(Artificial) Neural Networks in TensorFlow

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POSTECH

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1. Recall Supervised Learning Setup

- Input features $x^{(i)} \in \mathbb{R}^n$
- Ouput $y^{(i)}$

- Model parameters $\theta \in \mathbb{R}^k$
- Hypothesis function $h_\theta : \mathbb{R}^n \rightarrow y$

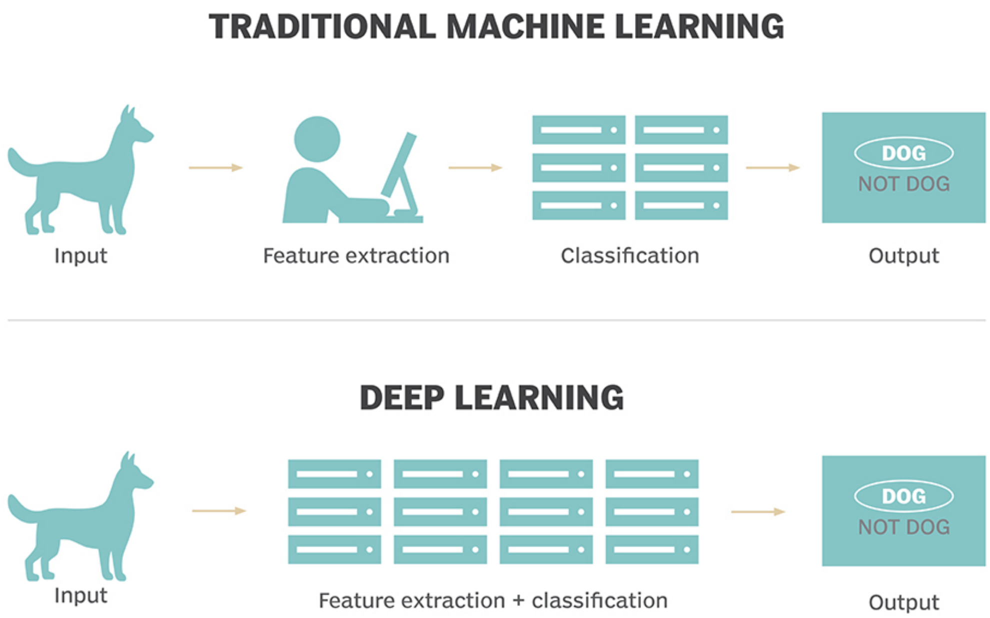
- Loss function $\ell : y \times y \rightarrow \mathbb{R}_+$

- Machine learning optimization problem

$$\min_\theta \sum_{i=1}^{m} \ell\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$$

(possibly plus some additional regularization)

- But, many specialized domains required highly engineered special features

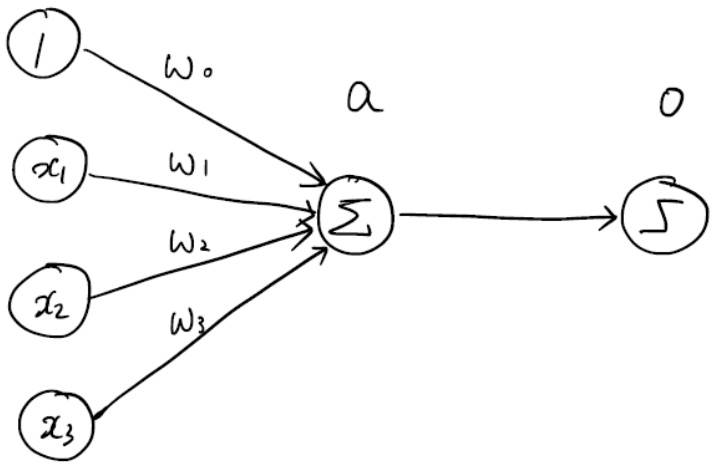


2. Artificial Neural Networks

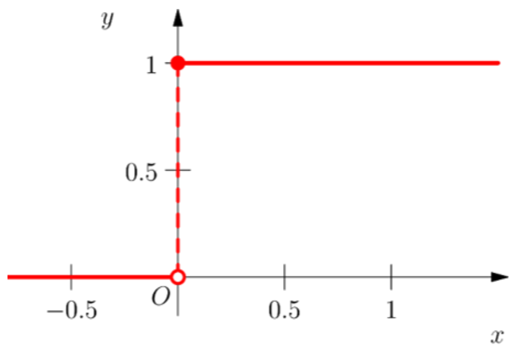
2.1. Perceptron for $h(\theta)$ or $h(\omega)$

- Neurons compute the weighted sum of their inputs
- A neuron is activated or fired when the sum a is positive

$$
\begin{aligned}
a &= \omega_0 + \omega_1 x_1 + \cdots \\
o &= \sigma(\omega_0 + \omega_1 x_1 + \cdots)
\end{aligned}
$$



