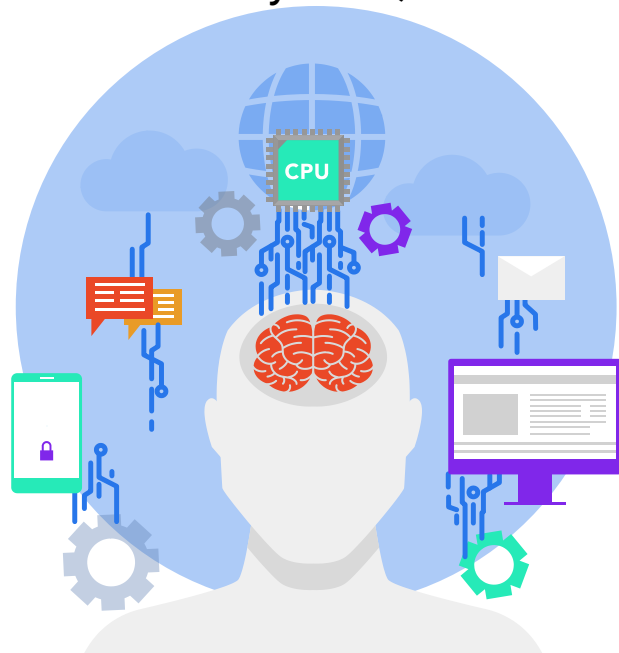


NETS Python Workshop Day 1

February 25th, 2023



What is Python



In short, Python is...

- a **high-level, interpreted** programming language
- relative good **code-readability** and **simplisticity**
- **widely-used** for scientific computing, data analysis, machine learning, automation, etc.
- support from a huge community of independent and institutional developers

Why do engineers need Python?

Versatility

Can be used in a wide range of applications

01

Ease of use

Simple and straightforward syntax

02

Large community

Lots of available resources and help

03

Job demand

Better job prospects and earning potential

04

This you, the engineer →



Choosing a text editor

Visual Studio Code



- Supports many languages
- Vast collections of extension and plugins
- Lightweight and fast
- Free

Jupyterlab



- Simple user interface
- Enhanced readability
- Can be installed onto Visual Studio Code
- Free

PyCharm



- Professional-grade integrated environment
- Wide range of features suitable for large and complex projects
- Free (with ucsd email)



Install Python Environment

Python Environment

A way to keep track of all the versions of Python packages you have installed

If your laptop specs are:

- Intel Core i3 7th gen and older
- Total storage less than 256 GB
- Total memory less than 12 GB

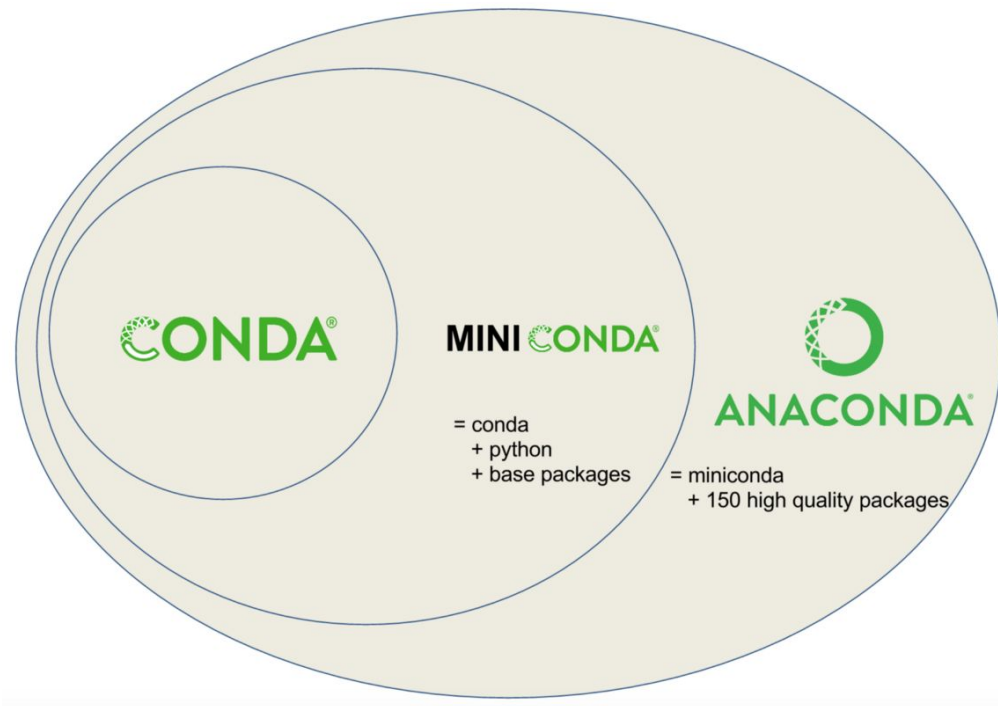
☐ Install Miniconda

<https://docs.conda.io/en/latest/miniconda.html>

Otherwise,

☐ Install Anaconda

<https://www.anaconda.com/>



Install Jupyter Notebook/Lab

Windows

Open Anaconda prompt

Mac and Linux

Open Terminal

Type in...

