NETS Python Workshop Day 1

February 18th, 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

Ease of use
Simple and straightforward syntax

Large community
Lots of available resources and help

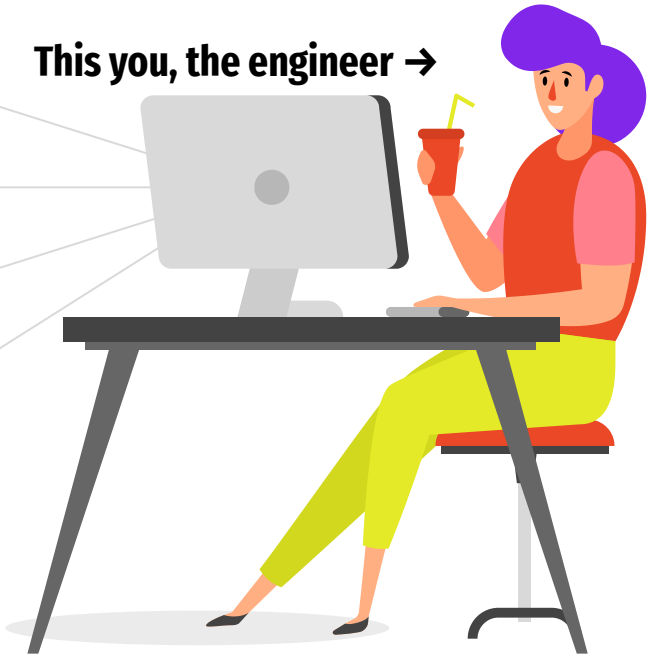
Job demand
Better job prospects and earning potential

01

02

03

04



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

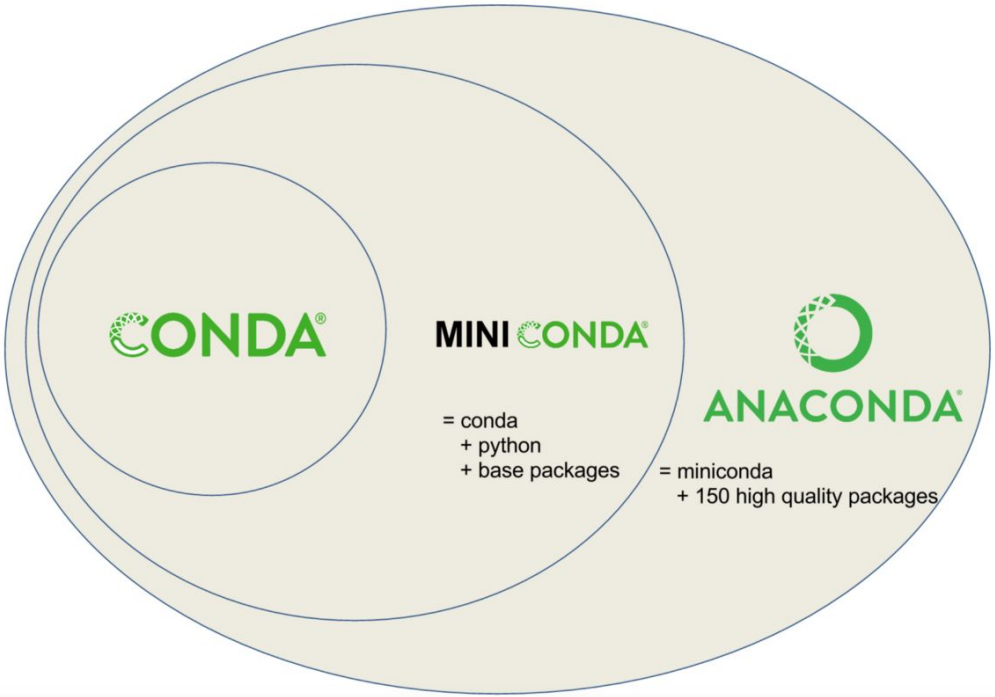
- Professional-grade integrated environment
- Wide range of features suitable for large and complex projects
- Free (with ucsd email)


