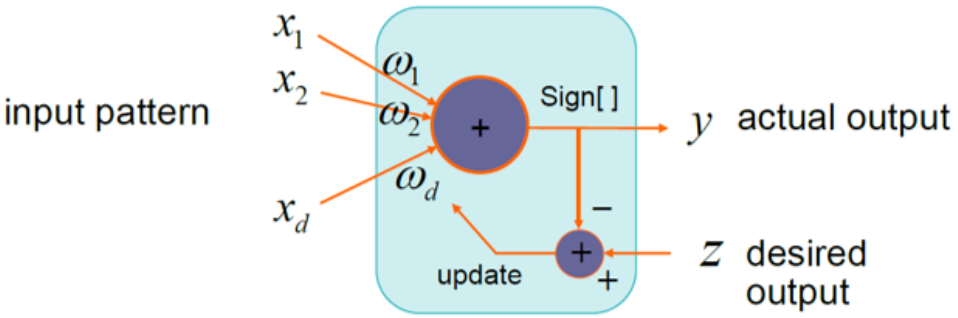
(Artificial) Neural Networks in TensorFlow

By Prof. Seungchul Lee
Industrial AI Lab
http://isystems.unist.ac.kr/
POSTECH

Table of Contents

1. Recall Supervised Learning Setup

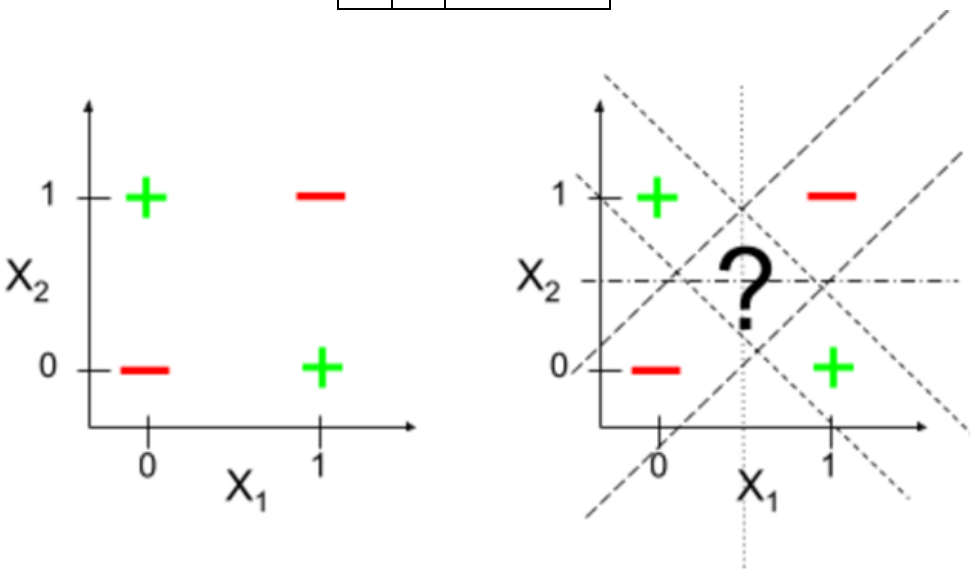
Perceptron



XOR Problem

- Minsky-Papert Controversy on XOR
  - not linearly separable
  - limitation of perceptron

x_1	x_2	x_1 **XOR** x_2
0	0	0
0	1	1
1	0	1
1	1	0

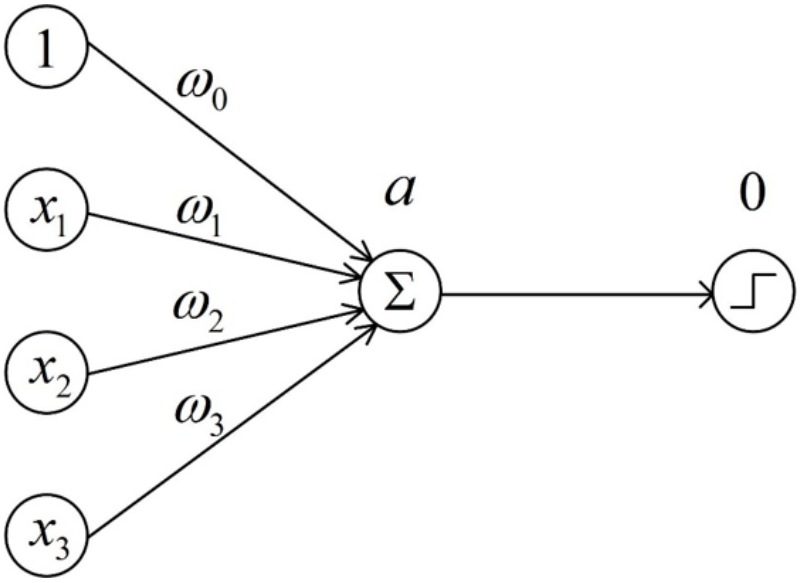


2. Artificial Neural Networks

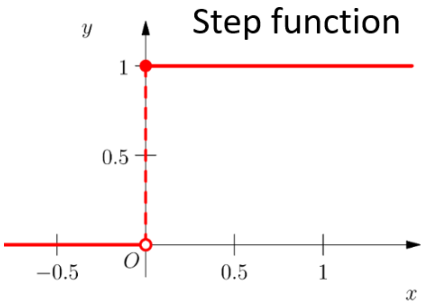
2.1. Perceptron for $h(\theta)$ or $h(\omega)$

