Selecting Hyperparameter for Multilayer Perceptron

COMP 4211 - Tutorial 05

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Objective

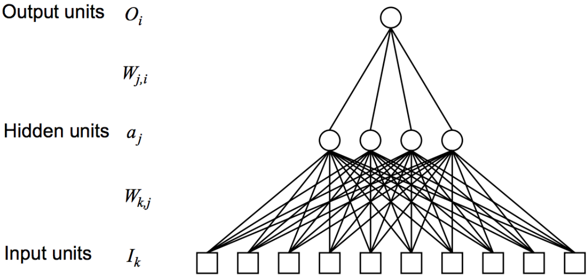
In this tutorial, you will learn the basic terminology and workflow in TensorFlow.

Agenda

1. What is TensorFlow?
2. How can you setting up an environment to run TensorFlow?
3. How to use TensorFlow?

Recap

- Multilayer perceptron/deep neural network.

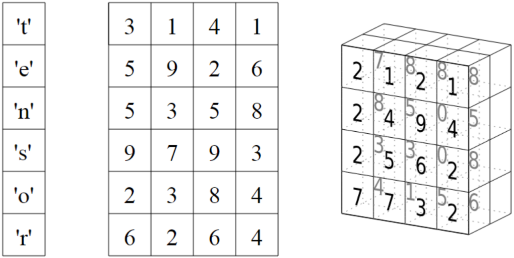


TensorFlow

What is TensorFlow?

What is TensorFlow?

- It is a **deep learning library** supported by Google.
- It provides lots of functions on tensors (n-dimensional array) for automatically computing their derivatives.

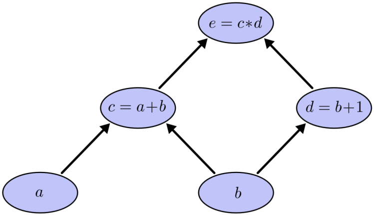


tensor of dimensions [6] (vector of dimension 6) | tensor of dimensions [6,4] (matrix 6 by 4) | tensor of dimensions [4,4,2]

Example of tensor

Why does it call TensorFlow?

- Tensorflow is basically a package for you to define a **computation graph**.



- This defines **how the tensors should be flowed in the graph** during computation.

Tensorflow vs Numpy

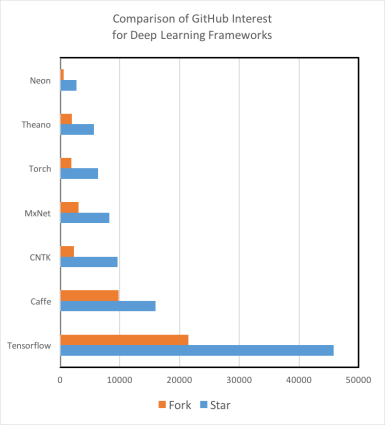
- Both provides API to deal with tensor.
- Tensorflow support tensor operation on both GPU and CPU, while Numpy support CPU solely.
- TensorFlow does the computation based on a defined computation graph. (Declarative programming). Numpy can do the computation on-the-fly. (Imperative programming)

Other Deep Learning Libraries

	Languages	Tutorials and training materials	CNN modeling capability	RNN modeling capability	Architecture: easy-to-use and modular front end	Speed	Multiple GPU support	Keras compatible
Theano	Python, C++	++	++	++	+	++	+	+
Tensor-Flow	Python	+++	+++	++	+++	++	++	+
Torch	Lua, Python (new)	+	+++	++	++	+++	++	
Caffe	C++	+	++		+	+	+	
MXNet	R, Python, Julia, Scala	++	++	+	++	++	+++	
Neon	Python	+	++	+	+	++	+	
CNTK	C++	+	+	+++	+	++	+	

Extract from https://svds.com/getting-started-deep-learning/

Other Deep Learning Libraries



Extract from https://svds.com/getting-started-deep-learning/

Personal Comments

As of March 2018, I found that most of them support a high level interface similar to scikit-learn, so below is the comments about the pros and cons on the low-level interface.

