Elements Of Data Science - F2024

Introduction to Data Science Tools

09/09/2024

TODOs

- **Read** Preface of PDSH
- **Read** Ch 1 of PDSH
- **Skim** Ch 2 of PDSH: Introduction to NumPy

- Weekly Quiz 01

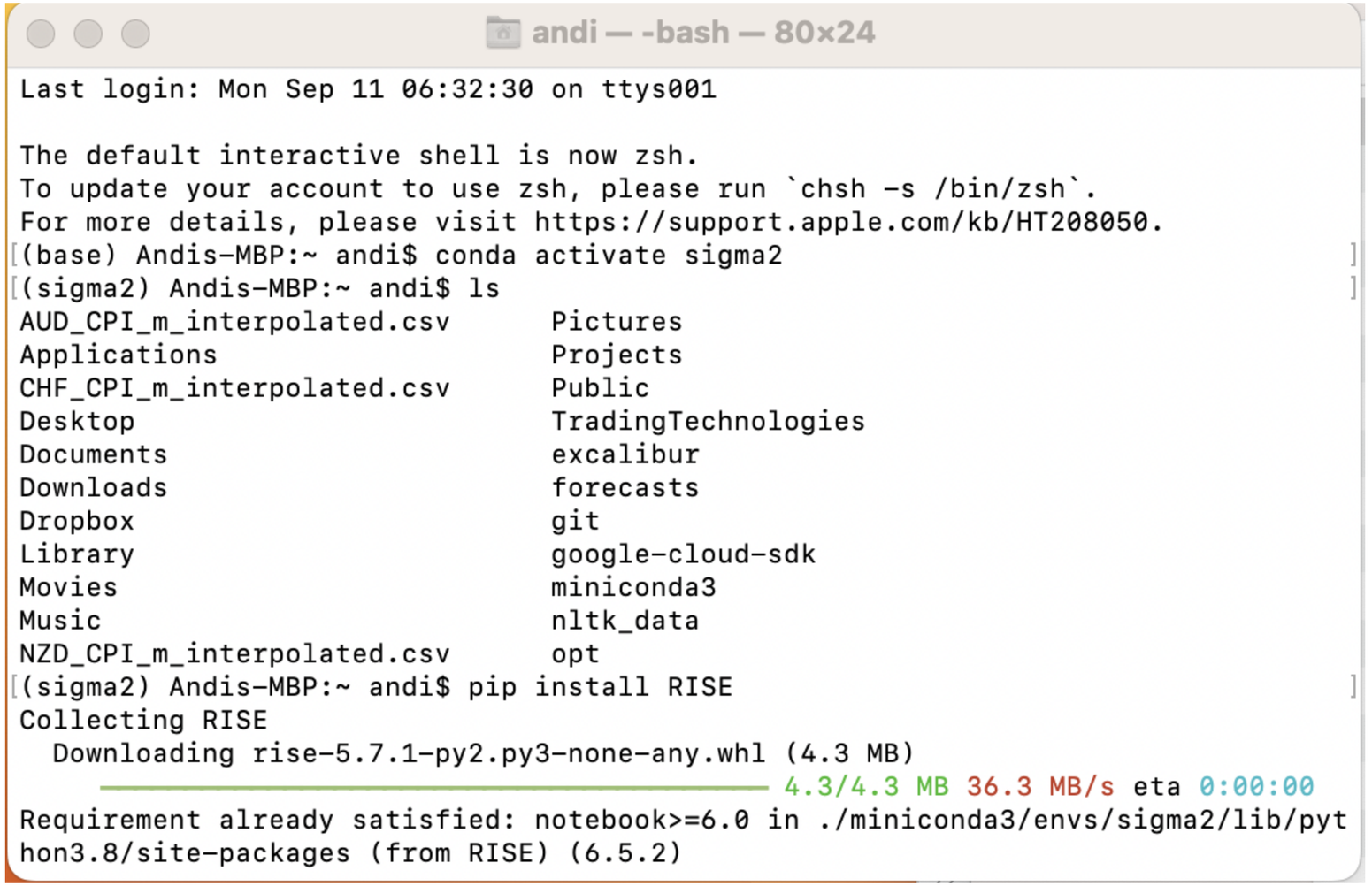
TODAY

- Software tools we'll be using

Our Python Data Science Stack

- Python (3.10): Programming language
- Anaconda : Package maintenance and environments
- Jupyter : IDE
- Git : Source control and versioning

Aside: The Terminal and The Shell



- If not familiar, get aquainted

Aside: Common Shell Commands

- **cd** : change directory
- **pwd** : where am i
- **ls** : list directory contents
- **head/tail** : print the beginning/end of a file
- **cat** : print entire file
- **less** : open a file in a pager
- **rm** : remove file
- **which** : path to executable
- ...

