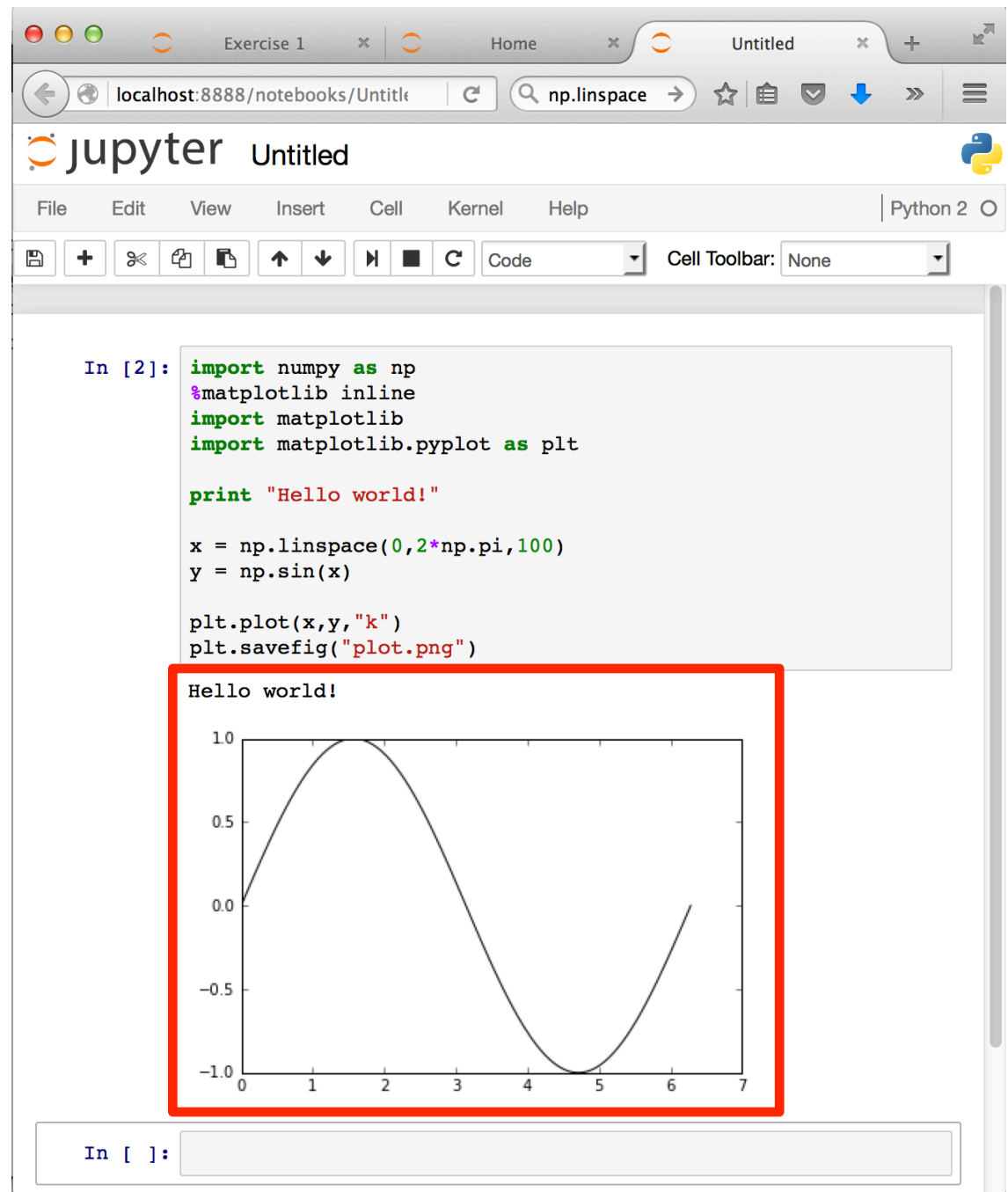
# Hello World!

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`.