- TensorFlow:
  - + Safe bet for most projects because there is a huge community.
  - + TensorBoard for visualization
  - − Support declarative programming only. (Imperative programming is supported in Tensorflow1.5, yet it is not stable.)
  - − Not easy to learn (if only declarative programming is supported.)
  - − Not efficient in terms of runtime and memory allocation.
- MXNet
  - + Support both declarative and imperative programming.
  - + Efficient in terms of runtime and memory allocation.
  - + Support lots of programming languages.
  - − Not easy to learn. (Getting better when Gluon is introduced in ver. 1.0.)

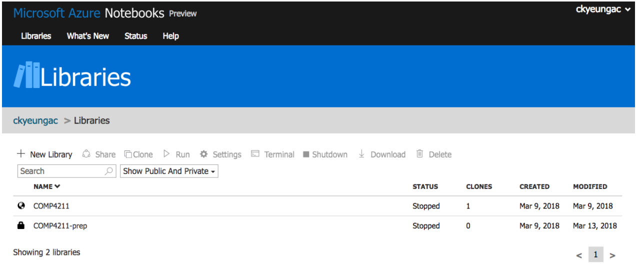
Personal Comments

- PyTorch
  - $+$ Support both declarative and imperative programming.
  - $+$ Efficient in terms of runtime and memory allocation.
  - $+$ Easier to learn if you know numpy already.
  - $-$ Not many high level interface is supported. We have to write our training code. (Yet, they provides automatic gradient function.)
  - $-$ No commercial support. It is in early development stage.
  - $-$ Limited tutorials. (The situation will be getting better.)
- Keras
  - $+$ High level interface for TensorFlow/MXNet.
  - $+$ Easy to learn. (Similar to scikit-learn.)
  - $-$ Runtime performance is bad.
  - $-$ Not flexible to make changes in neural network architecture.

Setting up the working environment

Getting ready for TensorFlow.

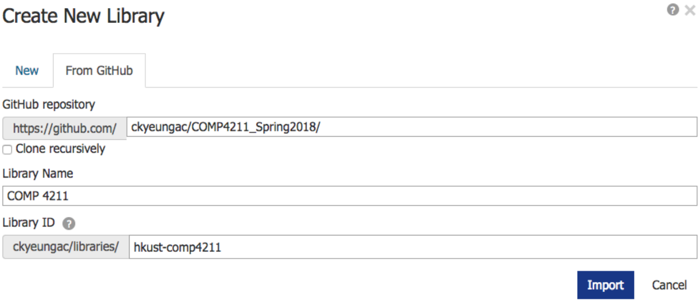
1. As Azure ML Studio does not support TensorFlow, it is better for us to set-up an environment using Azure Notebook (`https://notebooks.azure.com/`).
2. Set up your account in Azure Notebook.
3. Go to the libraries page. (https://notebooks.azure.com/<your_username>/libraries)



4. Click "+ New Library"

After clicking “+ New Library”

5. Click “From Github”.
6. Do the following configuration in the canvas



7. Click “Import”

Let's code

Having a taste in TensorFlow.

To better understand today tutorial, the following .ipynb is covered:

- T05_Single_Layer_Neural_Network_with_TensorFlow.ipynb

Importing TensorFlow

```python
import tensorflow as tf
print(tf.__version__)    # return '1.X.X'
```

Placeholder

Placeholder is dummy nodes that provide entry points for data to computational graph. Let's say we have a dataset where there are 786 features with 10 labels. We can use placeholder to define the our input.

```
# defining the input to the computation graph
x = tf.placeholder(tf.float32, shape=[None, 786]) # None means
                                                    not specified
y_true = tf.placeholder(tf.float32, shape=[None, 10])
```

Variable

Variable is shared, persistent state manipulated by the program. A `tf.Variable` represents a tensor whose value can be changed by running ops on it.

```
# defining the variables to be optimized
weights = tf.Variable(tf.zeros([784, 10]))
biases = tf.Variable(tf.zeros([10]))
```

