Introduction

Seongok Ryu

Department of Chemistry, KAIST

Contents

- Introduction

  - python, python libraries and deep learning frameworks

  - Installation of necessary python libraries

Why Python?

"Life is too short, You need Python."

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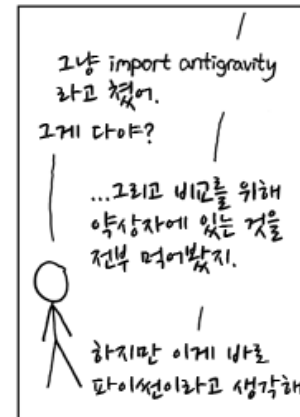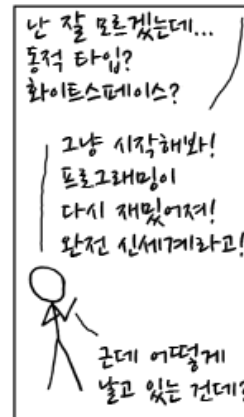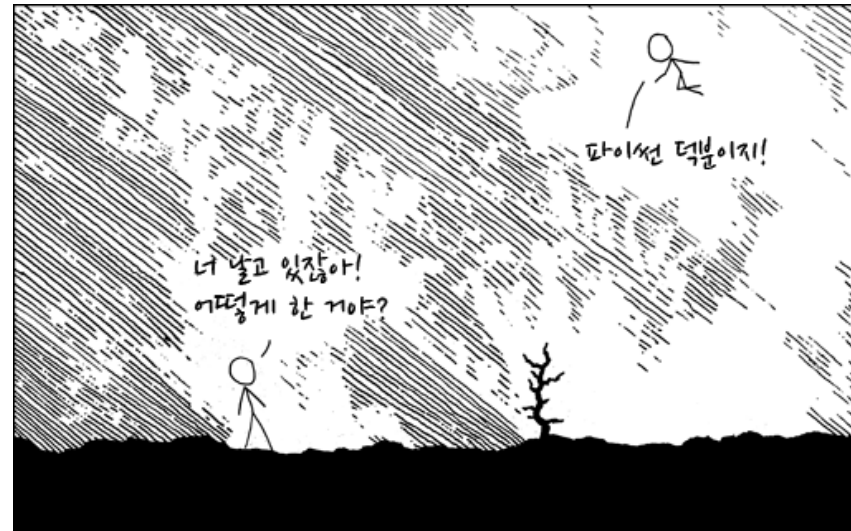```

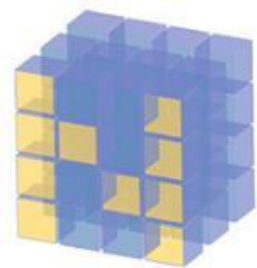Python 2.x

```
1. print 'hello world!'
```
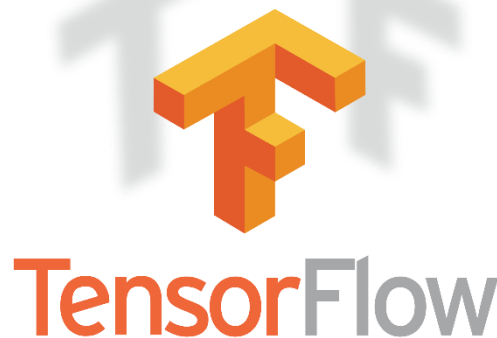
Python 2.6 ~ 3.x

```
1.  print('hello world!')
```

Why Python?