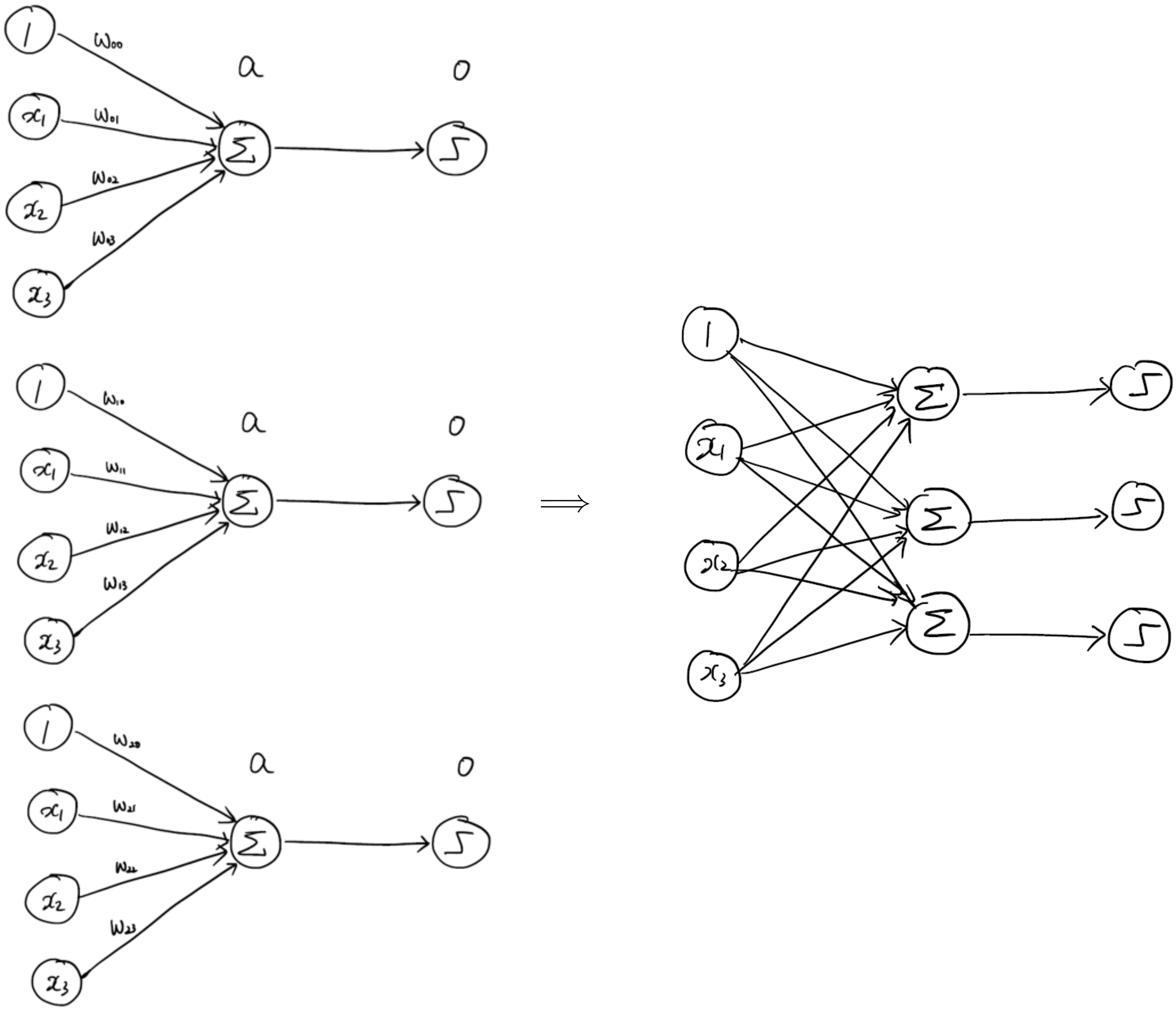
- A step function is not differentiable



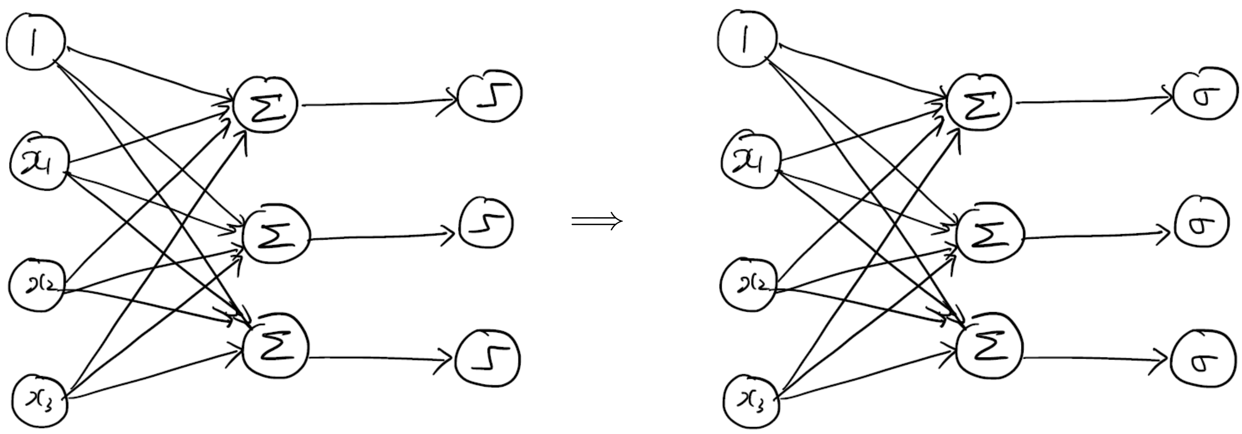
- One layer is often not enough

2.2. Multi-layer Perceptron = Artificial Neural Networks (ANN)

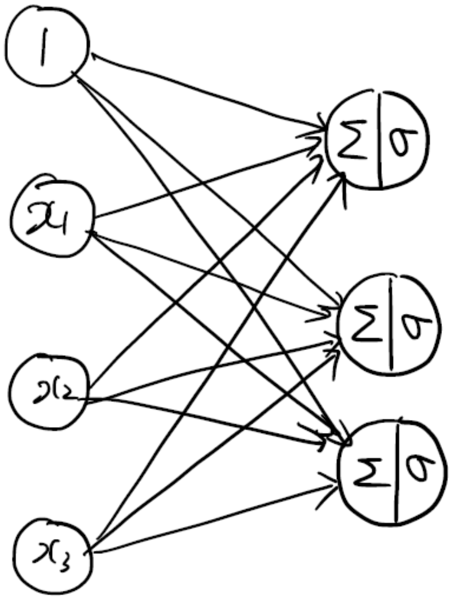
multi-neurons



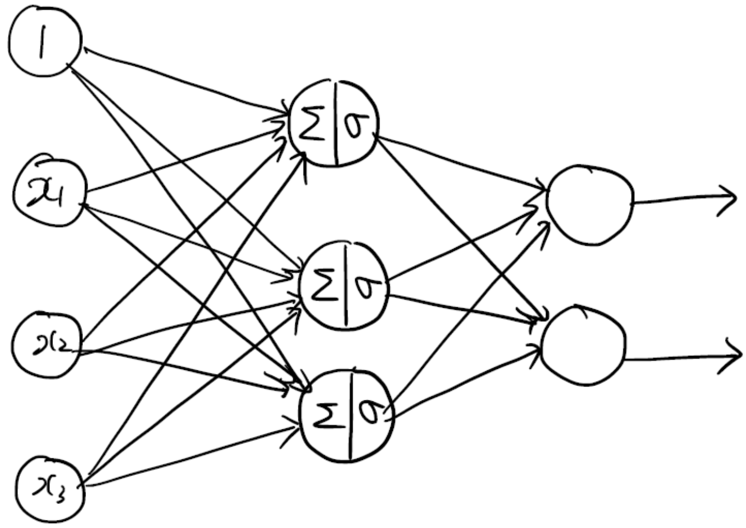
differentiable activation function



in a compact representation



multi-layer perceptron

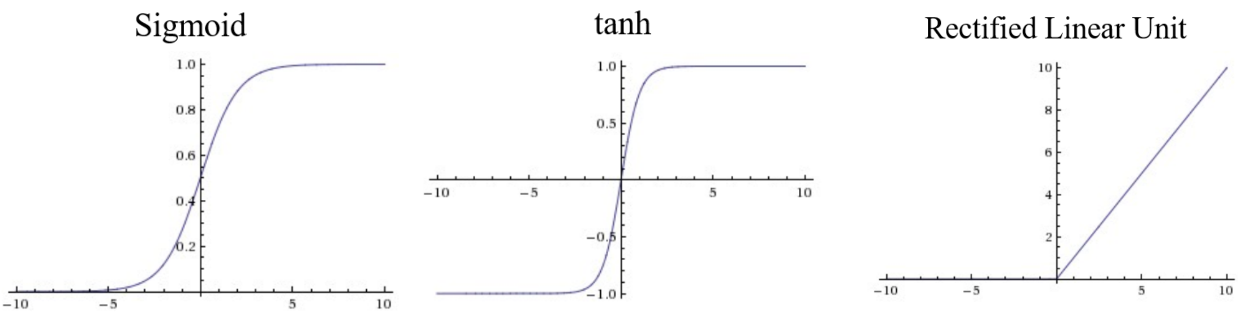


Transformation

- Affine (or linear) transformation and nonlinear activation layer (notations are mixed: $g = \sigma, \omega = \theta, \omega_0 = b$)

$$o(x) = g\left(\theta^T x + b\right)$$

- Nonlinear activation functions ($g = \sigma$)