1. Create virtual environment

```
conda create --name NETS python=3.9
```

2. Activate virtual environment

```
conda activate NETS
```

3. Install Jupyter and other necessary libraries

```
conda install --yes numpy matplotlib pandas jupyter  
seaborn scikit-learn
```

4. Open Jupyter Lab

```
jupyter lab
```

1. Create virtual environment

```
conda create --name NETS python =3.9
```

Proceed by typing 'y'

```
vc                      pkgs/main
vs2015_runtime          pkgs/main
wheel                   pkgs/main
wincertstore             pkgs/main
```

```
Proceed ([y]/n)? y
```

2. Activate virtual environment

```
conda activate NETS
```

```
(base) C:\Users\2018m>conda activate NETS
```

```
(NETS) C:\Users\2018m>
```

```
Anaconda Prompt (anaconda) x + v - □ x
(base) C:\Users\2018m>conda create --name NETS python=3.9.0
```

```
Collecting package metadata (current_repodata.json): done
Solving environment: failed with repodata from current_repod
ata.json, will retry with next repodata source.
Collecting package metadata (repodata.json): done
Solving environment: done
```

```
==> WARNING: A newer version of conda exists. <==
current version: 22.9.0
latest version: 23.1.0
```

```
Please update conda by running
```

```
$ conda update -n base -c defaults conda
```

```
## Package Plan ##
```

```
environment location: C:\Users\2018m\anaconda3\envs\NETS
```

```
added / updated specs:
- python=3.9.0
```


3. Install Jupyter and other necessary libraries

```
conda install --yes numpy matplotlib pandas jupyter  
seaborn scikit-learn
```

Download the necessary/basic python packages with conda install (IMPORTANT to note which version of the packages you used so your work can be replicated without bugs and errors)

1. **Numpy**
2. **Pandas**
3. **Seaborn**
4. **Matplotlib**
5. **Math**
6. **Scikit-Learn**
7. SciPy
8. Keras
9. TensorFlow
10. PyTorch

```
Anaconda Prompt (anaconda) x + v - □ x  
(NETS) C:\Users\2018m>conda install --yes numpy matplotlib p  
andas jupyter seaborn scikit-learn  
Collecting package metadata (current_repodata.json): done  
Solving environment: done  
  
==> WARNING: A newer version of conda exists. <==  
current version: 22.9.0  
latest version: 23.1.0  
  
Please update conda by running  
  
$ conda update -n base -c defaults conda
```

4. Open Jupyter Lab

```
jupyter lab
```

```
Anaconda Prompt (anaconda) x + v - □ x  
(NETS) C:\Users\2018m>jupyter lab  
[I 2023-02-11 16:11:18.873 ServerApp] jupyterlab | extension  
was successfully linked.  
[I 2023-02-11 16:11:18.873 ServerApp] nbclassic | extension  
was successfully linked.  
[I 2023-02-11 16:11:19.318 ServerApp] notebook_shim | extens  
ion was successfully linked.  
[I 2023-02-11 16:11:19.344 ServerApp] notebook_shim | extens
```