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

$$a = \omega_0 + \omega_1 x_1 + \cdots$$
$$o = \sigma(\omega_0 + \omega_1 x_1 + \cdots)$$



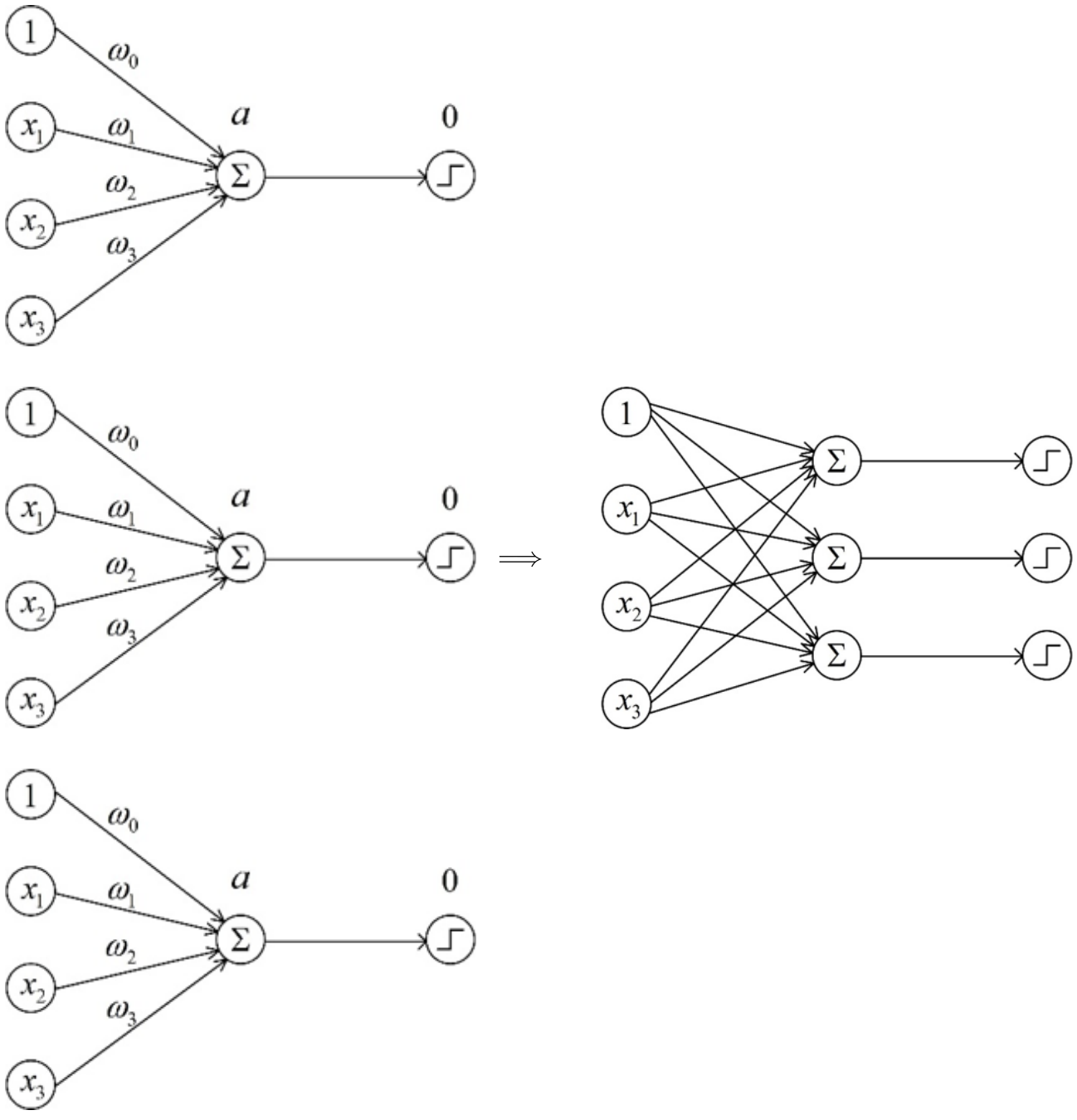