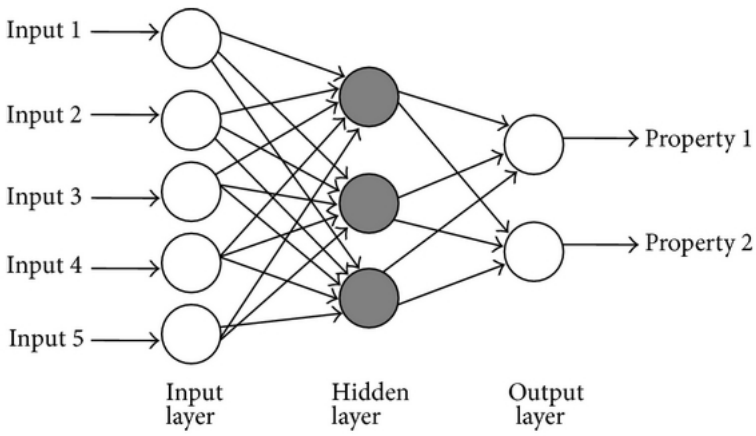
$$g(x) = \frac{1}{1 + e^{-x}} \qquad g(x) = \tanh(x) \qquad g(x) = \max(0, x)$$

Structure

A single layer is not enough to be able to represent complex relationship between input and output

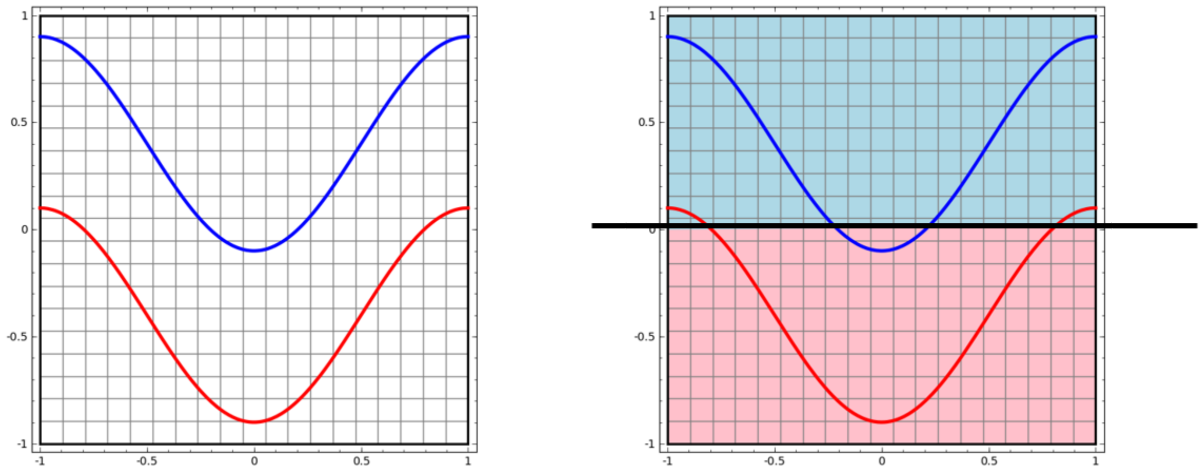
$\Longrightarrow$ perceptrons with many layers and units

$$o_2 = \sigma_2\left(\theta_2^T o_1 + b_2\right) = \sigma_2\left(\theta_2^T \sigma_1\left(\theta_1^T x + b_1\right) + b_2\right)$$



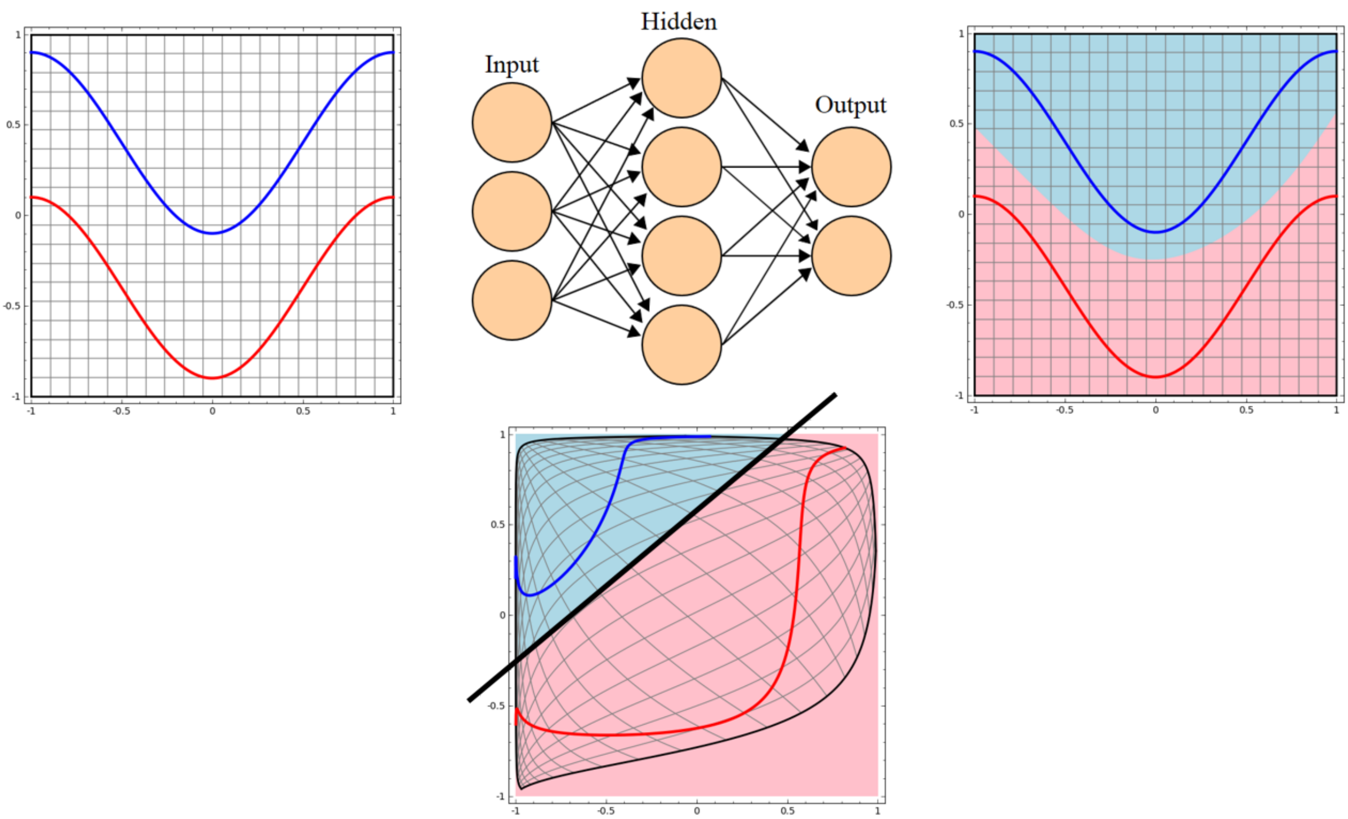
Linear Classifier

- Perceptron tries to separate the two classes of data by dividing them with a line



Neural Networks

- The hidden layer learns a representation so that the data is linearly separable



3. Training Neural Networks

$=$ Learning or estimating weights and biases of multi-layer perceptron from training data

3.1. Optimization

3 key components

1. objective function $f(\cdot)$
2. decision variable or unknown θ
3. constraints $g(\cdot)$

In mathematical expression

$$\begin{array}{rll} \min\limits_{\theta} & f(\theta) & \\ \text{subject to} & g_i(\theta) \leq 0, & \qquad i = 1, \cdots, m \end{array}$$