Quick Demo of data processing

01

Open Jupyter lab
with Prompt/Terminal

02

Go to Github

<https://tinyurl.com/NETS-Python-Workshop>

03

**Download from
Repository**

04

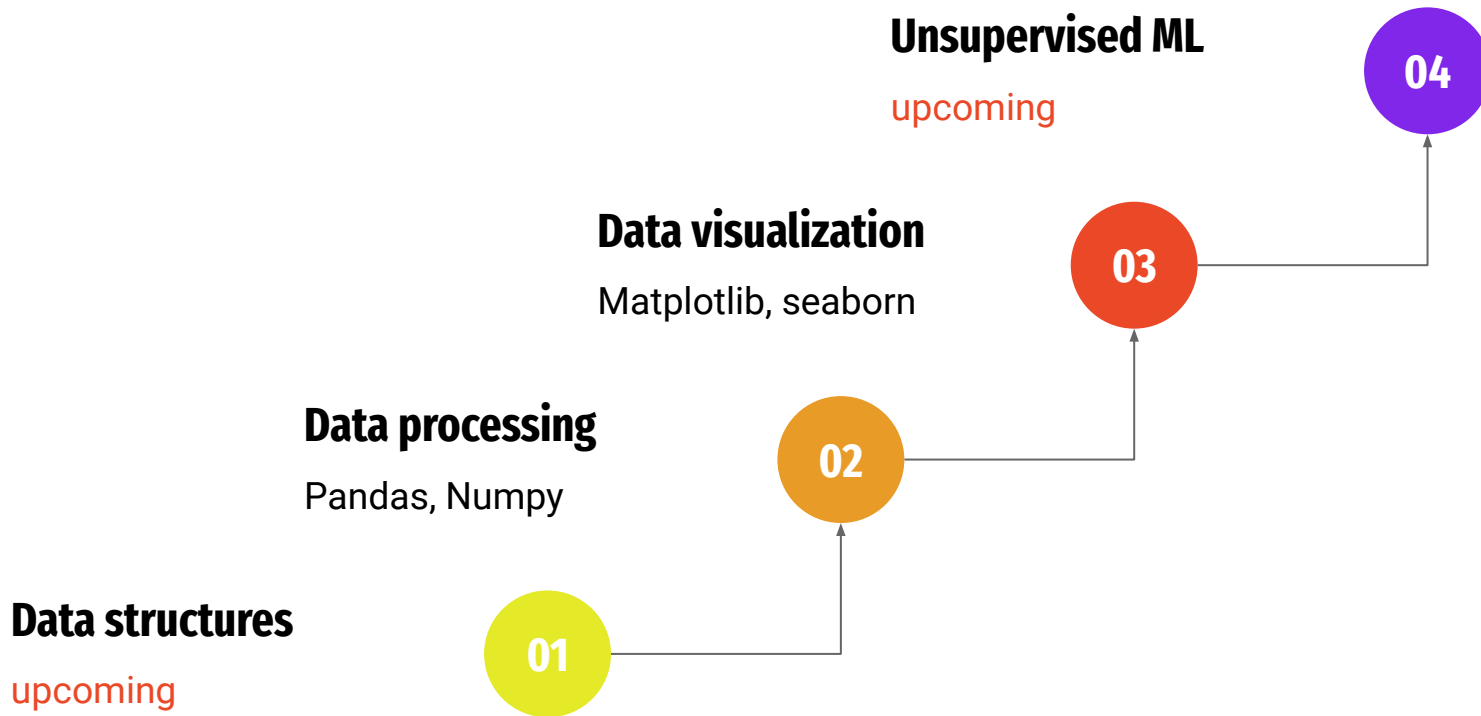
Make New Folder
and extract the files
from Github

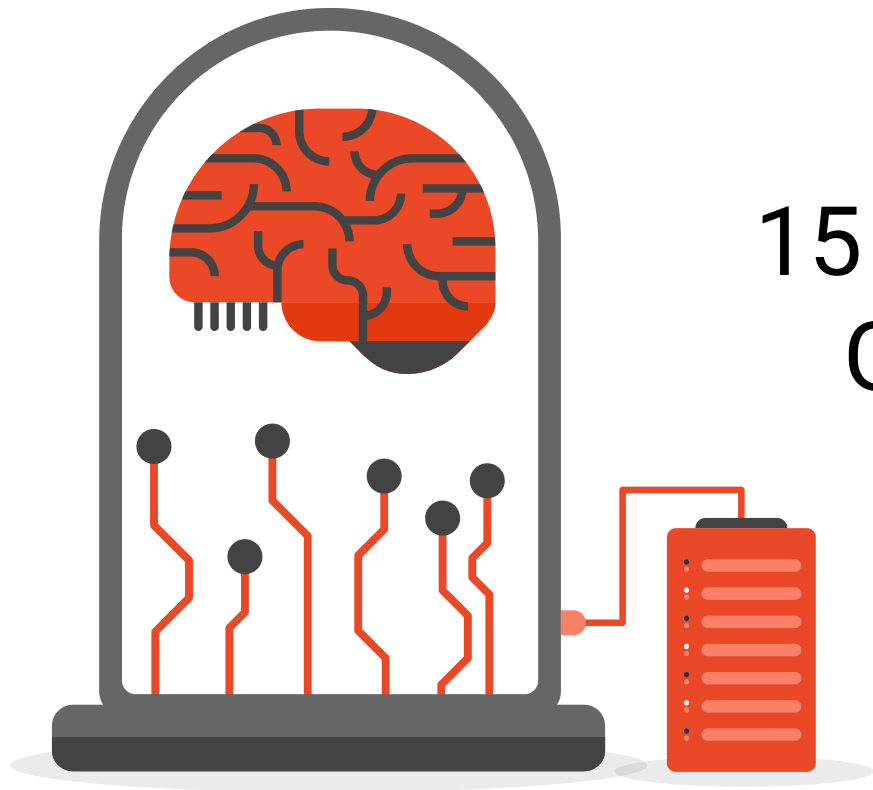
05

Open Notebook
Day_1_Part_A.ipynb



Recap on what we have done so far...

