

# **Practice 01**

Seongok Ryu KAIST Chemistry



### **Contents**

- Why do we use python?
- Python packages for data science and machine learning
- Virtual environment with Anaconda
- Python coding convention
- Linear regression with TensorFlow

## Why do we use python?



```
public class HelloWorld {
   public static void main(String[] args) {
       System.out.println("Hello, world!");
```

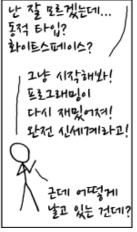
```
Python 2.x
  1. print 'hello world!'
Python 2.6 \sim 3.x
     print('hello world!')
```

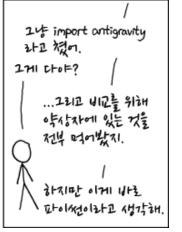
## Why do we use python?



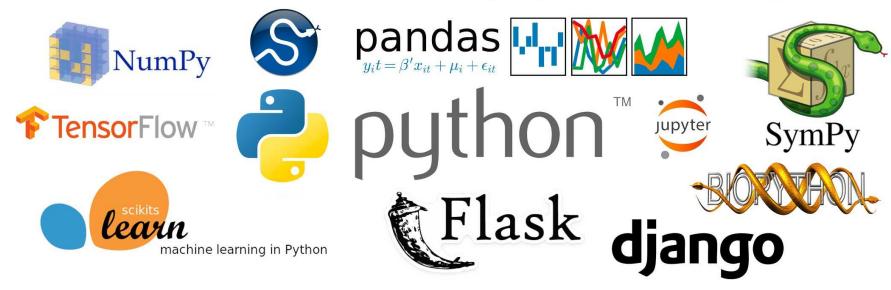








## We offer the following Python training



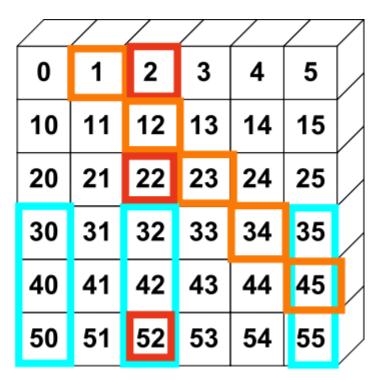
- Scientific works numpy, scipy, cvxopt
- Statistics & Visualization pandas, matplotlib, seaborn
- Web programming Flask, django
- Machine learning scikit-learn, tensorflow, keras, pytorch

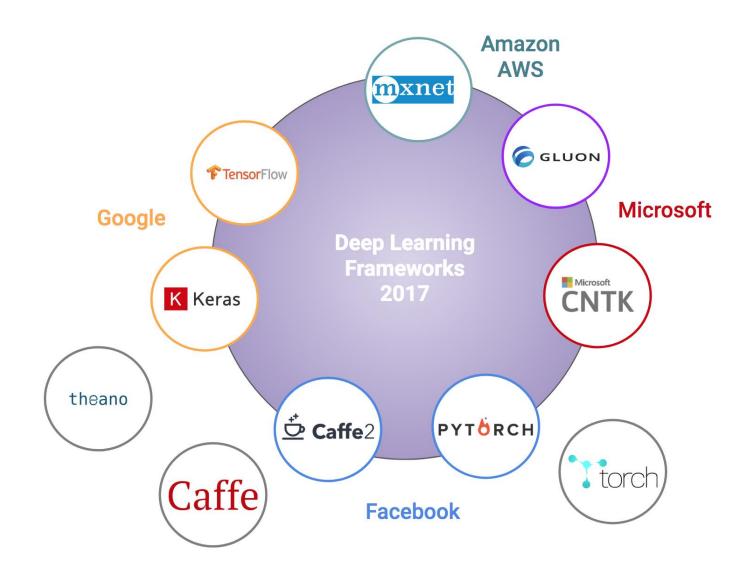


Python libraries



```
>>> a[(0,1,2,3,4),(1,2,3,4,5)]
array([ 1, 12, 23, 34, 45])
>>> a[3:,[0, 2, 5]]
array([[30, 32, 35],
        [40, 42, 45]])
        [50, 52, 55]])
>>>  mask = array([1,0,1,0,0,1],
                   dtype=bool)
>>> a[mask,2]
array([2,22,52])
```





- Tensorflow → This practice will mainly use tensorflow for practices.
  - Google에서 만들고 제공하는 deep learning framework
  - 가장 많은 user 들이 사용 → many practice codes on GitHub
  - Static computational graph