3.2. Loss Function

- Measures error between target values and predictions

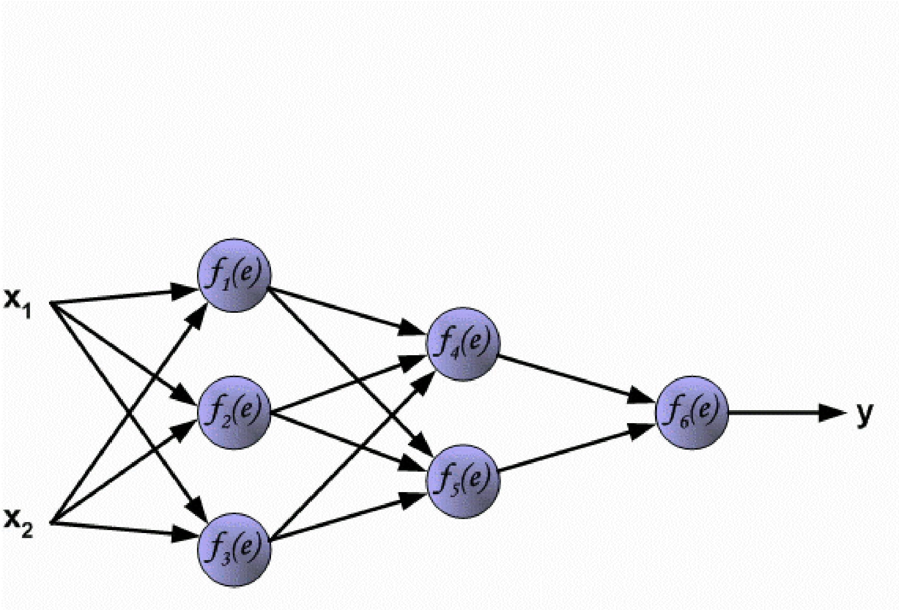
$$\min_{\theta} \sum_{i=1}^{m} \ell\left(h_{\theta}\left(x^{(i)}\right), y^{(i)}\right)$$

- Example
  - Squared loss (for regression):
$$\frac{1}{N} \sum_{i=1}^{N} \left(h_{\theta}\left(x^{(i)}\right) - y^{(i)}\right)^2$$
  - Cross entropy (for classification):
$$-\frac{1}{N} \sum_{i=1}^{N} y^{(i)} \log\left(h_{\theta}\left(x^{(i)}\right)\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_{\theta}\left(x^{(i)}\right)\right)$$

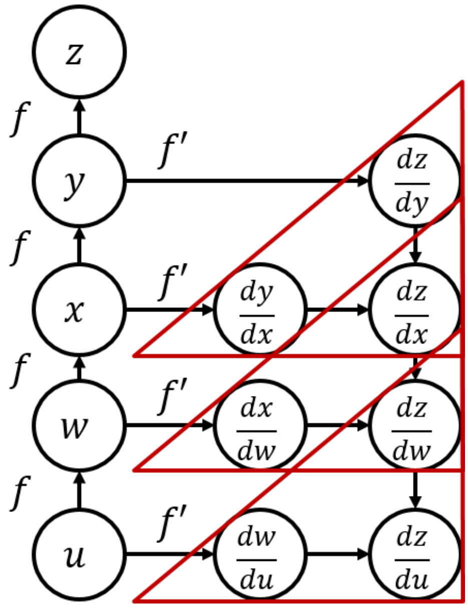
3.3. Learning

Backpropagation

- Forward propagation
  - the initial information propagates up to the hidden units at each layer and finally produces output
- Backpropagation
  - allows the information from the cost to flow backwards through the network in order to compute the gradients



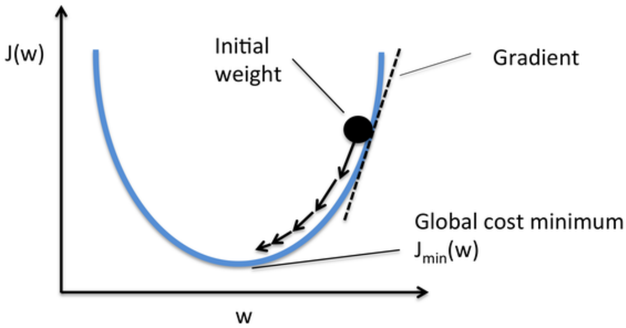
- Chain Rule
  - Computing the derivative of the composition of functions
    - $f(g(x))' = f'(g(x))g'(x)$
    - $\frac{dz}{dx} = \frac{dz}{dy} \bullet \frac{dy}{dx}$
    - $\frac{dz}{dw} = (\frac{dz}{dy} \bullet \frac{dy}{dx}) \bullet \frac{dx}{dw}$
    - $\frac{dz}{du} = (\frac{dz}{dy} \bullet \frac{dy}{dx} \bullet \frac{dx}{dw}) \bullet \frac{dw}{du}$
- Backpropagation
  - Update weights recursively

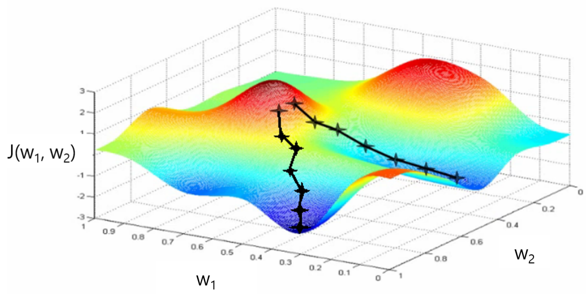


(Stochastic) Gradient Descent

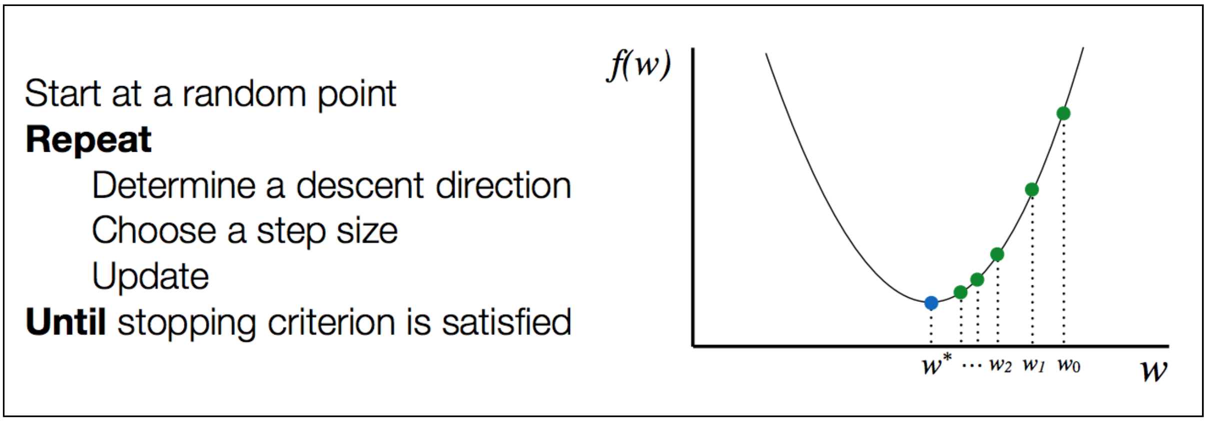
- Negative gradients points directly downhill of the cost function
- We can decrease the cost by moving in the direction of the negative gradient (α is a learning rate)

$$\theta := \theta - \alpha \nabla_\theta \left(h_\theta \left(x^{(i)} \right), y^{(i)} \right)$$