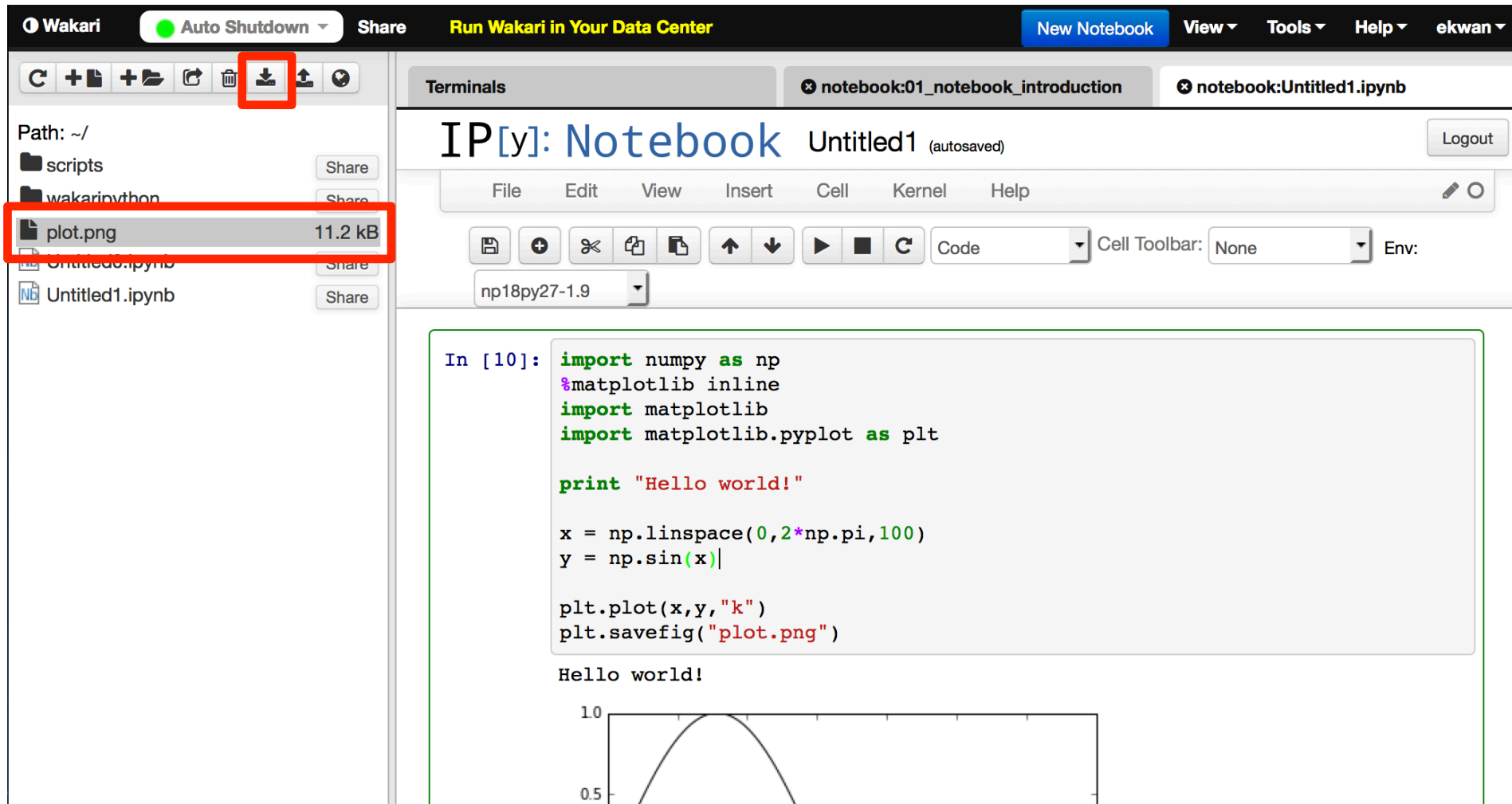
```
Last login: Sat Jan 9 23:41:36 on ttys006
~ $ cd kinetics_tutorial/
~/kinetics_tutorial $ ipython notebook
[W 13:04:06.148 NotebookApp] ipywidgets package not installed. Widgets are unavailable.
[I 13:04:06.155 NotebookApp] The port 8888 is already in use, trying another random port.
[I 13:04:06.252 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.



The screenshot displays the Wakari web interface. On the left, a file explorer shows the directory structure: `Path: ~/`, `scripts`, `wakarienv`, and `plot.png` (11.2 kB). The `plot.png` file is highlighted with a red box. Above the file explorer, a toolbar contains icons for file operations, with the download icon (a downward arrow) also highlighted by a red box. The main area on the right is titled "IP[y]: Notebook Untitled1 (autosaved)". It features a menu bar (File, Edit, View, Insert, Cell, Kernel, Help) and a toolbar with icons for saving, adding cells, and running code. Below the toolbar, the code cell shows the following Python code:

```
In [10]: import numpy as np
import 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")
```

The output of the code is "Hello world!" and a plot of a sine wave. The plot shows a single cycle of a sine wave, starting at (0,0) and ending at (2π,0), with a peak at π. The x-axis ranges from 0 to 2π, and the y-axis ranges from -1 to 1.

# 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.