Python libraries will be used in this class

Deep Learning

Deep learning Frameworks
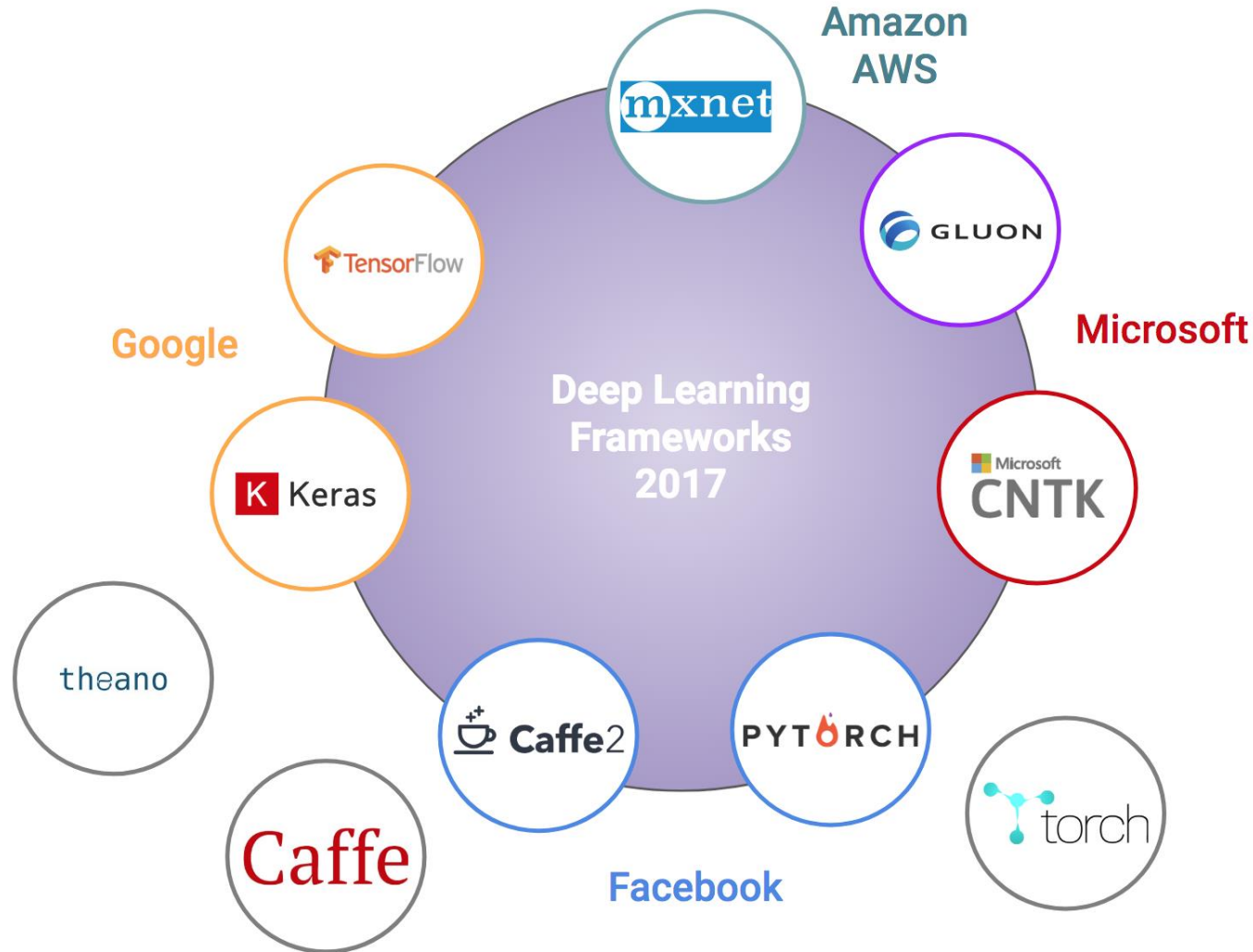
Deep learning Frameworks