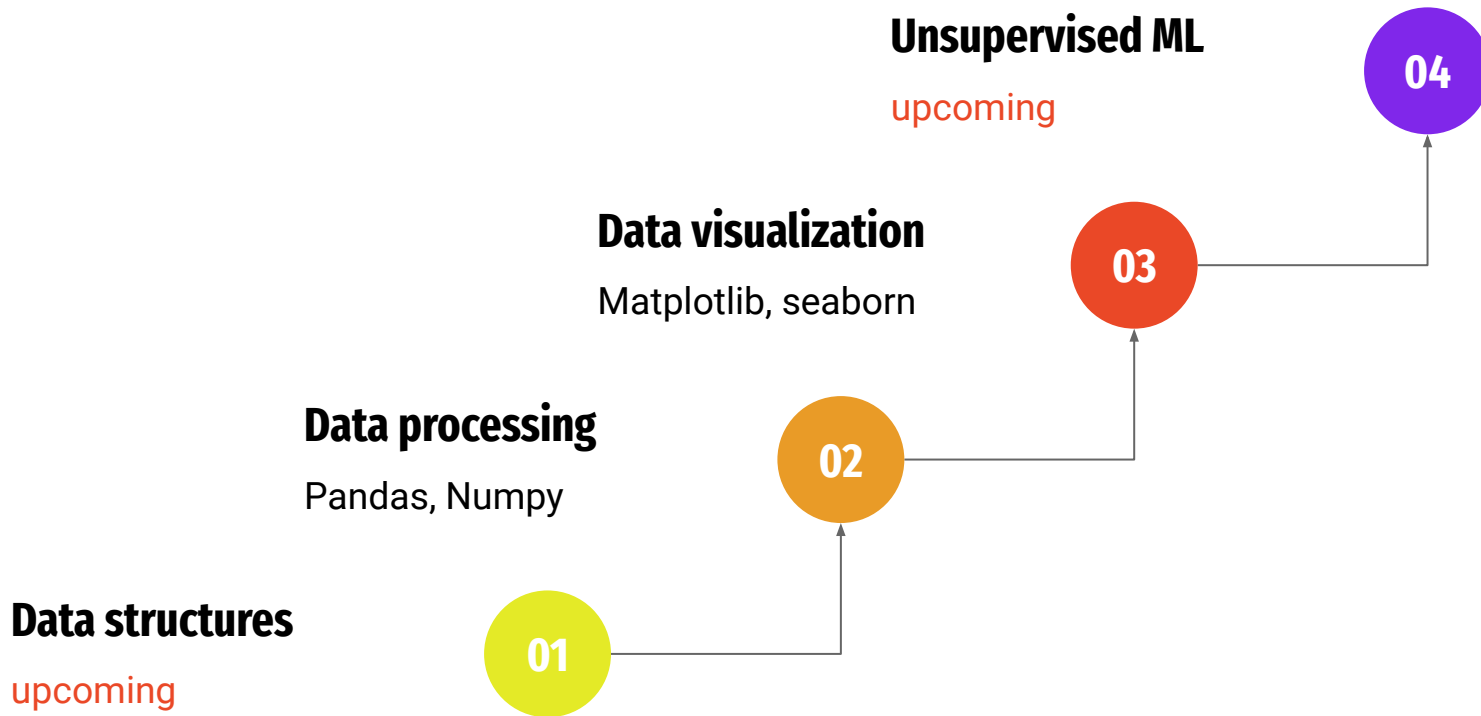




15 minutes break
Grab a bagel!