- Link to Tutorial

Data Science Life Skills

- Data munging
- Visualization
- Statistical analysis
- Machine learning
- Reporting
- Prototyping
- Productionizing...

Why Python?

- Robust and active DS stack
- Cross-platform
- Relatively low learning curve
- Fast to answers and prototypes

- Many other good languages and frameworks (R, Julia, etc.)

Why Python?

- But isn't python slow?
- **Issues:**
    - dynamic typing
        - The Python interpreter does type checking only as code runs, and the type of a variable is allowed to change over its lifetime.
- **Solutions:**
    - numpy + vectorization
    - multiprocessing
    - distributed processing with pyspark?

```
In [15]:
1 a = 'andi'
```

```
In [16]:
1 type(a)
```

```
Out[16]: str
```

The Python DS Stack

- **Data munging** : pandas, numpy
- **Visualization** : matplotlib, seaborn, plotly
- **Statistical analysis** : scipy, statsmodels, patsy
- **Machine learning** : scikit-learn, tensorflow, pytorch
- **Reporting** : jupyter+ipython, dash
- **Prototyping** : flask
- **Productionizing...**

Python 2 vs 3

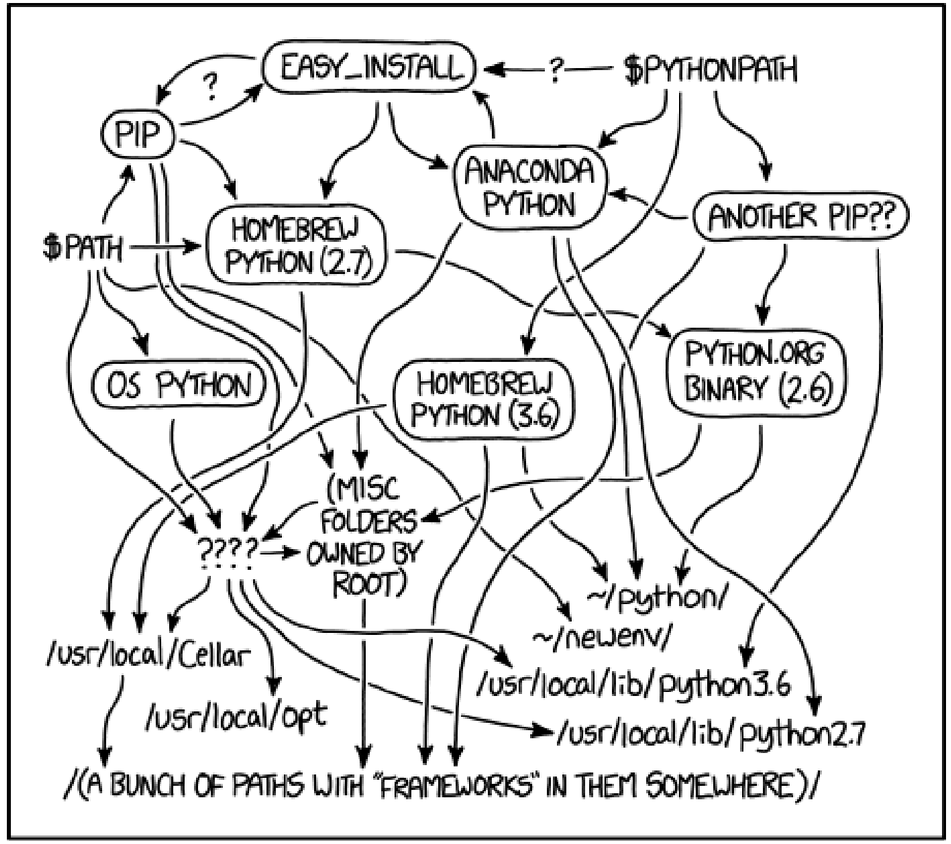
- We'll be using Python 3.10
- Python 2 end of life was Jan 1, 2020

- Need python 2 for another class? Virtual environments!