jupyter

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

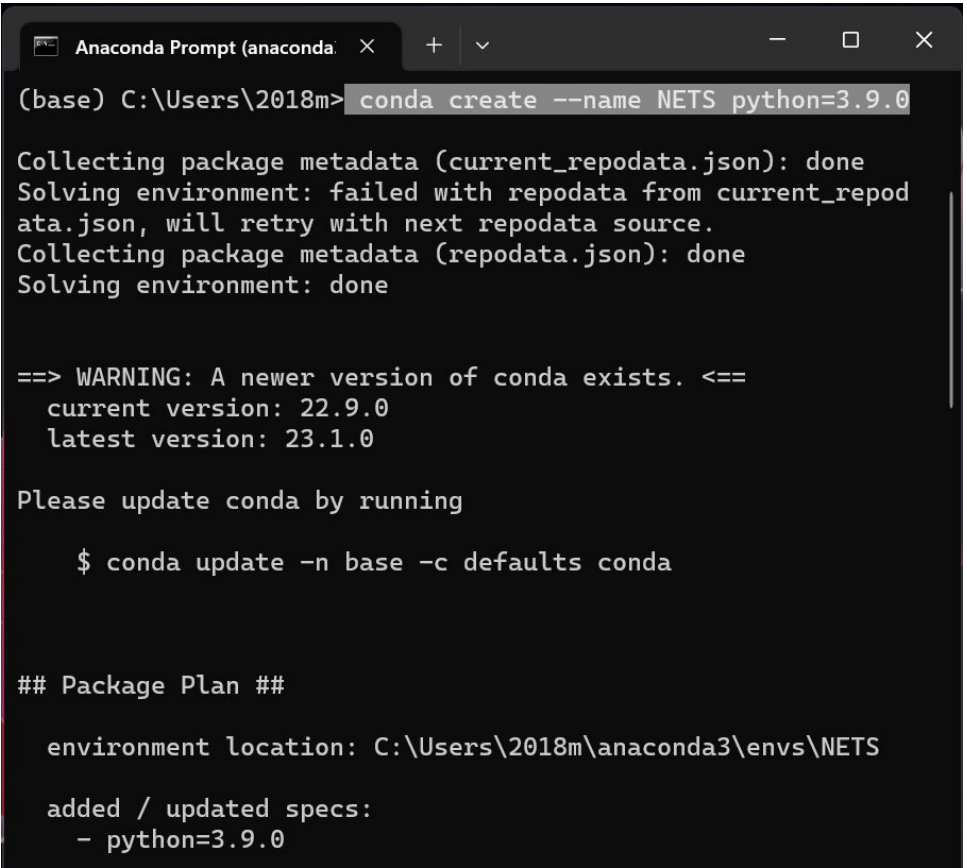
```
conda install --yes numpy matplotlib pandas jupyter seaborn scikit-learn
```

4. Open Jupyter Lab

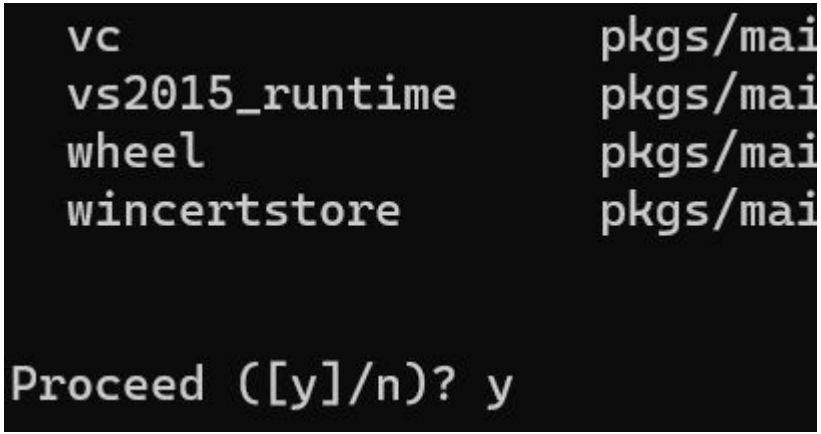
```
jupyter lab
```

1. Create virtual environment

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

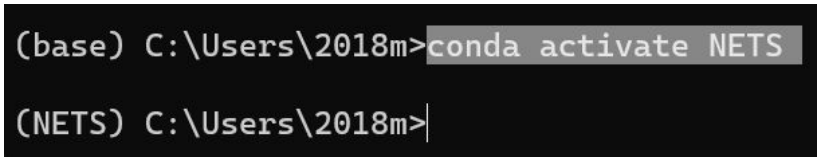


Proceed by typing ‘y’