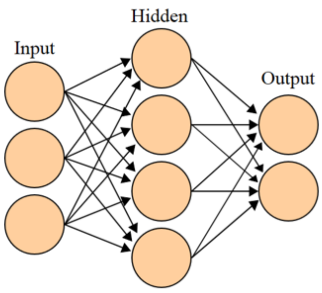
Optimization procedure



- It is not easy to numerically compute gradients in network in general.
  - The good news: people have already done all the "hardwork" of developing numerical solvers (or libraries)
  - There are a wide range of tools

Summary

- Learning weights and biases from data using gradient descent



$$x \longrightarrow \boxed{\hat{y} = f_{\omega_1,\cdots,\omega_k}(x)} \longrightarrow y$$

3.4. Deep Learning Libraries

Caffe

- Platform: Linux, Mac OS, Windows
- Written in: C++
- Interface: Python, MATLAB

Theano

- Platform: Cross-platform
- Written in: Python
- Interface: Python

Tensorflow

- Platform: Linux, Mac OS, Windows
- Written in: C++, Python
- Interface: Python, C/C++, Java, Go, R

4. TensorFlow

- `TensorFlow` (https://www.tensorflow.org) is an open-source software library for deep learning.

Computational Graph

- `tf.constant`
- `tf.Variable`
- `tf.placeholder`

In [1]:

```
import tensorflow as tf

a = tf.constant([1, 2, 3])
b = tf.constant([4, 5, 6])

A = a + b
B = a * b
```

In [2]:

```
A
```

Out[2]:

```
<tf.Tensor 'add:0' shape=(3,) dtype=int32>
```

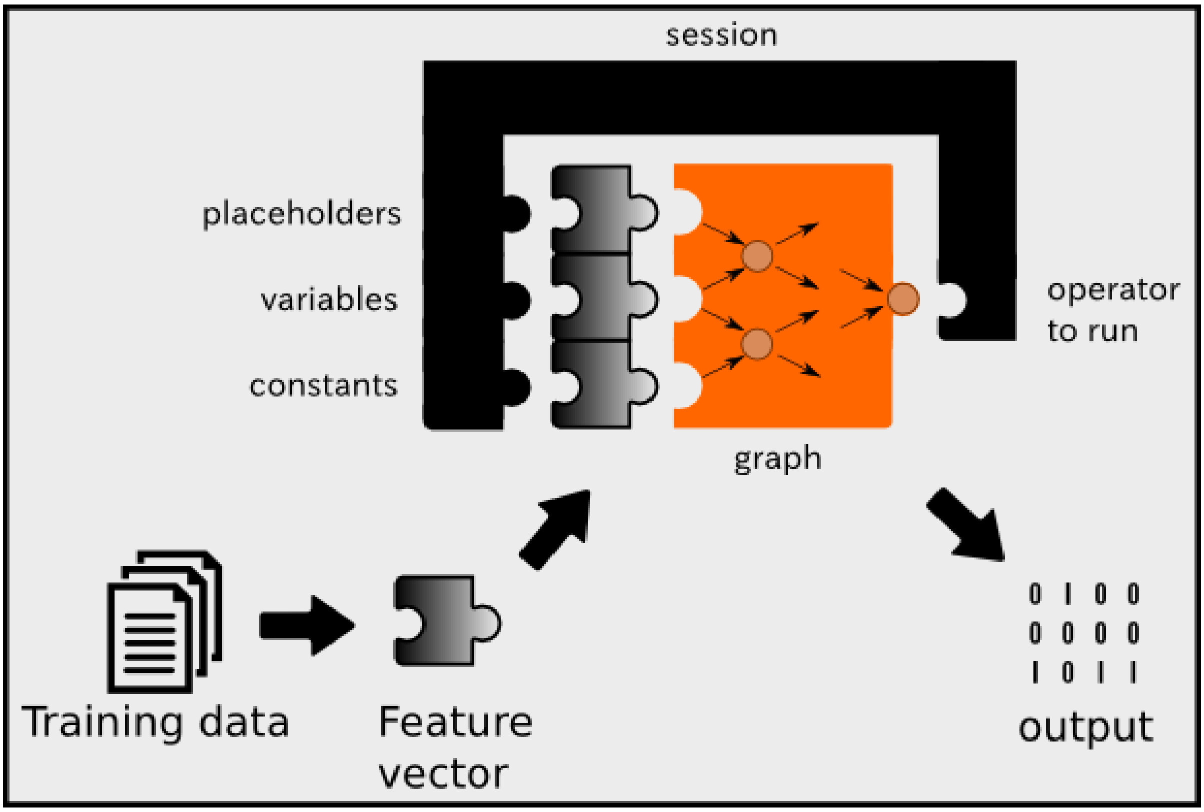
In [3]:

```
B
```

Out[3]:

```
<tf.Tensor 'mul:0' shape=(3,) dtype=int32>
```

To run any of the three defined operations, we need to create a session for that graph. The session will also allocate memory to store the current value of the variable.



In [4]:

```
sess = tf.Session()
sess.run(A)
```

Out[4]:

```
array([5, 7, 9], dtype=int32)
```

In [5]:

```
sess.run(B)
```

Out[5]:

```
array([ 4, 10, 18], dtype=int32)
```

`tf.Variable` is regarded as the decision variable in optimization. We should initialize variables to use `tf.Variable`.

In [6]:

```
w = tf.Variable([1, 1])
```

In [7]:

```
init = tf.global_variables_initializer()
sess.run(init)
```

In [8]:

```
sess.run(w)
```

Out[8]:

```
array([1, 1], dtype=int32)
```

The value of `tf.placeholder` must be fed using the `feed_dict` optional argument to `Session.run()`.

In [9]:

```
x = tf.placeholder(tf.float32, [2, 2])
```

In [10]:

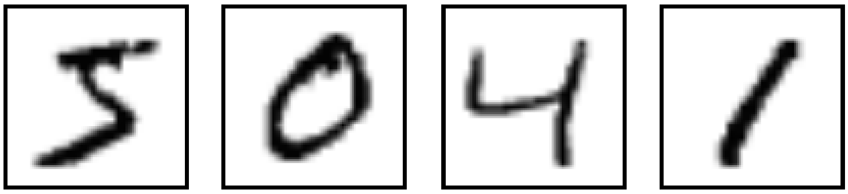
```
sess.run(x, feed_dict={x : [[1,2],[3,4]]})
```

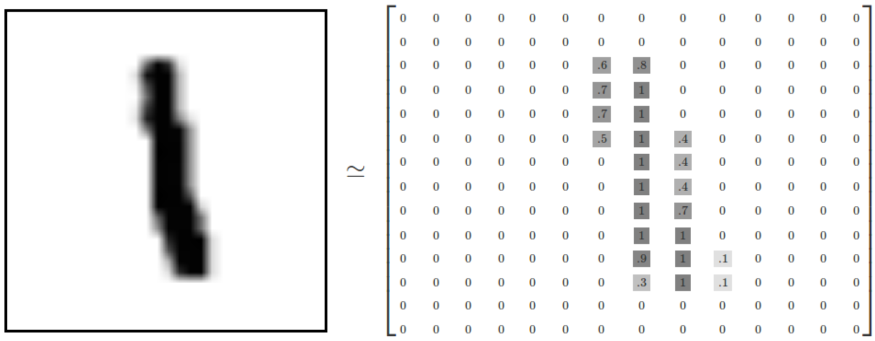
Out[10]:

```
array([[ 1.,  2.],
       [ 3.,  4.]], dtype=float32)
```