- A step function is not differentiable



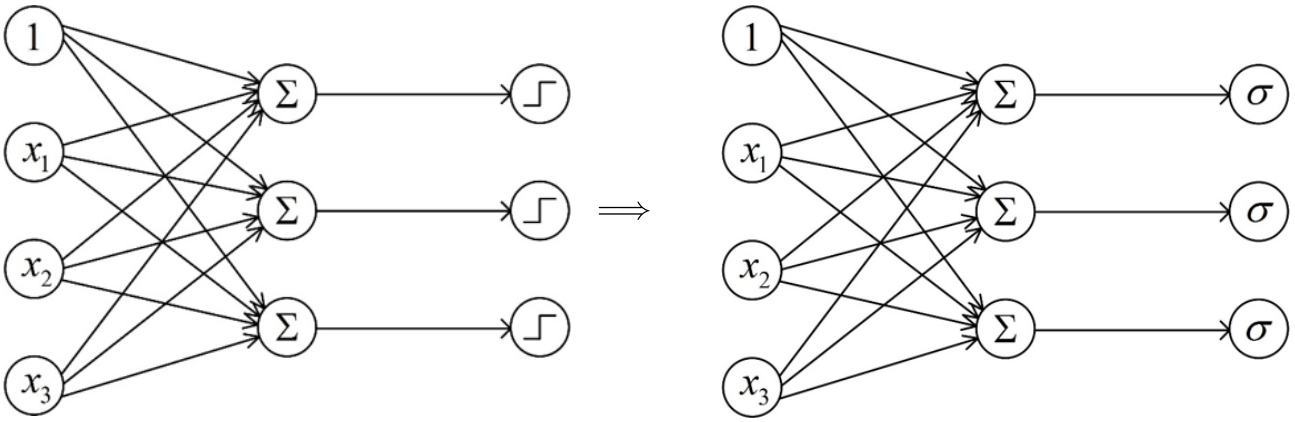
- One layer is often not enough

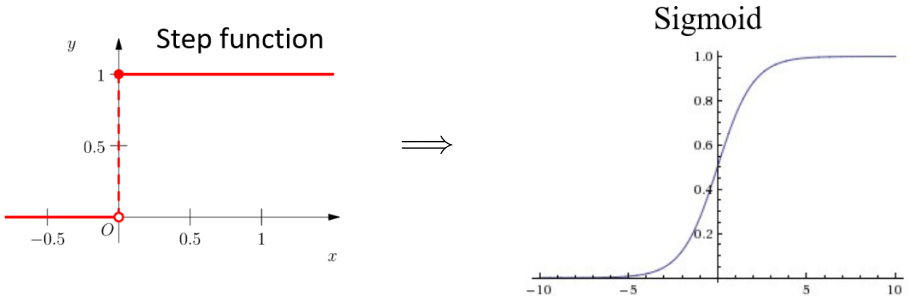
2.2. Multi-layer Perceptron = Artificial Neural Networks (ANN)