2. Activate virtual environment

```
conda activate NETS
```

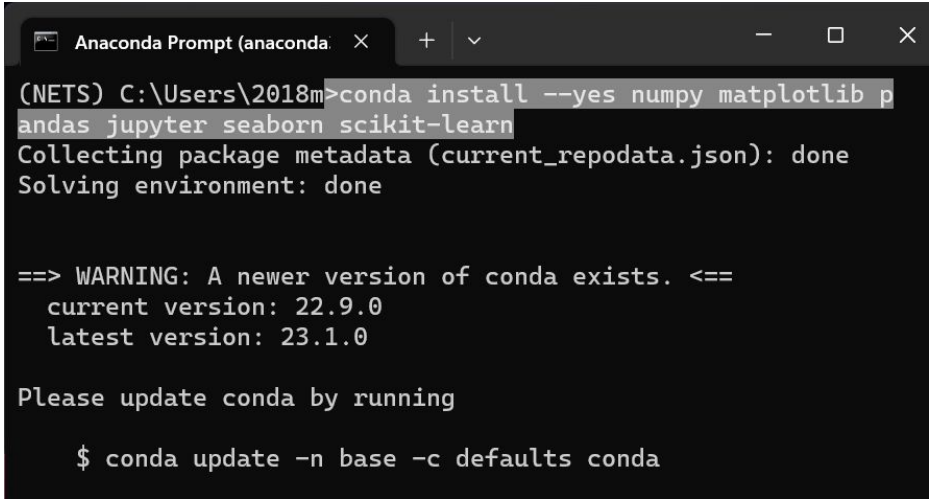


3. Install Jupyter and other necessary libraries

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

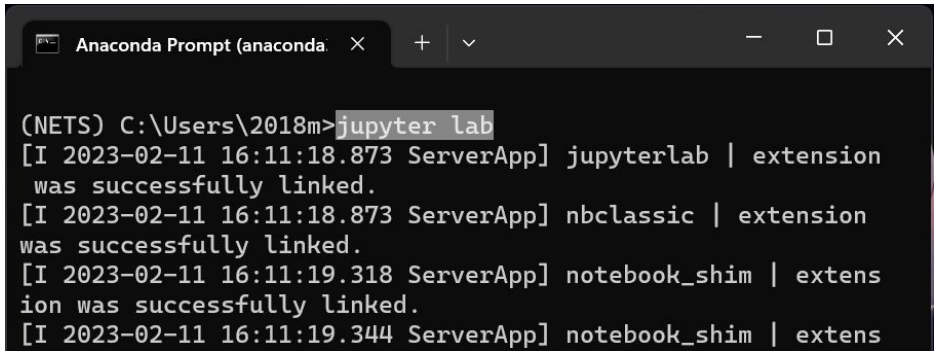
Download the necessary/basic python packages with conda install (IMPORTANT to note which version of the packages you used so your work can be replicated without bugs and errors)