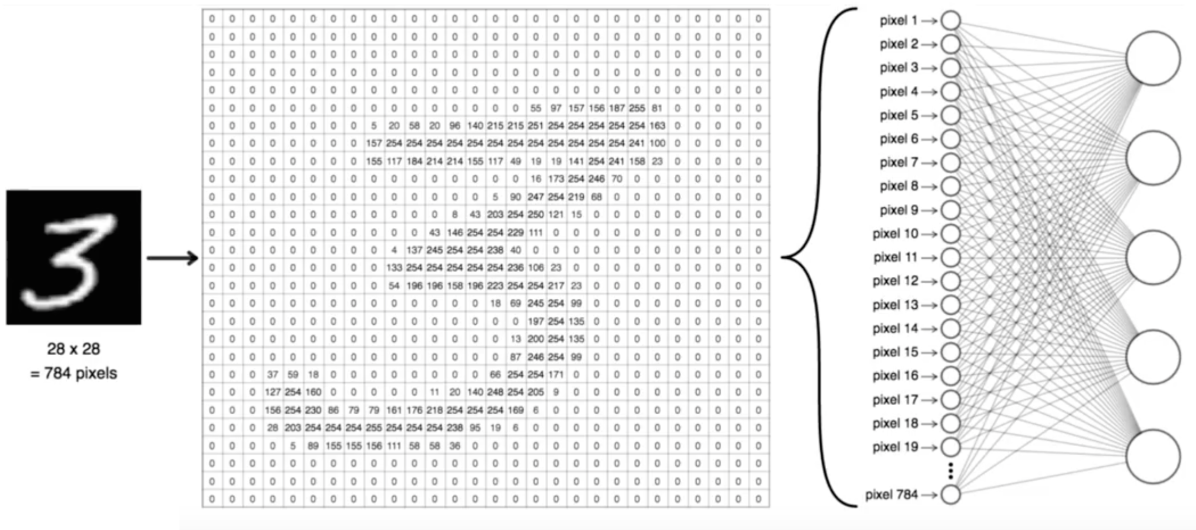
ANN with TensorFlow

- MNIST (Mixed National Institute of Standards and Technology database) database
  - Handwritten digit database
  - 28×28 gray scaled image
  - Flattened matrix into a vector of $28 \times 28 = 784$

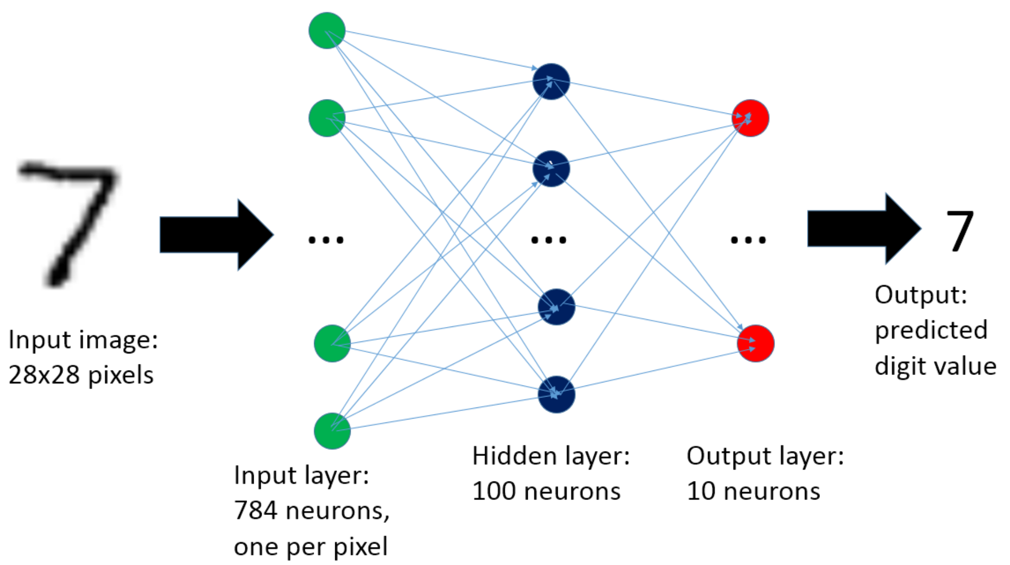




- feed a gray image to ANN

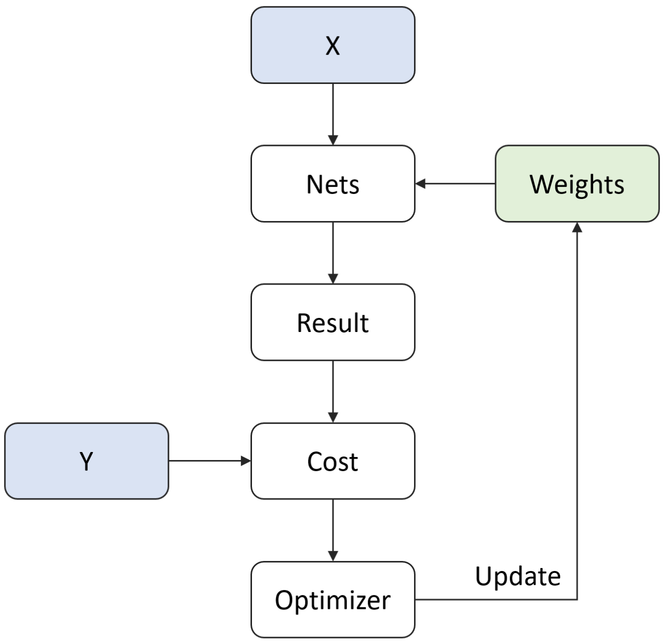


- our network model



$$
\begin{aligned}
\min_{\theta} \quad & f(\theta) \\
\text{subject to} \quad & g_i(\theta) \leq 0
\end{aligned}
$$

$$
\theta := \theta - \alpha \nabla_\theta \left(h_\theta \left(x^{(i)} \right), y^{(i)} \right)
$$



4.1. Import Library

In [11]:

```
# Import Library
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
```

4.2. Load MNIST Data

- Download MNIST data from tensorflow tutorial example

In [12]:

```
from tensorflow.examples.tutorials.mnist import input_data
mnist = input_data.read_data_sets("MNIST_data/", one_hot=True)
```

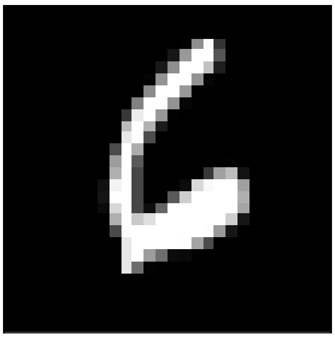
```
Extracting MNIST_data/train-images-idx3-ubyte.gz
Extracting MNIST_data/train-labels-idx1-ubyte.gz
Extracting MNIST_data/t10k-images-idx3-ubyte.gz
Extracting MNIST_data/t10k-labels-idx1-ubyte.gz
```

In [13]:

```
train_x, train_y = mnist.train.next_batch(10)
img = train_x[3,:].reshape(28,28)

plt.figure(figsize=(5,3))
plt.imshow(img,'gray')
plt.title("Label : {}".format(np.argmax(train_y[3])))
plt.xticks([])
plt.yticks([])
plt.show()
```