multi-neurons

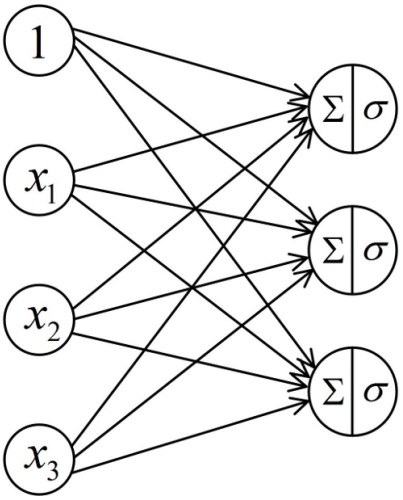


differentiable activation function

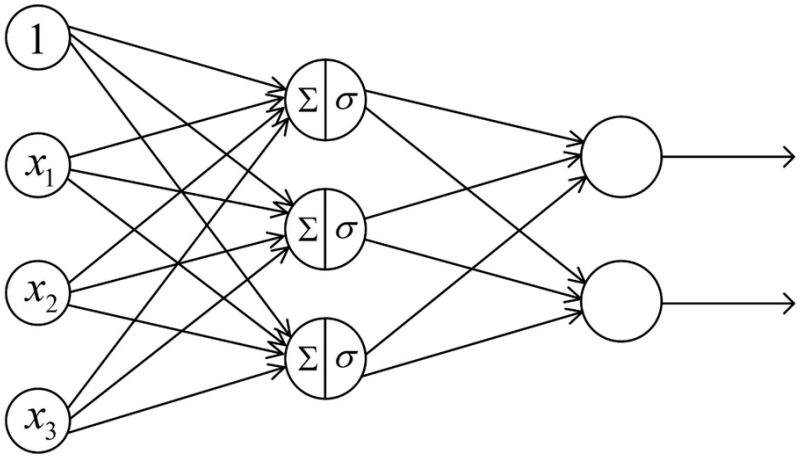




in a compact representation



multi-layer perceptron



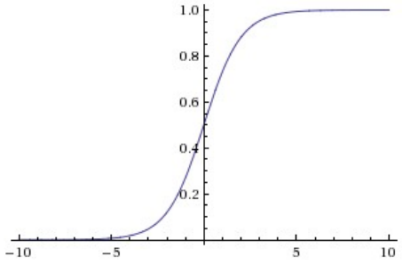
Transformation

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

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

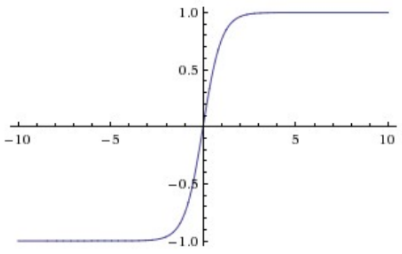
- Nonlinear activation functions ($g = \sigma$)

Sigmoid



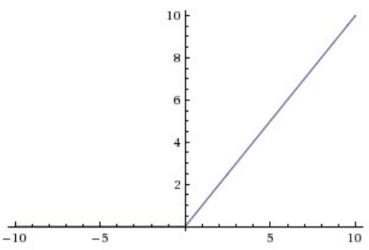
$$g(x) = \frac{1}{1 + e^{-x}}$$

tanh



$$g(x) = \tanh(x)$$

Rectified Linear Unit



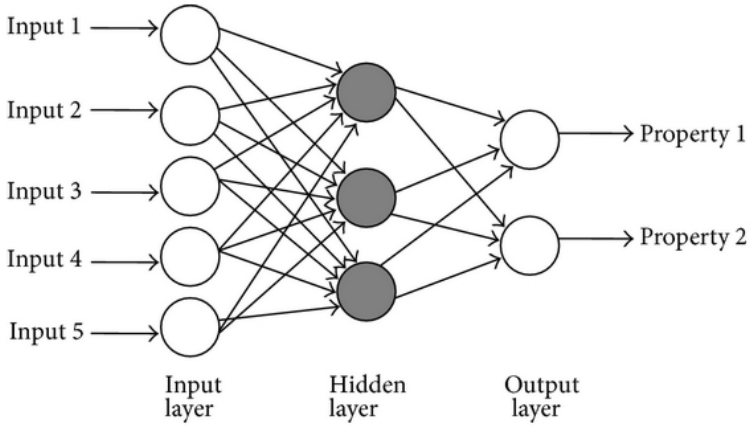
$$g(x) = \max(0, x)$$

Structure

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

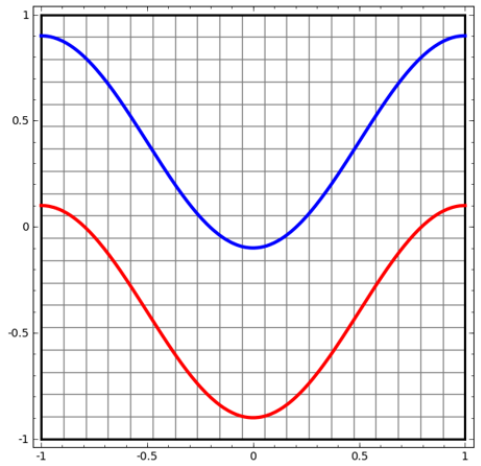
$\Longrightarrow$ perceptrons with many layers and units

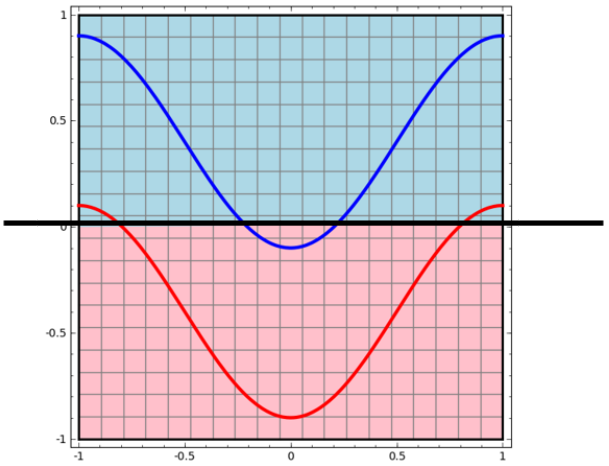
$$o_2 = \sigma_2\left(\theta_2^T o_1 + b_2\right) = \sigma_2\left(\theta_2^T \sigma_1\left(\theta_1^T x + b_1\right) + b_2\right)$$