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



4. Open Jupyter Lab

```
jupyter lab
```



Quick Demo of data processing

01

Open Jupyter lab

with Prompt/Terminal

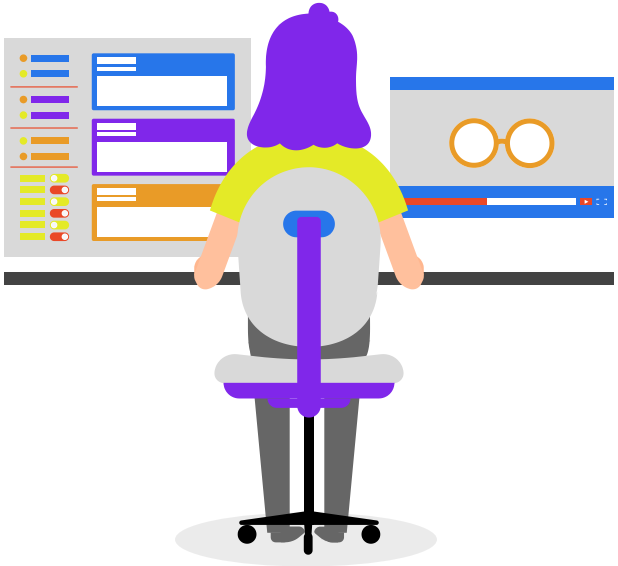
02

Go to Github

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

03

Download from Repository



04