15:00

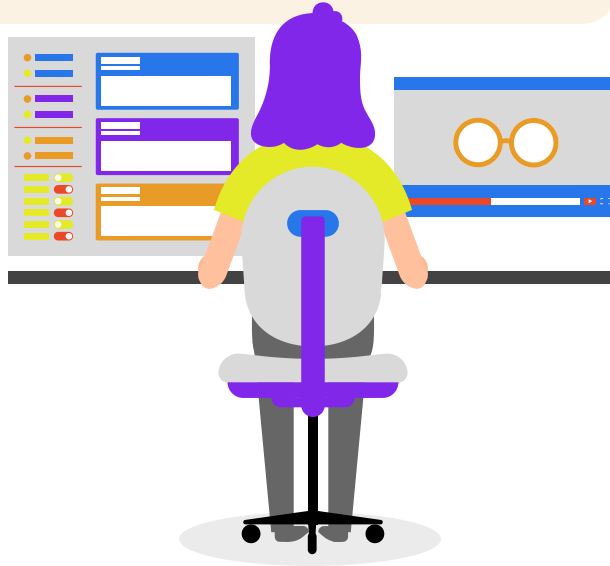
Recap on what we have done so far...



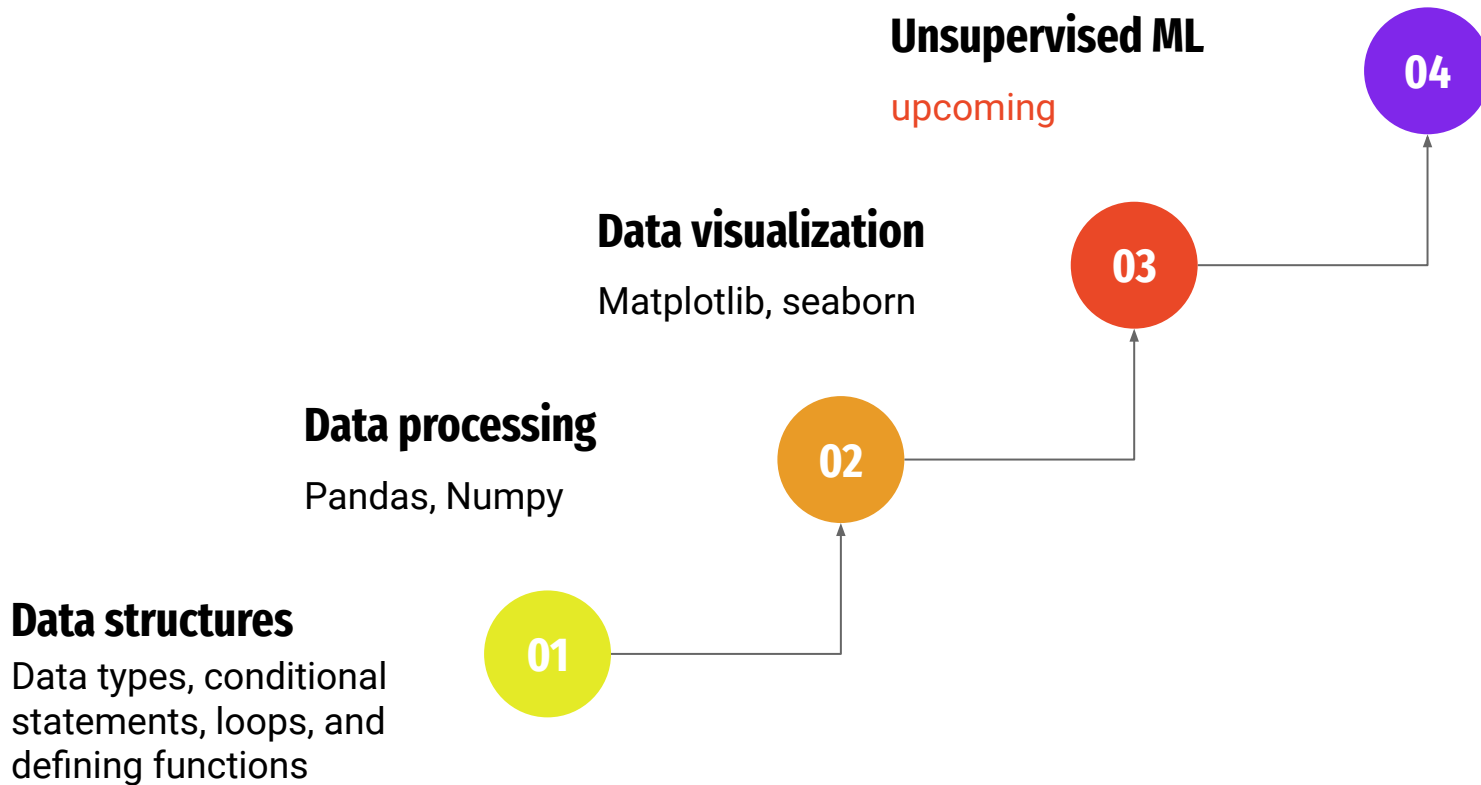