How To Get Python

- You might already have it
- But your OS needs it!
- Our solution: Anaconda

Why Anaconda?



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

https://imgs.xkcd.com/comics/python_environment.png

Why Anaconda?

- includes most of what we need by default
- package curation
- dependency control
- conda virtual environments
- cross-platform

Installing Anaconda / Anaconda NAvigator

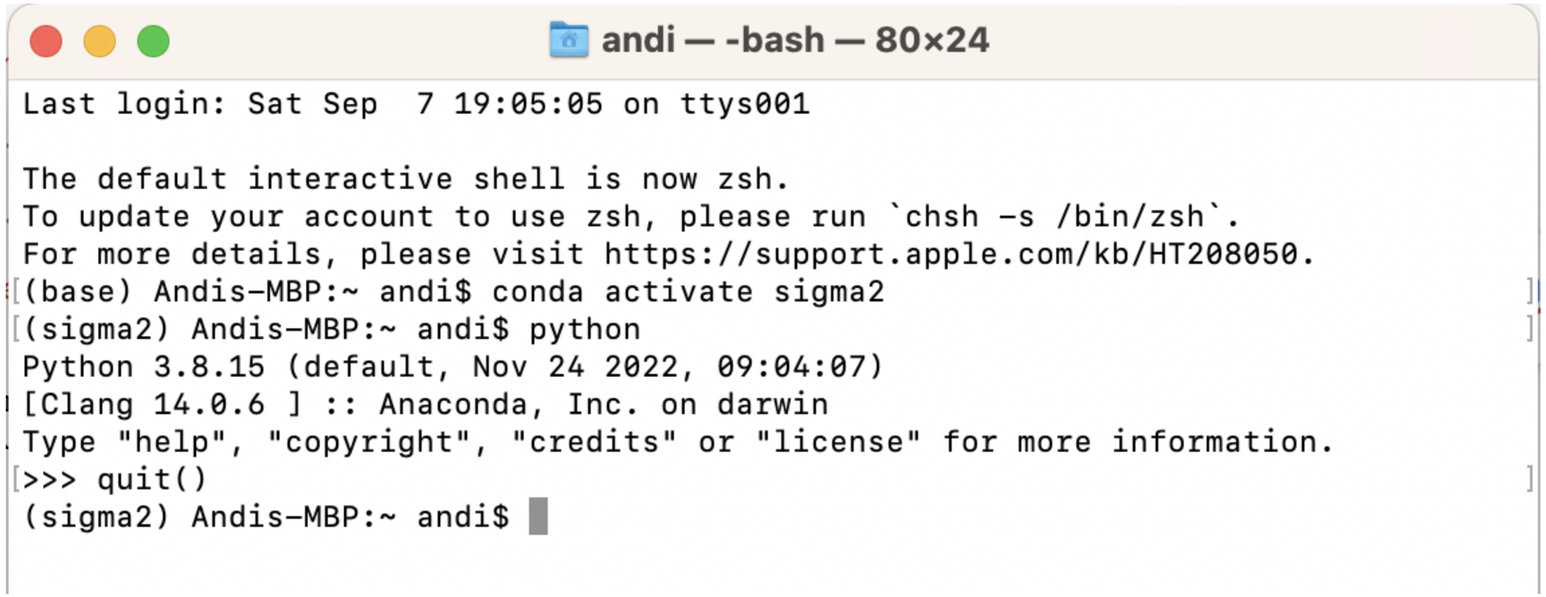
- Download via https://www.anaconda.com/products/individual
- Select OS and Grab Python 3.9 version
- Install somewhere easy to navigate to
    - /home/andi/anaconda3
    - C:\Users\andi\anaconda3
- Recommend letting installer run `conda init` to set up your shell
- Note: base environment activated by default
    - To Turn off: `conda config --set auto_activate_base false`

Running Python

- via terminal:
    - python REPL
    - python command line
    - python script
    - ipython REPL
- via jupyter
- via other IDE
- online via Google Colab
- ...