Make New Folder

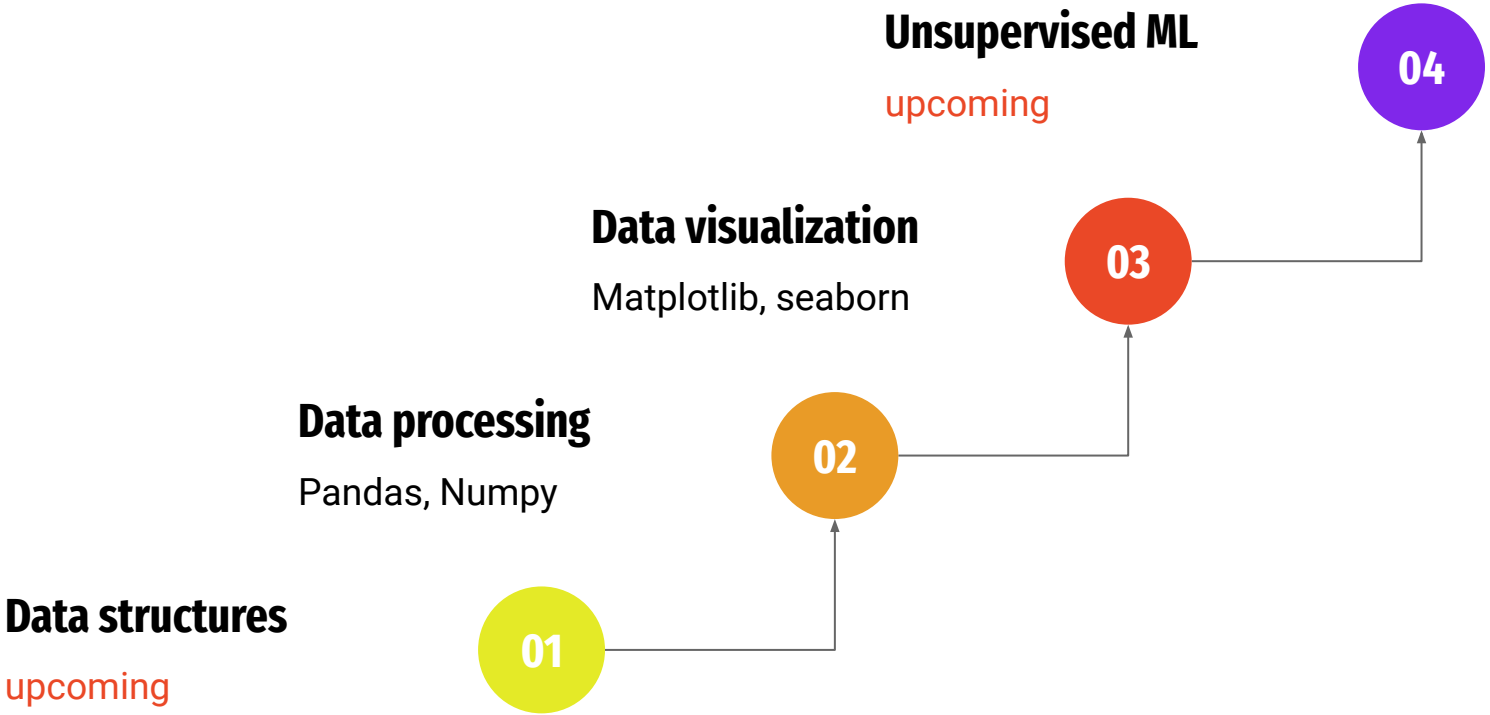
and extract the files from GitHub

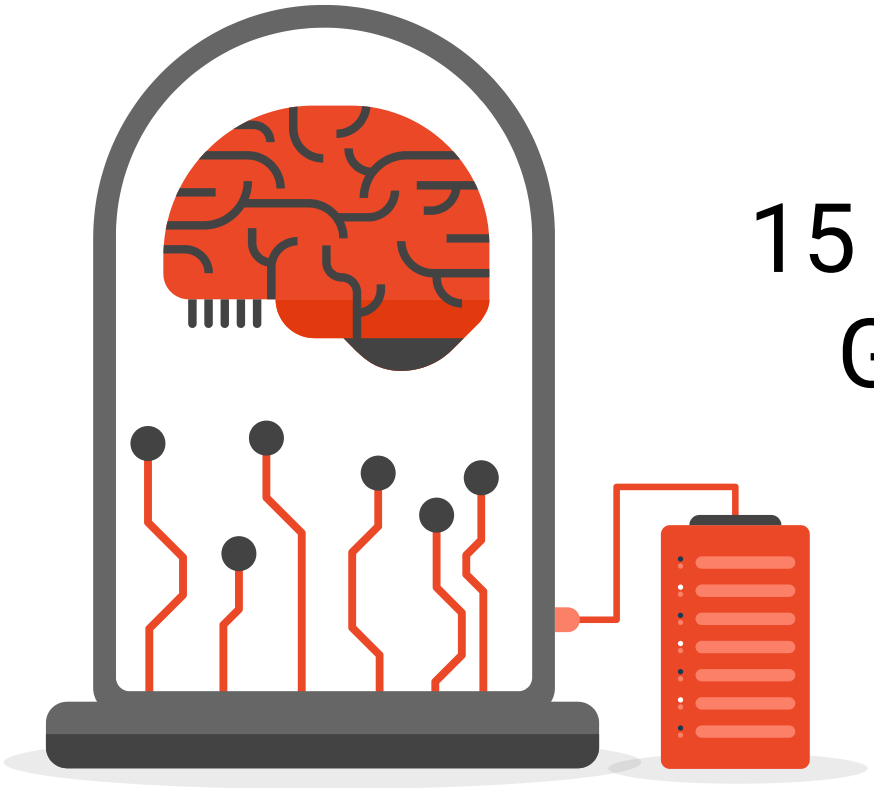
05

Open Notebook

Day_1_Part_A.ipynb

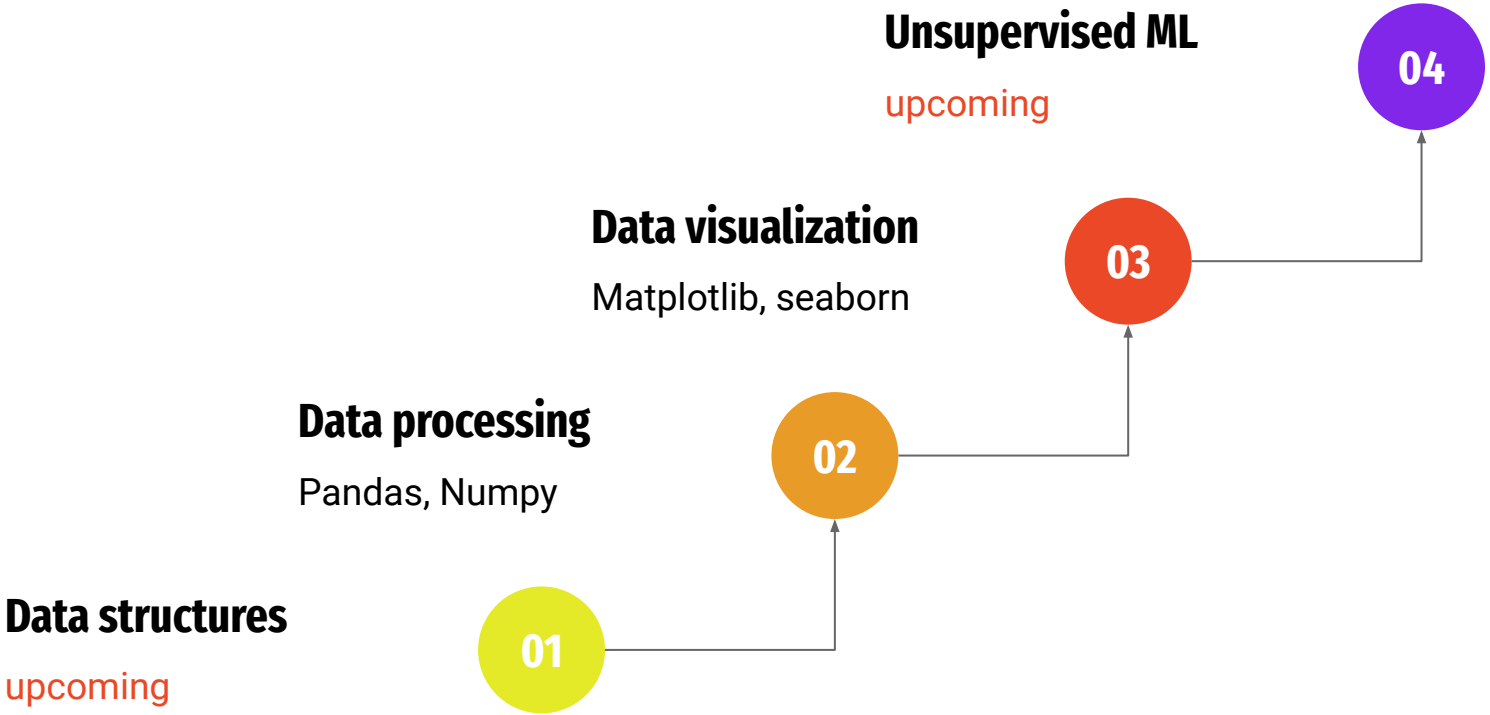
Recap on what we have done so far...





15 minutes break
Grab a bagel!

Recap on what we have done so far...