Linear Classifier

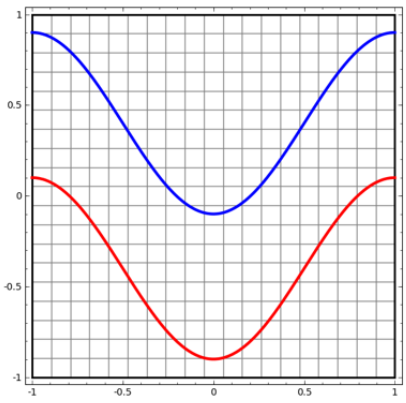
- Perceptron tries to separate the two classes of data by dividing them with a line

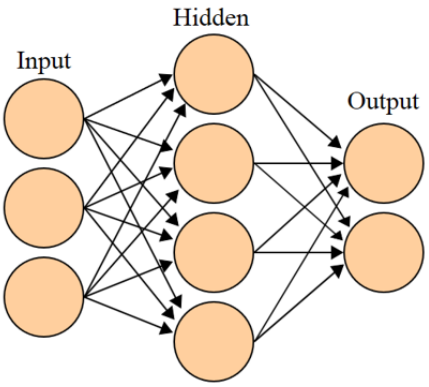


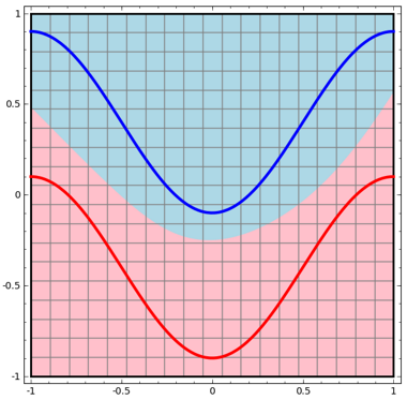


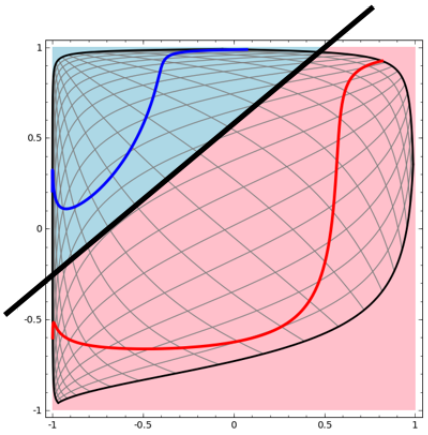
Neural Networks

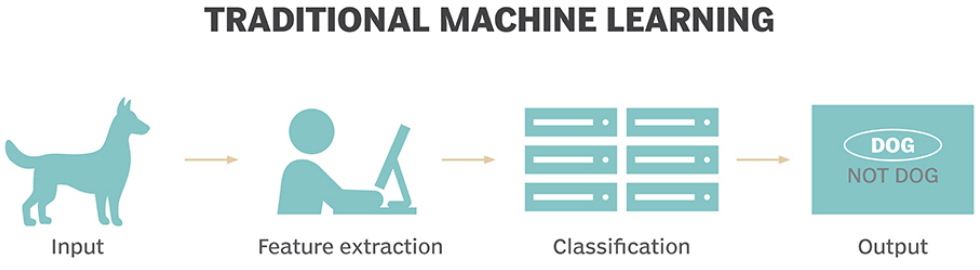
- The hidden layer learns a representation so that the data is linearly separable

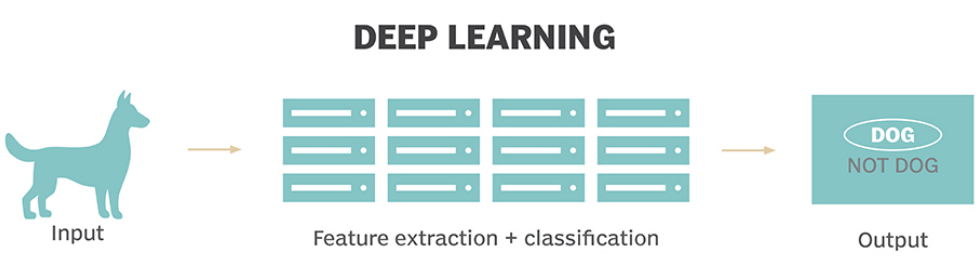












3. Training Neural Networks

$=$ 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

$$\begin{aligned} \min_{\theta} \quad & f(\theta) \\ \text{subject to} \quad & g_i(\theta) \leq 0, \qquad i = 1, \cdots, m \end{aligned}$$