Running Python

- Via REPL (Read–Eval–Print Loop)
  - `$ conda activate`
  - `(base)$ python`



- quit() or Ctrl-D to exit

Running Python

Via command line

```
(base) Andis-MBP:~ andi$ python -c "print('hello')"
hello
```

Via script

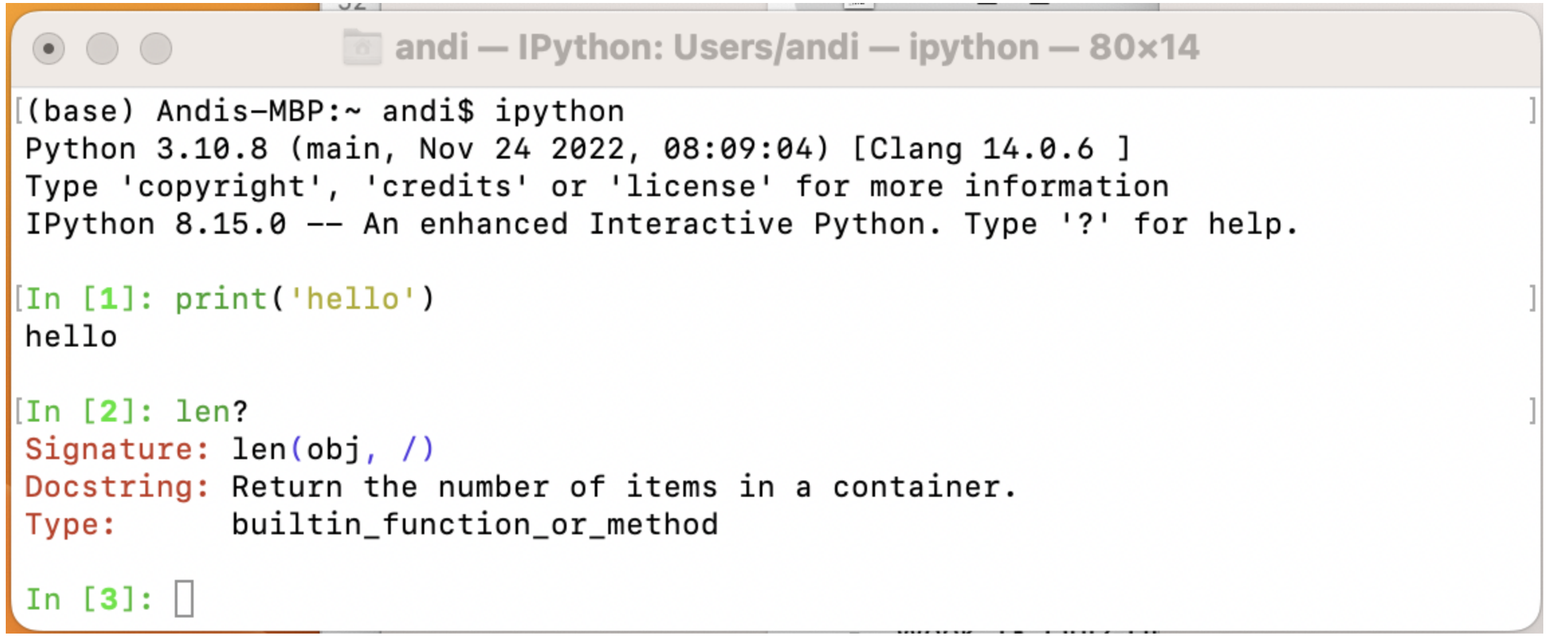
```
(base) Andis-MBP:~$ echo "print('hello from the other file')" > /tmp/say_hello.py
(base) Andis-MBP:~$ python /tmp/say_hello.py
hello
```

Ipython: Interactive Python

- history (`python` does this now as well)
- tab completion (`python` does this now as well)
- "magic" commands
- help via `?` (`python` has `help()` as well)
- (see PDSH Ch 1 for more info)

Ipython : REPL and Help

- `$conda activate` if (base) not activated



Ipython Magic Commands

- preceded by % for line, %% for cell

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# The output of the `echo` can be redirected to a file instead of displaying it on the
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In [6]:
```
!echo 'print("hello from Room 833, Sep 2024")' > /tmp/say_hello.py
!python /tmp/say_hello.py
```

```
hello from Room 833, Sep 2024
```

Ipython Magic Commands

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In [7]:
```
%run /tmp/say_hello.py
```