Deep learning framework search interest

TensorFlow
Keras
Caffe
Theano
Torch
Pytorch

7/1/2014   1/1/2015   7/1/2015   1/1/2016   7/1/2016   1/1/2017
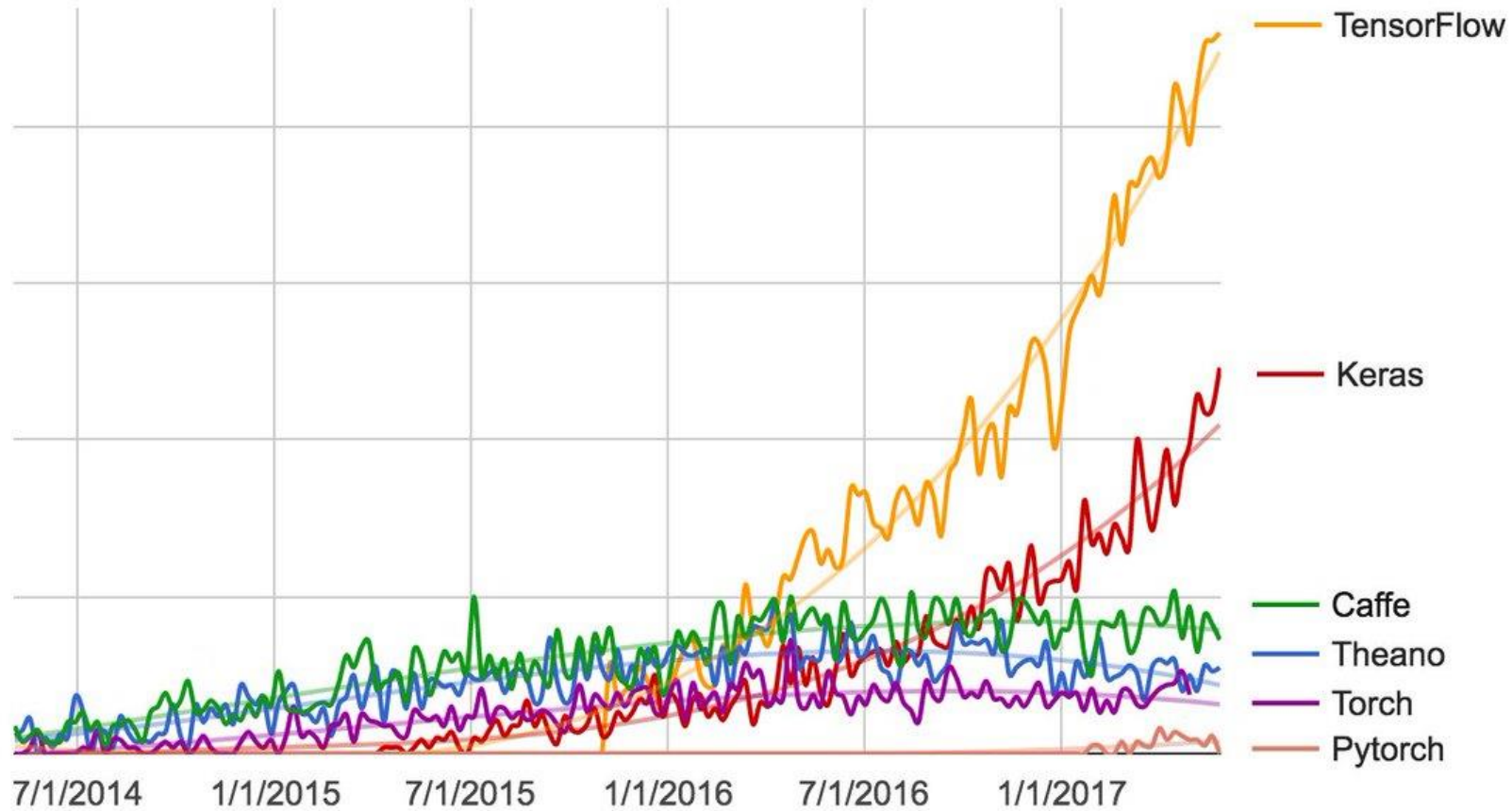
Deep learning Frameworks

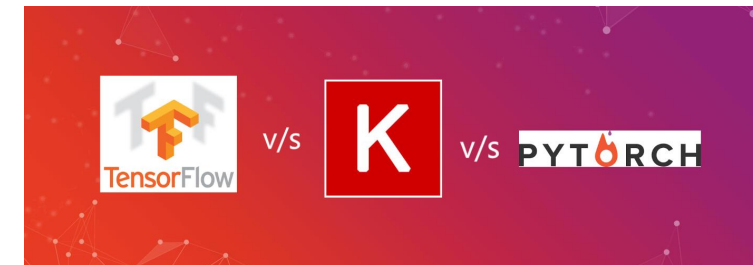- **TensorFlow – We will use this in this class.**