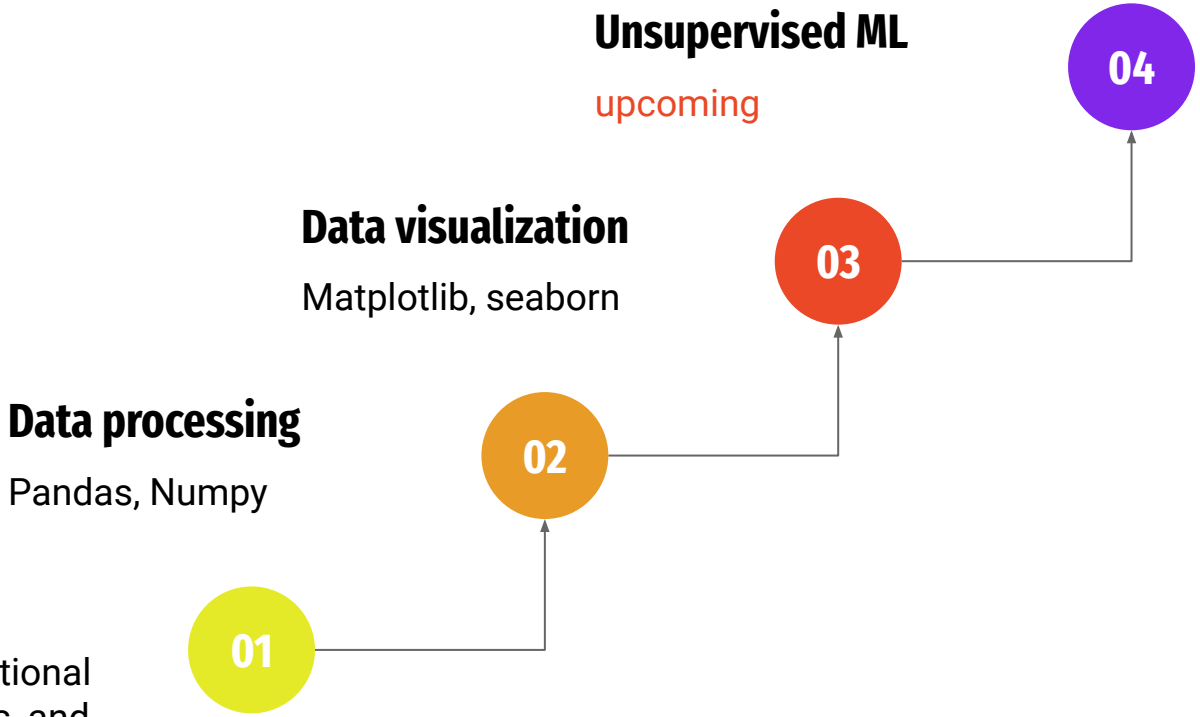


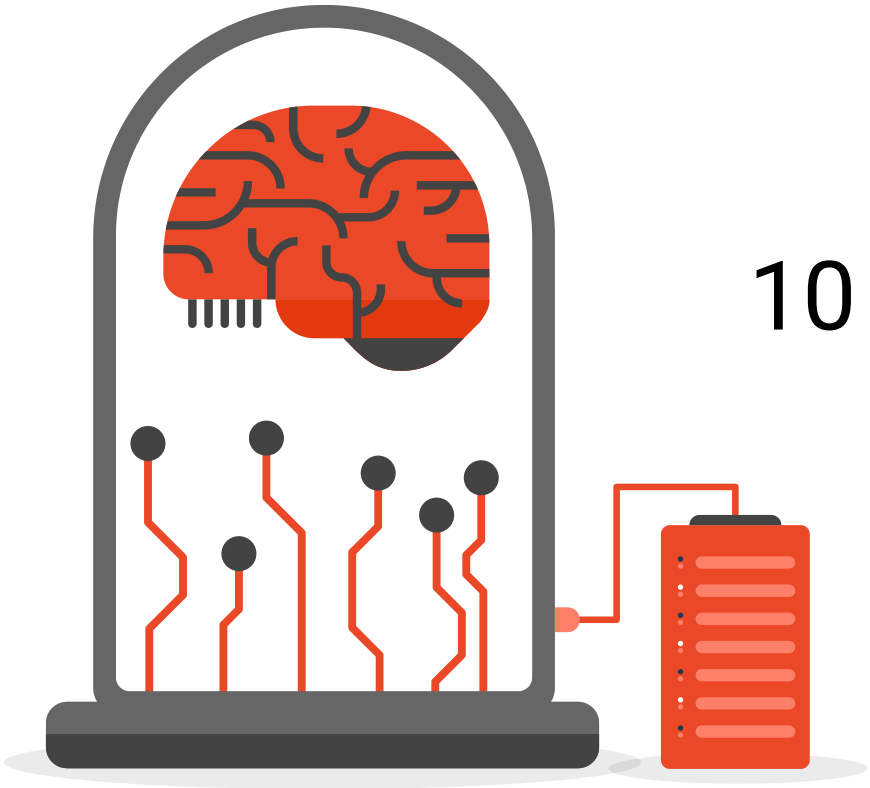
Quick Demo of data processing

Open Notebook

Day_1_Part_B.ipynb