Label : 6



One hot encoding

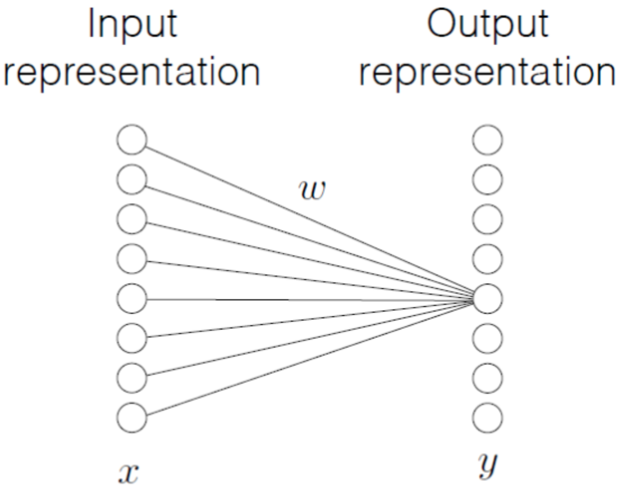
In [14]:

```
print ('Train labels : {}'.format(train_y[3, :]))
```

```
Train labels : [ 0.  0.  0.  0.  0.  0.  1.  0.  0.  0.]
```

4.3. Build a Model

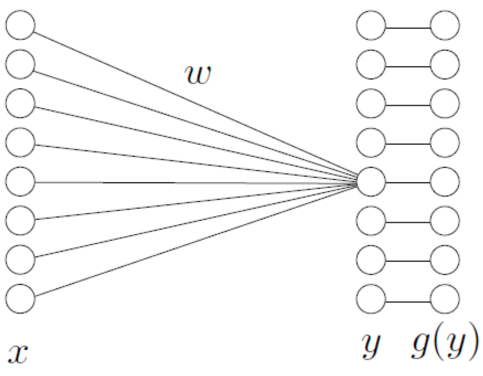
First, the layer performs several matrix multiplication to produce a set of linear activations

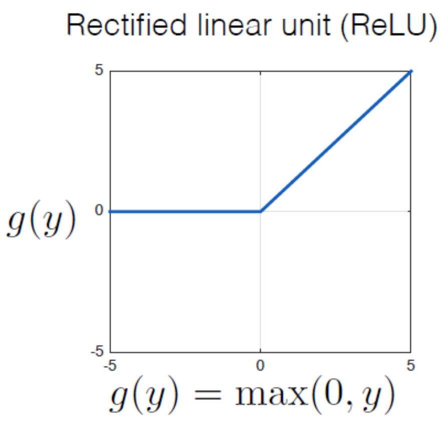


$$y_j = \left(\sum_i \omega_{ij} x_i\right) + b_j$$
$$y = \omega^T x + b$$

```
# hidden1 = tf.matmul(x, weights['hidden1']) + biases['hidden1']
hidden1 = tf.add(tf.matmul(x, weights['hidden1']), biases['hidden1'])
```

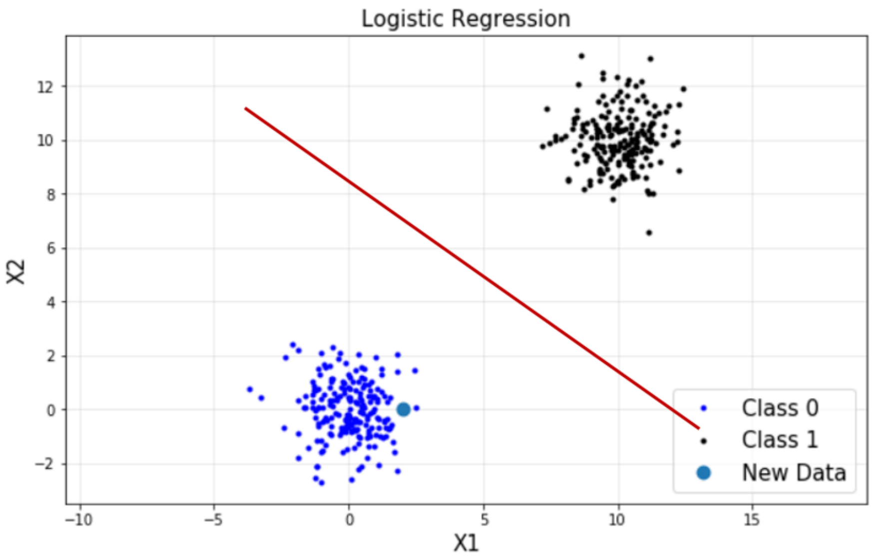
Second, each linear activation is running through a nonlinear activation function






```
hidden1 = tf.nn.relu(hidden1)
```

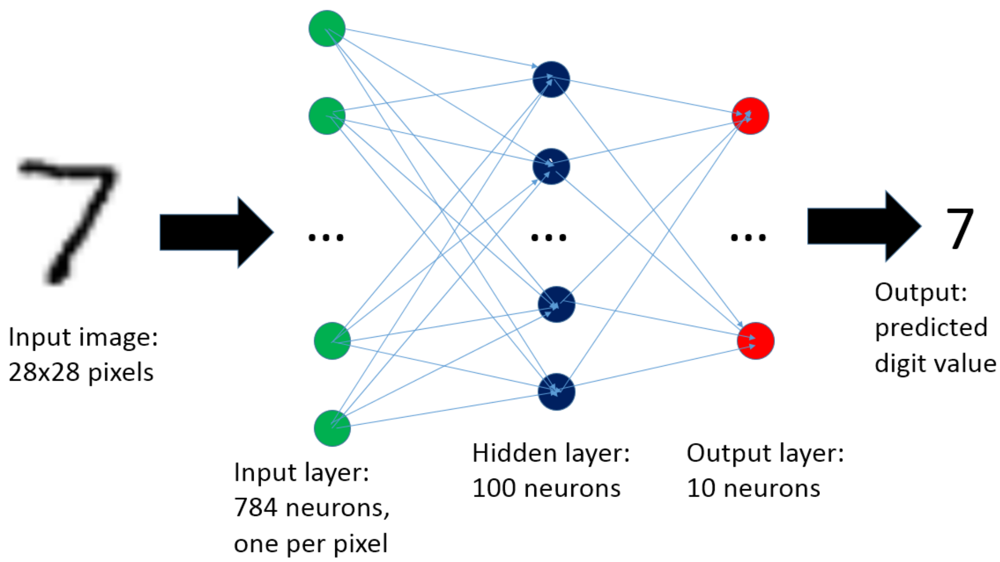
Third, predict values with an affine transformation




```
# output = tf.matmul(hidden1, weights['output']) + biases['output']
output = tf.add(tf.matmul(hidden1, weights['output']), biases['output'])
```

4.4. Define the ANN's Shape

- Input size
- Hidden layer size
- The number of classes



In [15]:

```
n_input = 28*28
n_hidden1 = 100
n_output = 10
```

4.5. Define Weights, Biases and Network

- Define parameters based on predefined layer size
- Initialize with normal distribution with $\mu = 0$ and $\sigma = 0.1$

In [16]:

```
weights = {
    'hidden1' : tf.Variable(tf.random_normal([n_input, n_hidden1], stddev = 0.1)),
    'output' : tf.Variable(tf.random_normal([n_hidden1, n_output], stddev = 0.1)),
}

biases = {
    'hidden1' : tf.Variable(tf.random_normal([n_hidden1], stddev = 0.1)),
    'output' : tf.Variable(tf.random_normal([n_output], stddev = 0.1)),
}

x = tf.placeholder(tf.float32, [None, n_input])
y = tf.placeholder(tf.float32, [None, n_output])
```