Quick Demo of data processing

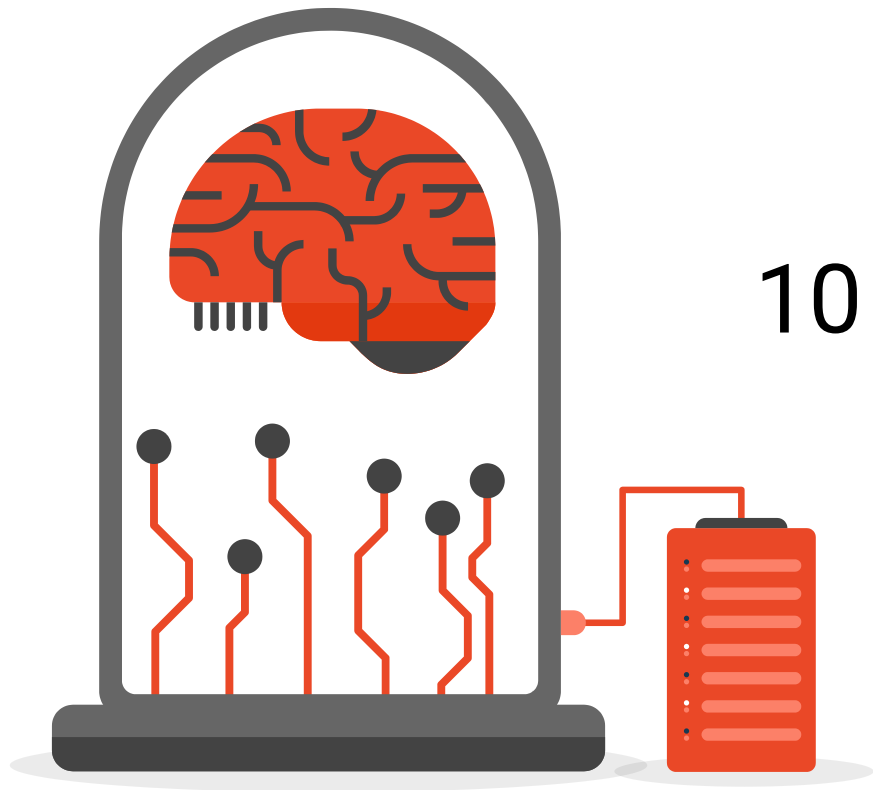
Open Notebook

Day_1_Part_B.ipynb



Recap on what we have done so far...