3.2. Loss Function

- Measures error between target values and predictions

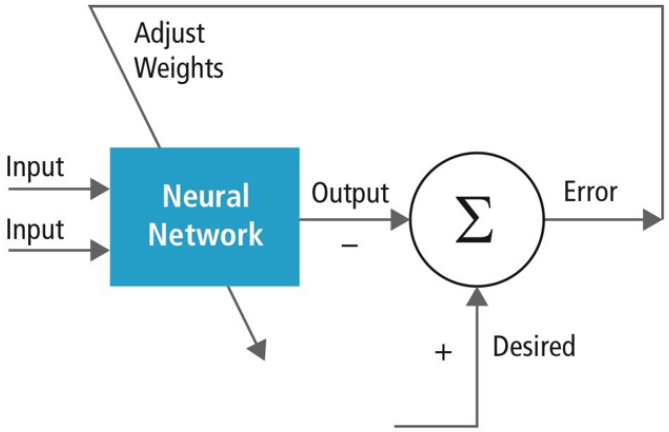
$$\min_{\theta} \sum_{i=1}^{m} \ell \left(h_\theta \left(x^{(i)} \right), y^{(i)} \right)$$

- Example
  - Squared loss (for regression):

$$\frac{1}{N} \sum_{i=1}^{N} \left(h_\theta \left(x^{(i)} \right) - y^{(i)} \right)^2$$

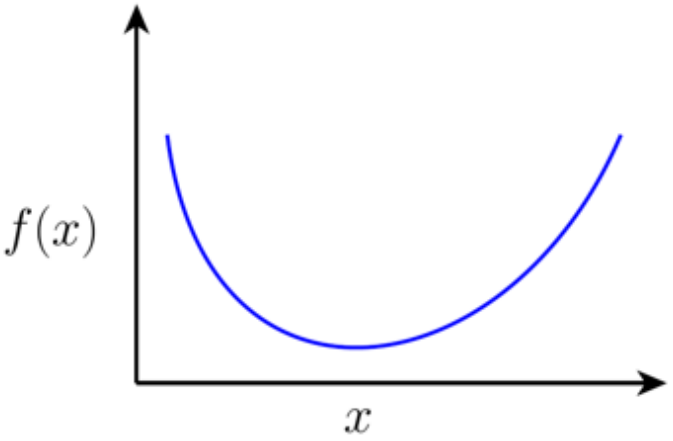
  - Cross entropy (for classification):

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



Solving Optimization Problems

- Starting with the unconstrained, one dimensional case



  - To find minimum point x^*, we can look at the derivative of the function $f'(x)$: any location where $f'(x) = 0$ will be a “flat” point in the function

- For convex problems, this is guaranteed to be a minimum

- Generalization for multivariate function $f : \mathbb{R}^n \rightarrow \mathbb{R}$
  - the gradient of f must be zero

$$\nabla_x f(x) = 0$$

- For defined as above, gradient is a n-dimensional vector containing partial derivatives with respect to each dimension

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

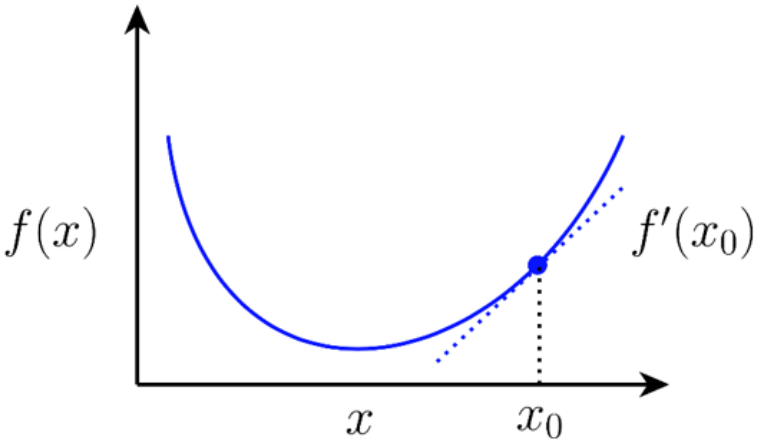
- For continuously differentiable f and unconstrained optimization, optimal point must have $\nabla_x f(x^*) = 0$

How do we Find $\nabla_x f(x) = 0$

- Direct solution
  - In some cases, it is possible to analytically compute x^* such that $\nabla_x f(x^*) = 0$

$$
\begin{aligned}
f(x) &= 2x_1^2 + x_2^2 + x_1 x_2 - 6x_1 - 5x_2 \\
\implies \nabla_x f(x) &= \begin{bmatrix} 4x_1 + x_2 + 6 \\ 2x_2 + x_1 + 5 \end{bmatrix} \\
\implies x^\star &= \begin{bmatrix} 4 & 1 \\ 1 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}
\end{aligned}
$$

- Iterative methods
  - More commonly the condition that the gradient equal zero will not have an analytical solution, require iterative methods