#### Keras

- Tensorflow와 theano를 back-end로 하는 framework
- Very very easy to use
- Static computational graph

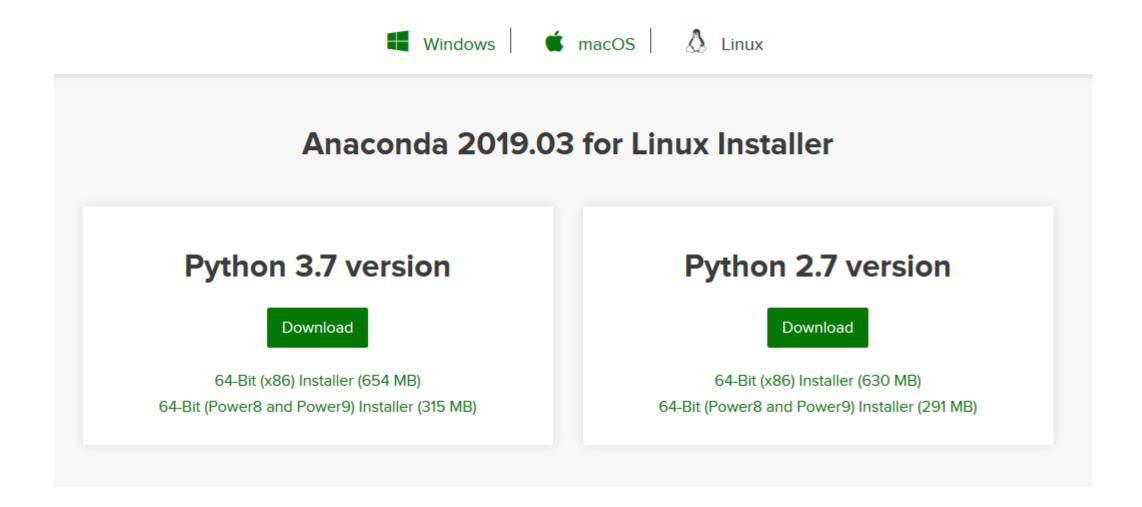
### PyTorch

- Facebook에서 만든 Torch(C++)를 Python으로 wrapping
- Dynamic computational graph





1. Install Anaconda https://www.anaconda.com/distribution/



2. Create your own virtual environment

```
[wykgroup@horus0 ~]$ conda create -n python_seongok
collecting package metadata (current_répodata.json): done
Solving environment: done
## Package Plan ##
  environment location: /home/wykgroup/appl/anaconda3/envs/python_seongok
Proceed ([y]/n)? y
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
  To activate this environment, use
      $ conda activate python_seongok
  To deactivate an active environment, use
      $ conda deactivate
```

3. Activate your virtual environment

```
(python_seongok) [wykgroup@horus0 ~]$ source deactivate python_seongok
DeprecationWarning: 'source deactivate' is deprecated. Use 'conda deactivate'.
```

<sup>\*</sup> Deactivation of your virtual environment

4. Install python packages in your virtual environment

```
(python_seongok) [wykgroup@horus0 ~]$ conda install numpy
Collecting package metadata (current_repodata.json): doné solving environment: done
## Package Plan ##
  environment location: /home/wykgroup/appl/anaconda3/envs/python_seongok
  added / updated specs:
    numpy
The following packages will be downloaded:
    package
                                                build
    blas-1.0
                                                  mk1
                                                                  6 KB
```

- numpy, scikit-learn
- tensorflow (tensorflow-gpu for GPU utilization)
- rdkit (for chemists), see <a href="https://anaconda.org/rdkit/rdkit">https://anaconda.org/rdkit/rdkit</a>

5. Check whether packages are successfully installed

```
(python_seongok) [wykgroup@horus0 ~]$ python
Python 3.7.3 (default, Mar 27 2019, 22:11:17)
[GCC 7.3.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> import tensorflow as tf
>>> import keras
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'keras'
>>>
```

<sup>\*</sup> I didn't install 'keras' in the virtual environment 'python\_seongok'.

## Python coding convention

See practice codes in <a href="https://github.com/SeongokRyu/ACE-Team-DLstudy/tree/master/practices/week01">https://github.com/SeongokRyu/ACE-Team-DLstudy/tree/master/practices/week01</a>

## **Linear regression with TensorFlow**

See practice codes in <a href="https://github.com/SeongokRyu/ACE-Team-DLstudy/tree/master/practices/week01">https://github.com/SeongokRyu/ACE-Team-DLstudy/tree/master/practices/week01</a>