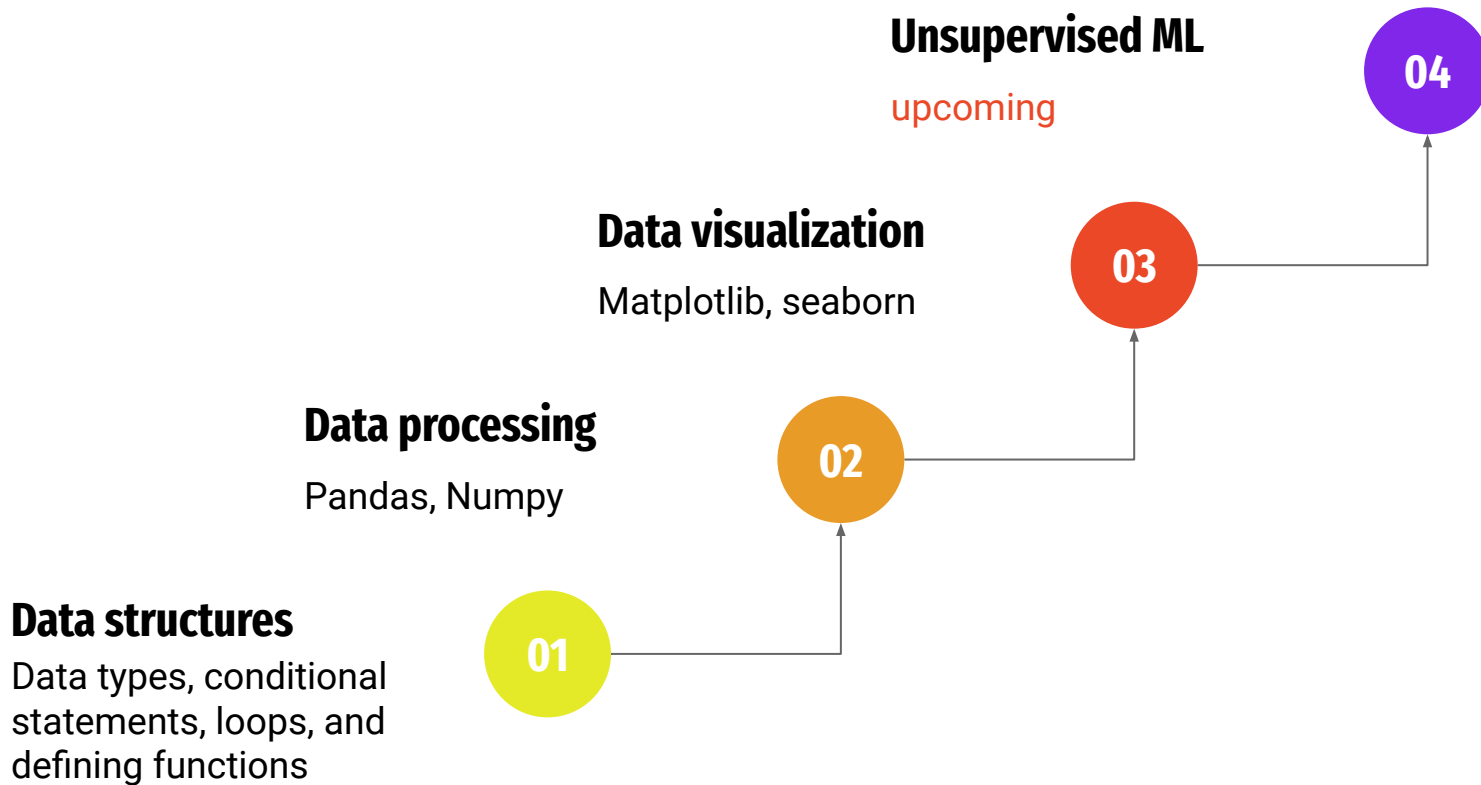




10 minutes break

10:00

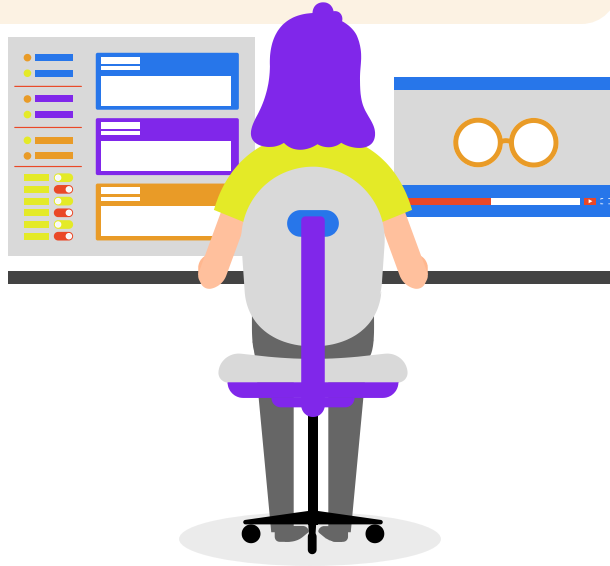
Recap on what we have done so far...