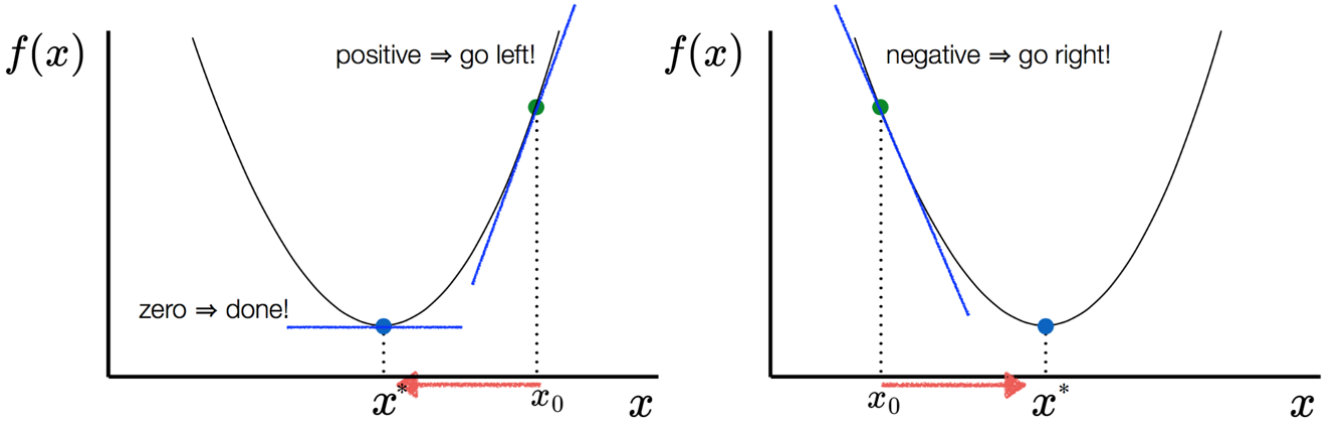


- The gradient points in the direction of "steepest ascent" for function f

Decent Direction (1D)

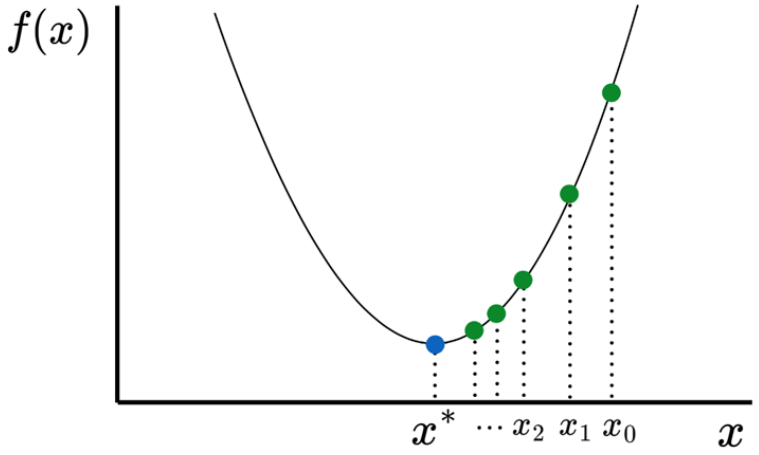
- It motivates the gradient descent algorithm, which repeatedly takes steps in the direction of the negative gradient

$$
x \leftarrow x - \alpha \nabla_x f(x) \qquad \text{for some step size } \alpha > 0
$$



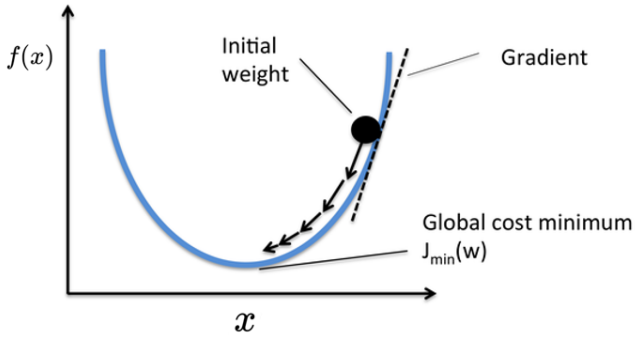
- Gradient Descent

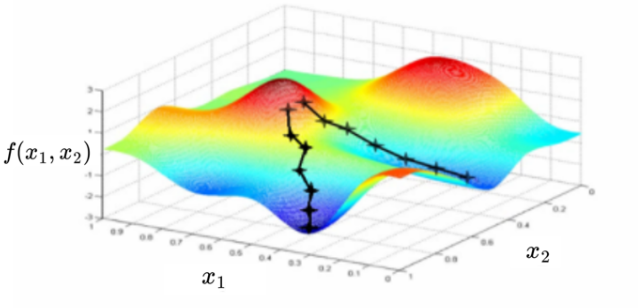
$$\text{Repeat}: x \leftarrow x - \alpha \nabla_x f(x) \qquad \text{for some step size } \alpha > 0$$