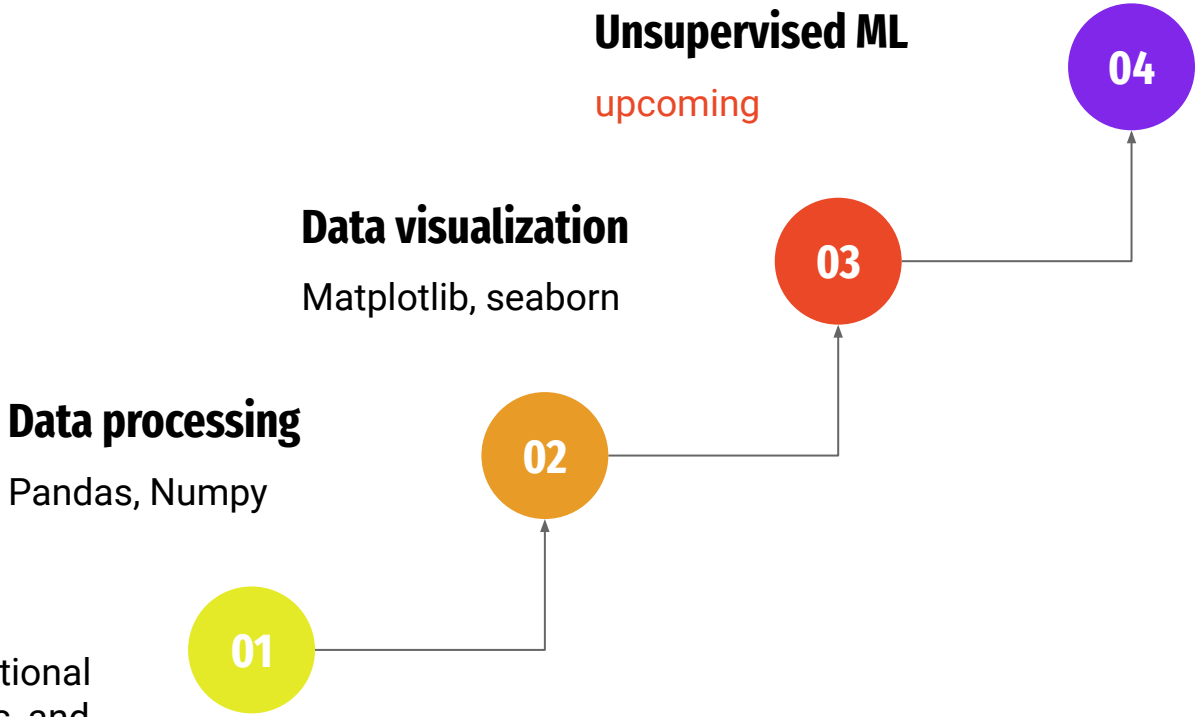
Recap on what we have done so far...





10 minutes break

Recap on what we have done so far...