Tensor Operation

Many tensor operations are available, google it when you need. Here are some useful ones:

```
# These are part of the operations supported by TensorFlow
logits = tf.matmul(x, weights) + biases # z = XW + b
y_pred = tf.nn.softmax(logits) # transform to a probability
                                distribution
y_pred_cls = tf.argmax(y_pred, axis=1) # pick the index with
                                the highest probability
cross_entropy = tf.nn.softmax_cross_entropy_with_logits(logits=
                                logits, labels=y_true) #
                                calculate the cross_entropy
                                loss for each sample
cost = tf.reduce_mean(cross_entropy) # take the mean of the
                                cross_entropy
```

Optimizer

In neural network, there is a cost/loss function you would like to minimize. Optimizer is a handy tool that provide means for you to optimize your network w.r.t your cost function.

```
# defining the optimation method
optimizer = tf.train.GradientDescentOptimizer(
    learning_rate=0.5
).minimize(cost)
```

Many different optimization algorithms are supported in Tensorflow[1], such as `MomentumOptimizer`, `AdamOptimizer`, etc..

[1] https://www.tensorflow.org/api_guides/python/train.

Running the Computation Graph

Once your network (computation graph) is defined, we would like to run our network. Let's say we would like to train our network, we would do:

```
# get the batch data
x_batch, y_true_batch = data.train.next_batch(batch_size)

# define the data that is fed to the network by dict
feed_dict_train = {x: x_batch,
                   y_true: y_true_batch}

# pass the feed_dict and run the computation graph
session.run(optimizer, feed_dict=feed_dict_train)
# the above code will run the optimize we defined with the
                                 feed_dict_train.
```

Appendix

The softmax function is used in various multiclass classification methods. It is defined as

$$\text{softmax}(\mathbf{z})_j = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

In MNIST dataset, we use the softmax in the output layer, and you can think of it as

$$\hat{\mathbf{y}} = \frac{1}{\sum_{k=0}^{9} \exp(z_k)} \begin{bmatrix} \exp(z_0) \\ \exp(z_1) \\ \vdots \\ \exp(z_9) \end{bmatrix} = \begin{bmatrix} P(y=0|\mathbf{x};\mathbf{W}) \\ P(y=1|\mathbf{x};\mathbf{W}) \\ \vdots \\ P(y=9|\mathbf{x};\mathbf{W}) \end{bmatrix}$$

i.e. each output node is a probability.

Appendix

Assume there is a single hidden layer neural network, with the hidden layer $l1$ of d_{l1} neurons. How a sample input $\mathbf{x} = (x_1, x_2, \dots, x_n)$ can be forward propagated in the neural network from the input layer to hidden layer with the weight matrix $\mathbf{W}$[2]

$$
\begin{aligned}
\mathbf{z} &= \mathbf{W}\mathbf{x} \\
&= \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1,n} \\ w_{21} & w_{22} & \cdots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{d_{l1},1} & w_{d_{l1},2} & \cdots & w_{d_{l1},n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \\
&= \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_{d_{l1}} \end{bmatrix}
\end{aligned}
$$

[2]The bias and activation function are omit here for simplicity.

Appendix

What about a dataset $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m)$, how would the whole dataset can be forward propagated in the neural network?

$$
\begin{aligned}
\mathbf{Z} &= \mathbf{X}\mathbf{W}^T \\
&= \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1,n} \\ x_{21} & x_{22} & \cdots & x_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \cdots & x_{m,n} \end{bmatrix} \begin{bmatrix} w_{11} & w_{21} & \cdots & w_{d_{l1},1} \\ w_{12} & w_{22} & \cdots & w_{d_{l1},2} \\ \vdots & \vdots & \ddots & \vdots \\ w_{1,n} & w_{2,n} & \cdots & w_{d_{l1},n} \end{bmatrix} \\
&= \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1,d_{l1}} \\ z_{21} & z_{22} & \cdots & z_{2,d_{l1}} \\ \vdots & \vdots & \ddots & \vdots \\ z_{m,1} & z_{m,2} & \cdots & z_{m,d_{l1}} \end{bmatrix}
\end{aligned}
$$

Then, a row $\mathbf{z}_i = (z_{i,1}, z_{i,2}, \ldots, z_{i,d_{l1}})$ in $\mathbf{Z}$ is the layer output of the sample $\mathbf{x}_i$.