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In [8]:
```
%timeit sorted([5,1,2,5])
```

```
174 ns ± 6.22 ns per loop (mean ± std. dev. of 7 runs, 10,000,000 loops each)
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%timeit sorted([5,1,2,5])
```

```
174 ns ± 6.22 ns per loop (mean ± std. dev. of 7 runs, 10,000,000 loops each)
```

In [9]:
```
%%timeit
x = []
for i in range(20):
    x.append(i**2)
```

```
3.57 µs ± 103 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
```

Help with Magic Commands

- get information about the %timeit magic function

```
%timeit?
```

- get info on all magic functions

```
%magic
```

- get list of magic functions

```
%lsmagic
```

Ipython Notebooks with Jupyter

- Jupyter: application that combines code, markup and visualizations
- interact via web browser
- notebooks are easily sharable
- Jupyter can run other kernels as well: R, Julia, C#, etc.
- To launch via command line:

```
(base) Andis-MBP:~ andi$ cd ~/proj
(base) Andis-MBP:~ andi~/proj$ jupyter notebook
```

- launches dashboard in your default browser
- Ctrl-C to kill server

Other IDEs

- jupyterlab
- spyder
- pycharm
- visual studio code ...

Arguments for Notebooks

- fast to iterate
- easy to test new ideas
- wide adoption

Arguments against notebooks

- out of order execution
- messy code
- issues with version control
- slides by Joel Grus

How to deal with version issues? Virtual Environments

- encapsulate python executable and packages
- allow for easy experimentation
- workaround versioning issues

- two major implementations: virtualenv and conda (we'll be using conda)

Virtual Environments with Conda

Example for creating a new environment called py2 with python=2.7:

```
(base) Andis-MBP:~ andi$ conda create -n py2 python=2.7
...

(base) Andis-MBP:~ andi$ conda activate py2

(py2) Andis-MBP:~ andi$ which python
/Users/andi/miniconda3/envs/py2/bin/python
```

```
(py2) Andis-MBP:~ andi$ python --version
Python 2.7.18 :: Anaconda, Inc.

(py2) Andis-MBP:~ andi$ conda deactivate

(base) Andis-MBP:~ andi$ which python
/Users/andi/miniconda3/bin/python

(base) Andis-MBP:~ andi$ python --version
Python 3.10.8
```

Managing Conda Enviroments

- `conda create -n [env_name]`
- `conda create -n [env_name] [package] [package]=[version]`

- **`conda env create --file [requirementsfile].yml`**

- `conda activate [name]`
- `conda deactivate`

- `conda env list`

- For more information see: https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html

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1. first, try conda (with conda-forge):

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conda install -n [env_name] -c conda-forge [package]
```

2. next, try another channel : eg. bioconda

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3. then, try pip:

```
conda activate [env_name]
pip install [package]
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conda activate [env_name]
pip install [package]
```

- when you can, double check the path to your env

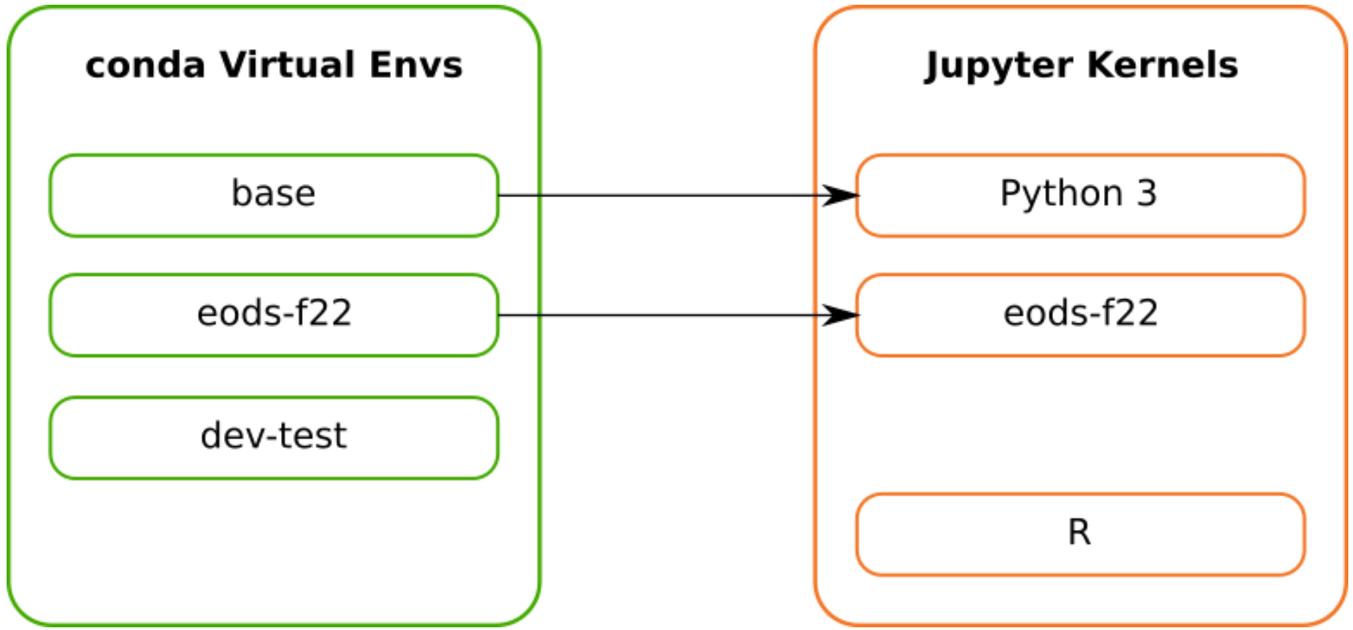
Conda Channels: default vs conda-forge

- channels: locations where packages are stored
    - default: Anaconda terms specify only used in non-commercial application
    - conda-forge: where all of the good stuff is anyway