In [17]:

```
# Define Network
def build_model(x, weights, biases):
    # first hidden layer
    hidden1 = tf.add(tf.matmul(x, weights['hidden1']), biases['hidden1'])
    # non linear activate function
    hidden1 = tf.nn.relu(hidden1)

    # Output layer with linear activation
    output = tf.add(tf.matmul(hidden1, weights['output']), biases['output'])
    return output
```

4.6. Define Cost, Initializer and Optimizer

Loss

- Classification: Cross entropy
  - Equivalent to apply logistic regression

$$-\frac{1}{N}\sum_{i=1}^{N} y^{(i)} \log(h_\theta\left(x^{(i)}\right)) + (1-y^{(i)}) \log(1-h_\theta\left(x^{(i)}\right))$$

Initializer

- Initialize all the empty variables

Optimizer

- AdamOptimizer: the most popular optimizer

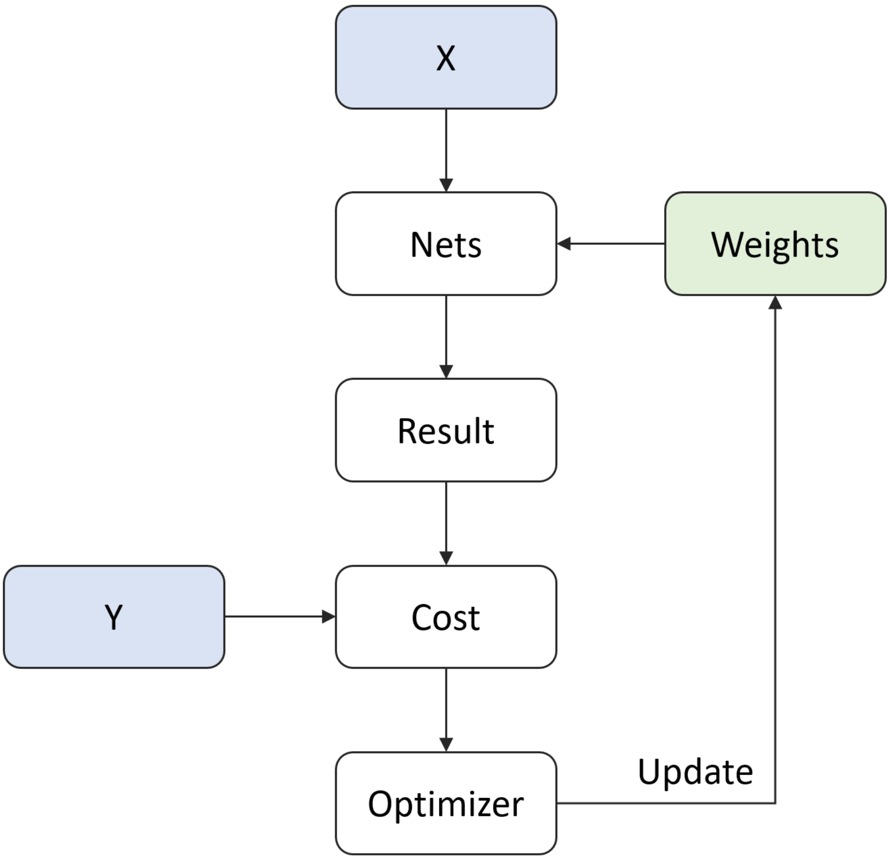
In [18]:

```
# Define Cost
pred = build_model(x, weights, biases)
loss = tf.nn.softmax_cross_entropy_with_logits(logits=pred, labels=y)
loss = tf.reduce_mean(loss)

# optimizer = tf.train.GradientDescentOptimizer(learning_rate).minimize(cost)
LR = 0.0001
optm = tf.train.AdamOptimizer(LR).minimize(loss)

init = tf.global_variables_initializer()
```

4.7. Summary of Model



4.8. Define Configuration

- Define parameters for training ANN
  - `n_batch`: batch size for stochastic gradient descent
  - `n_iter`: the number of learning steps
  - `n_prt`: check loss for every `n_prt` iteration

In [19]:

```
n_batch = 50     # Batch Size
n_iter = 2500    # Learning Iteration
n_prt = 250      # Print Cycle
```

4.9. Optimization

In [20]:

```
# Run initialize
# config = tf.ConfigProto(allow_soft_placement=True)  # GPU Allocating policy
# sess = tf.Session(config=config)
sess = tf.Session()
sess.run(init)

# Training cycle
for epoch in range(n_iter):
    train_x, train_y = mnist.train.next_batch(n_batch)
    sess.run(optm, feed_dict={x: train_x,  y: train_y})

    if epoch % n_prt == 0:
        c = sess.run(loss, feed_dict={x : train_x,  y : train_y})
        print ("Iter : {}".format(epoch))
        print ("Cost : {}".format(c))
```

```
Iter : 0
Cost : 2.49772047996521
Iter : 250
Cost : 1.4581751823425293
Iter : 500
Cost : 0.7719646692276001
Iter : 750
Cost : 0.5604625344276428
Iter : 1000
Cost : 0.4211314022541046
Iter : 1250
Cost : 0.5066109299659729
Iter : 1500
Cost : 0.32460322976112366
Iter : 1750
Cost : 0.412553608417511
Iter : 2000
Cost : 0.26275649666786194
Iter : 2250
Cost : 0.481355220079422
```

4.10. Test

In [21]:

```
test_x, test_y = mnist.test.next_batch(100)

my_pred = sess.run(pred, feed_dict={x : test_x})
my_pred = np.argmax(my_pred, axis=1)

labels = np.argmax(test_y, axis=1)

accr = np.mean(np.equal(my_pred, labels))
print("Accuracy : {}%".format(accr*100))
```

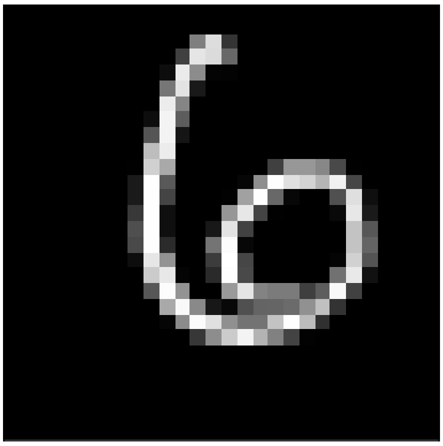
```
Accuracy : 96.0%
```

In [22]:

```
test_x, test_y = mnist.test.next_batch(1)
logits = sess.run(tf.nn.softmax(pred), feed_dict={x : test_x})
predict = np.argmax(logits)

plt.imshow(test_x.reshape(28,28), 'gray')
plt.xticks([])
plt.yticks([])
plt.show()

print('Prediction : {}'.format(predict))
np.set_printoptions(precision=2, suppress=True)
print('Probability : {}'.format(logits.ravel()))
```



```
Prediction : 6
Probability : [ 0.01  0.01  0.07  0.    0.01  0.01  0.89  0.    0.01  0.  
]
```

In [23]:

```
%%javascript
$.getScript('https://kmahelona.github.io/ipython_notebook_goodies/ipython_notebook_toc.
js')
```