    - Developed and maintained by Google

    - Most popular deep learning framework → many examples on gitHub

    - Static computational graph, *but dynamic computational graph is also supported now.*
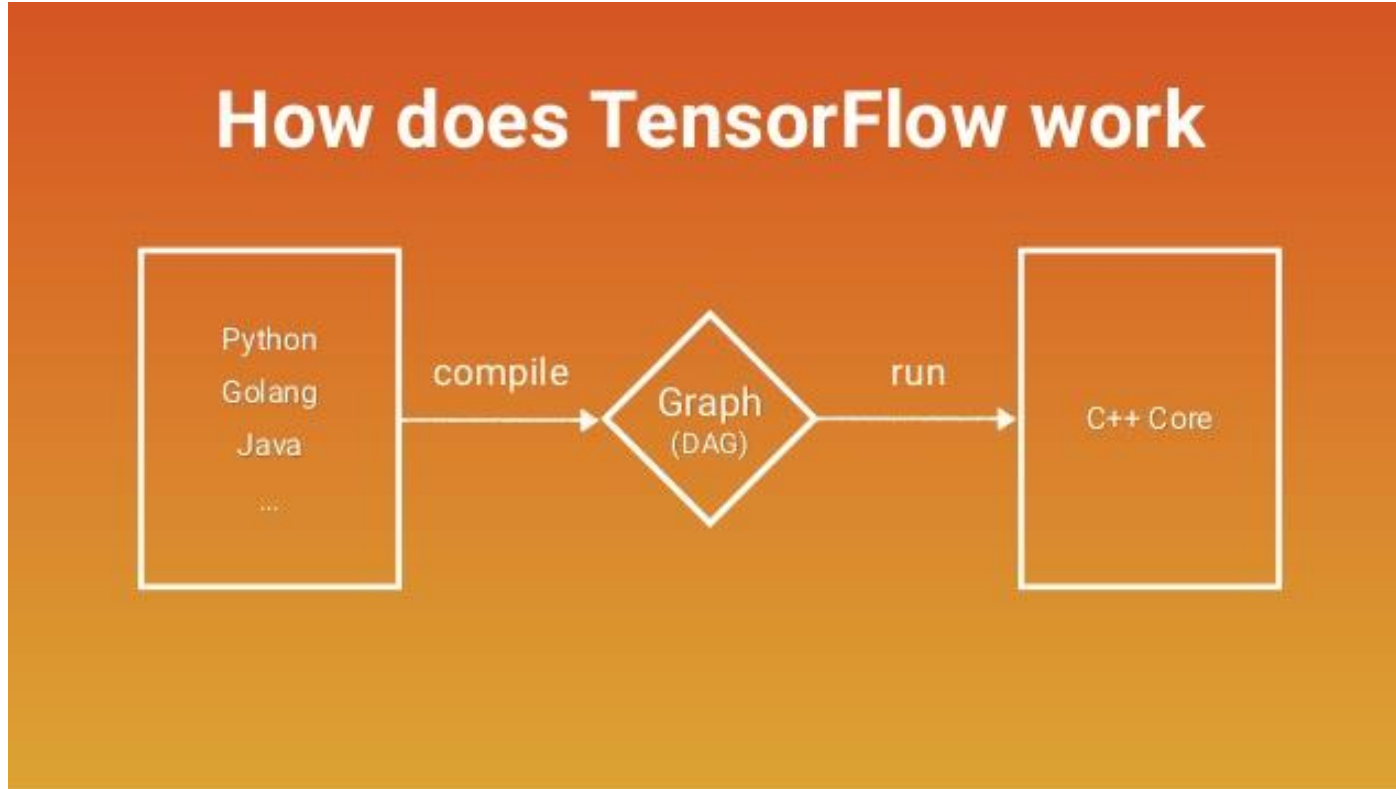
- **Keras**

    - Framework using tensorflow and theanoas back-end

    - Super super easy to use

    - Static computational graph

- **PyTorch**

    - Developed and maintained by Facebook

    - Dynamic Computational Graph

Deep learning Frameworks

How does TensorFlow work

Install python and necessary libraries

- Recommend environment : Linux with GPU

- Anaconda : a package which manages python and libraries

- Virtual Environment

    - http://thrillfighter.tistory.com/466

- Install python libraries

    - install numpy, scipy, scikit-learn, matplotlib, tensorflow

    - just type **"conda create numpy"**

- Install RDKit

    - "conda create –c rdkit my-rdkit-env rdkit"

    - reference : https://www.rdkit.org/docs/Install.html

Overall procedure

1. Excute 'Anaconda prompt'

2. Create a new virtual environment.
   - conda create –n python_ai

3. Activate the virtual environment
   - activate python_ai

4. Install rdkit and other necessary libraries
   - conda install –c rdkit rdkit
   - conda install tensorflow
   - conda install scikit-learn

5. Excute python and check installations.
   - python
   - from rdkit import Chem
   - import tensorflow as tf
   - …