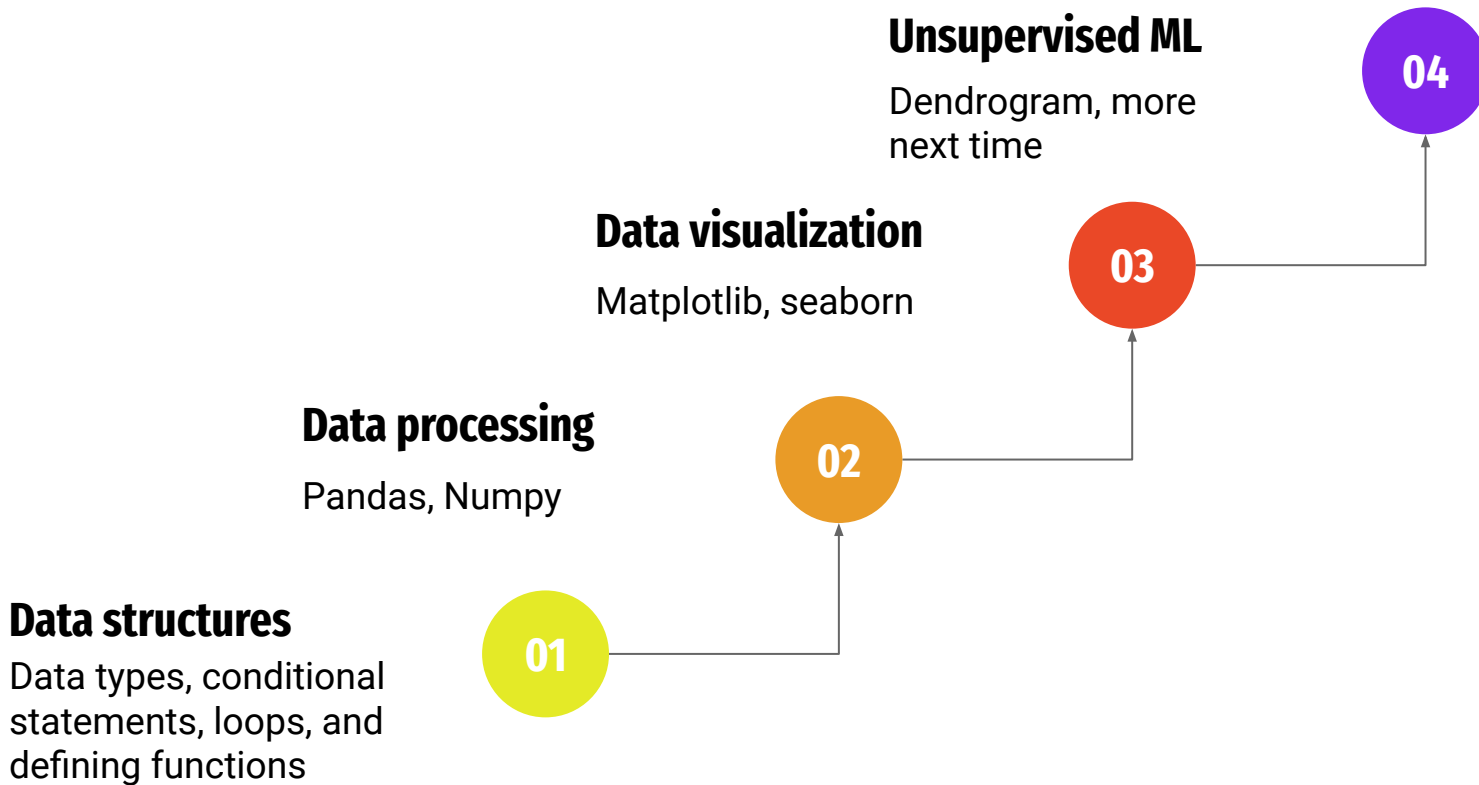
Quick Demo of data processing

Open Notebook

Day_1_Part_C.ipynb



Recap on what we have done so far...



Other Resources for YOU

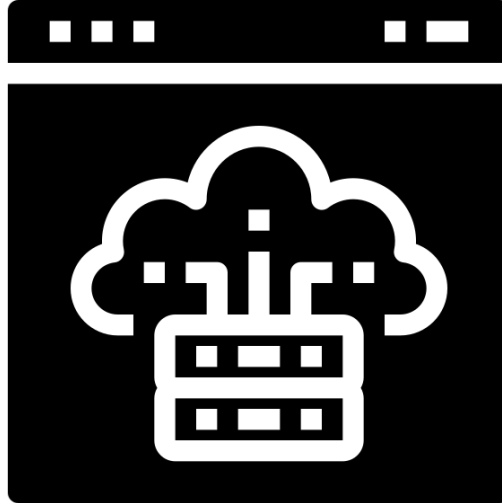
- General Python: <https://github.com/phillipai/100-days-of-code-python>
- Material Sciences: <https://github.com/materialsvirtuallab/nano281>
- Physics:
<https://deeplearningforphysicsresearchbook.github.io/deep-learning-physics/>
- Overview of ML for Material Science:
<https://towardsdatascience.com/machine-learning-in-materials-science-8c6c0db5ce7a>
- Competitions: <https://www.kaggle.com/competitions>

Sneak Peek at Tomorrow

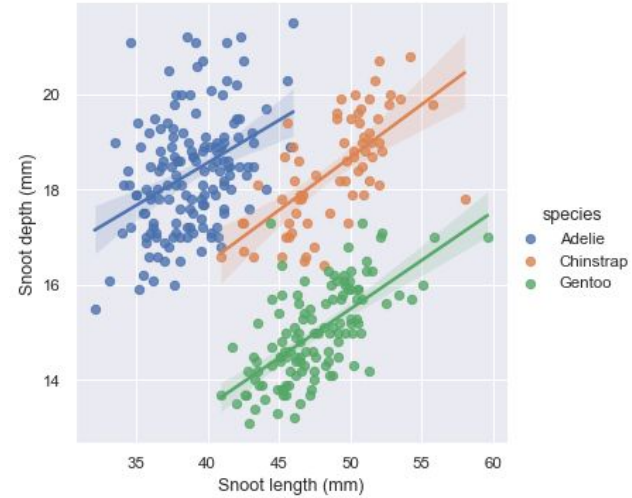
API with Ethan



Website with Duc



ML with Mai



Food and Goodbye.
See everyone again tomorrow.