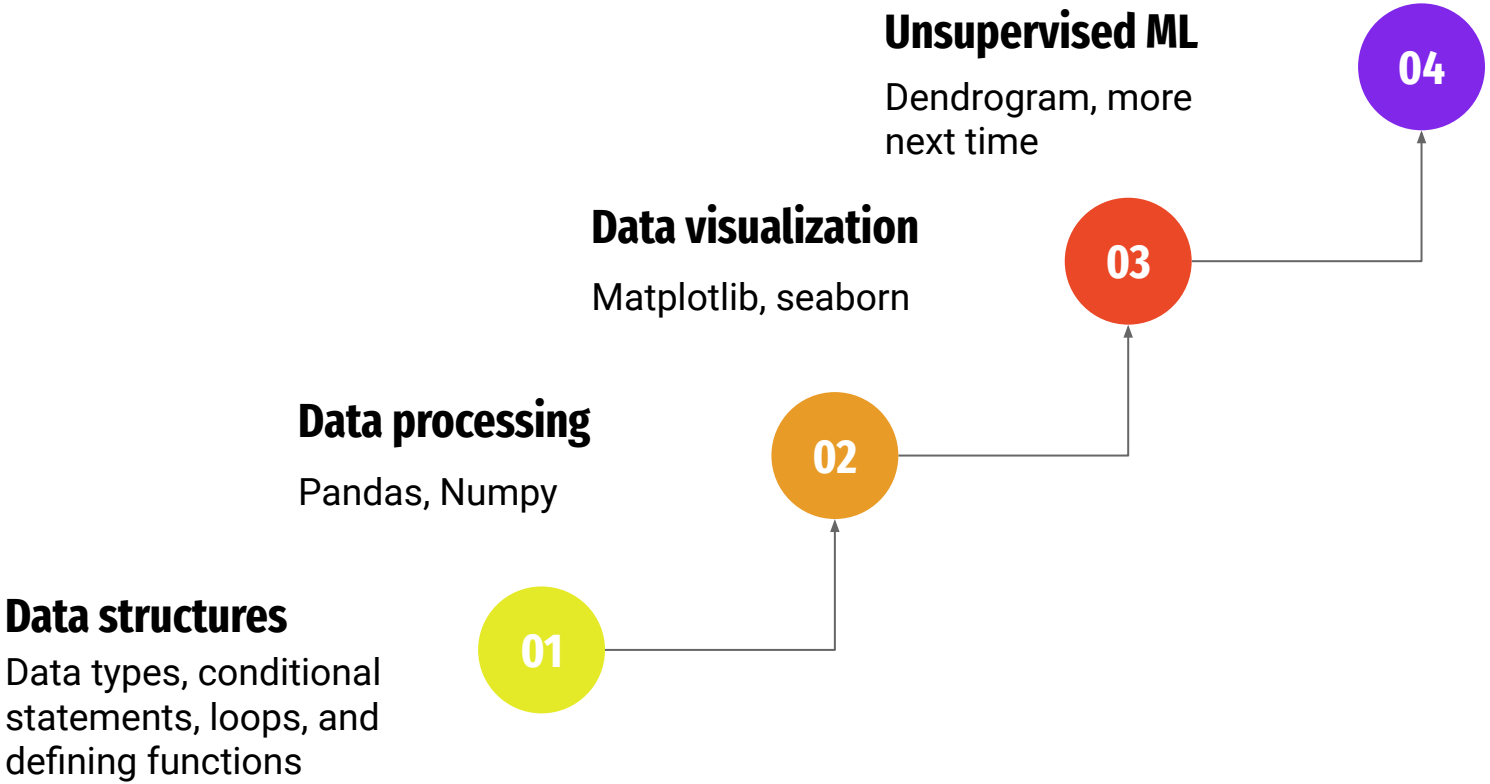


Quick Demo of data processing

Open Notebook

Day_1_Part_C.ipynb

Recap on what we have done so far...



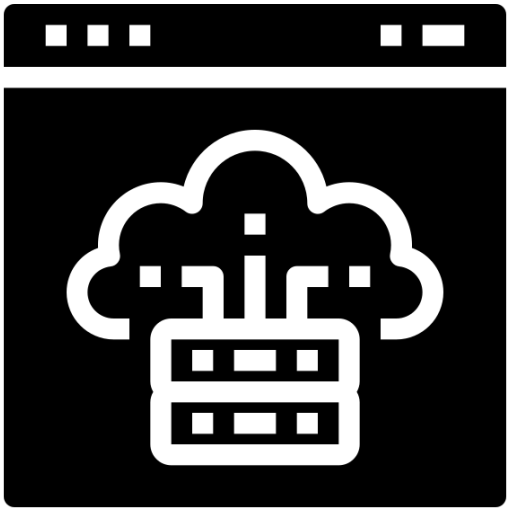
Other Resources for YOU

- 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

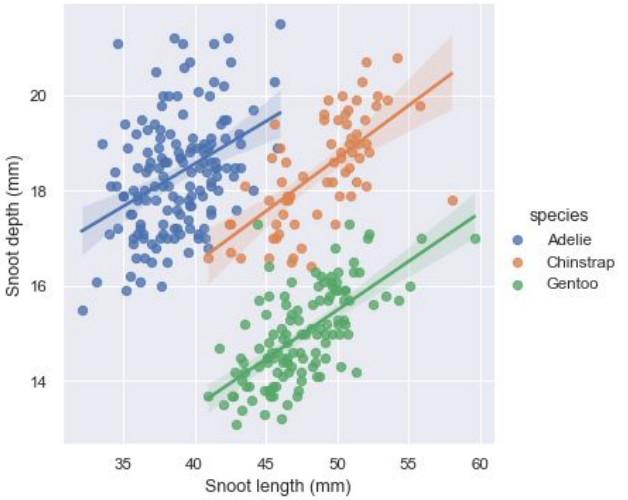
Sneak Peek at Tomorrow

API with Ethan

Website with Duc



ML with Mai



Food and Goodbye.
See everyone again tomorrow.