```
conda install -n [env_name] -c conda-forge [package]
```

Conda Virtual Envs and Jupyter Kernels

- jupyter can run many different kernels
- conda envs not automatically added as available kernels



Controlling Jupyter Kernels

- to install a new kernel in jupyter:

```
(base) $ conda activate py2
(py2) $ conda install -c conda-forge ipykernel
(py2) $ python -m ipykernel install --user --name py2
```

- to list kernels: `jupyter kernelspec list`

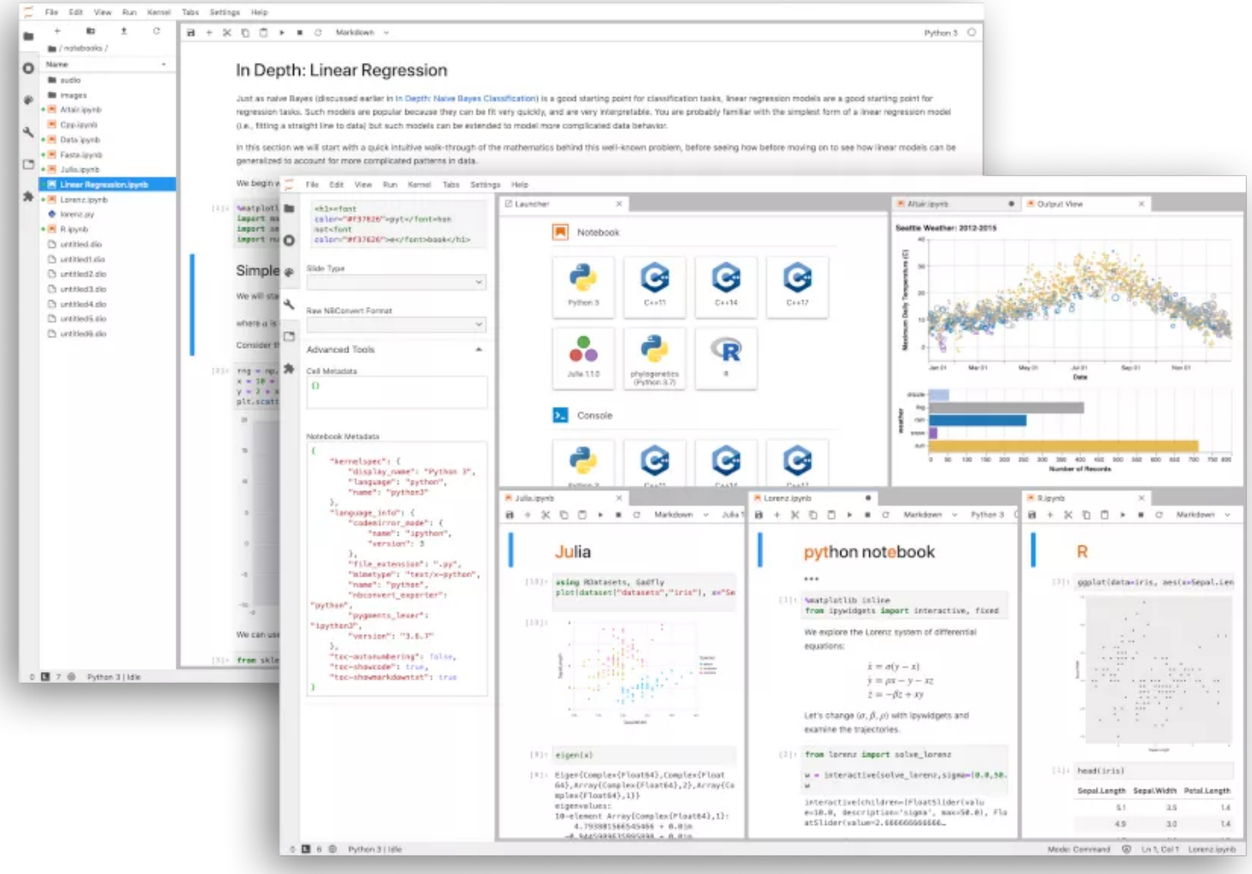
- to remove kernel: `jupyter kernelspec uninstall [name]`

Jupyter Demo

- Important: h for help
- Markdown syntax help: https://daringfireball.net/projects/markdown/syntax

Jupyter Classic vs JupyterLab

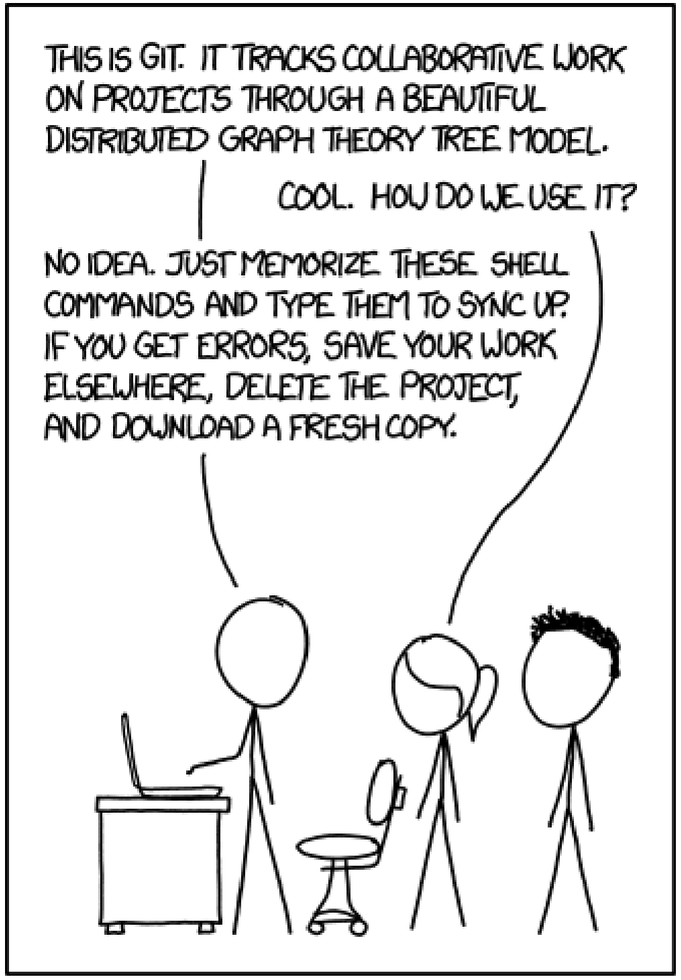
- start as either `jupyter notebook` or `jupyter lab`
- or replace `http://localhost:8888/tree` with `http://localhost:8888/lab`



Example Notebooks

Gallery of interesting Jupyter Notebooks

Git and Github



http://imgs.xkcd.com/comics/git.png

Git

- distributed version control
- for code, documentation, *small* data
- can be used locally or with remote collaborators

Github

- backup
- sharing
- used for both large and small projects
    - Ex: https://github.com/scikit-learn/scikit-learn

Getting course material

- Can view online at: TBA
- You'll also want to clone locally:

```
$ cd [your projects folder]
$ git clone **TBA**
```

Demo Week 1 Quiz

Questions?

- Next time: Python review, numpy and pandas