- Gradient Descent in High Dimension

$$\text{Repeat}: x \leftarrow x - \alpha \nabla_x f(x)$$





- Gradient Descent Example

$$\min \quad (x_1 - 3)^2 + (x_2 - 3)^2$$

$$= \min \quad \frac{1}{2}[x_1 \quad x_2]\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - [6 \quad 6]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + 18$$

- Update rule

$$X_{i+1} = X_i - \alpha_i \nabla f(X_i)$$

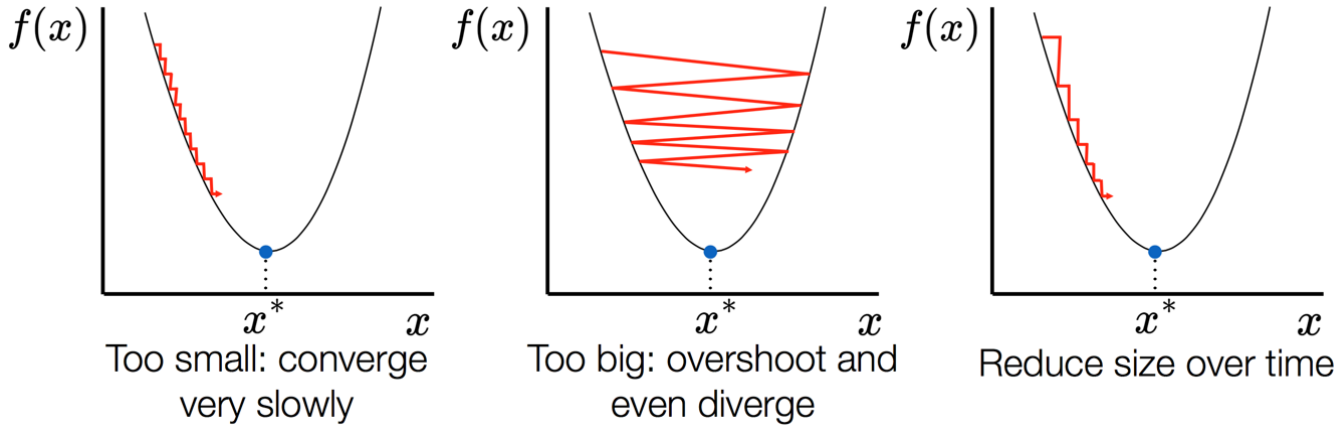
In [1]:
```
import numpy as np
```

In [2]:
```
H = np.array([[2, 0],[0, 2]])
f = -np.array([[6],[6]])

x =  np.zeros((2,1))
alpha = 0.2

for i in range(25):
    g = H.dot(x) + f
    x = x - alpha*g

print(x)
```

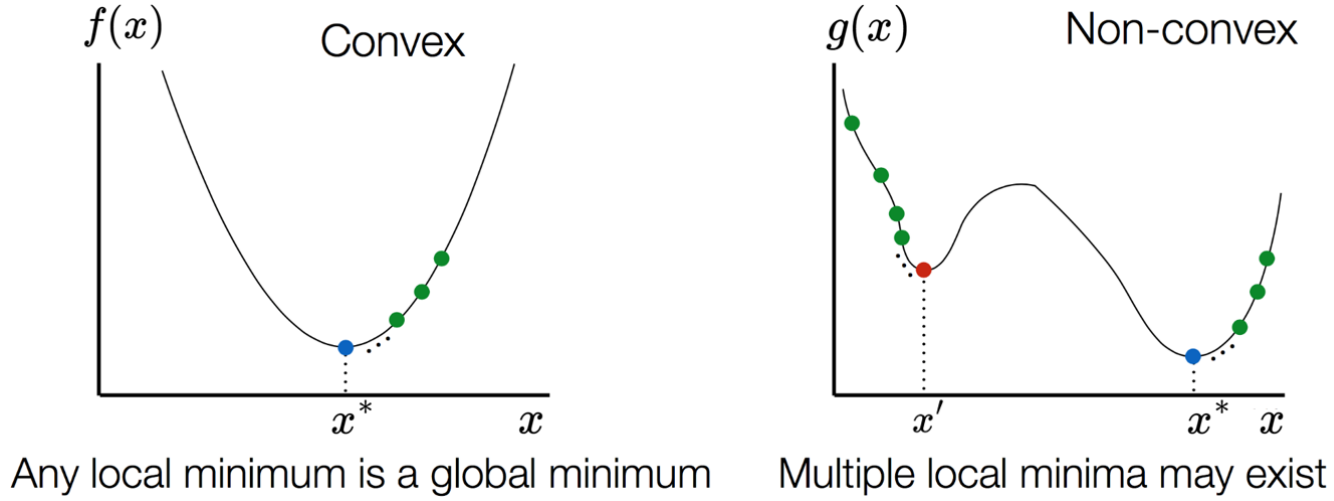
```
[[2.99999147]
 [2.99999147]]
```

Choosing Step Size α

- Learning rate



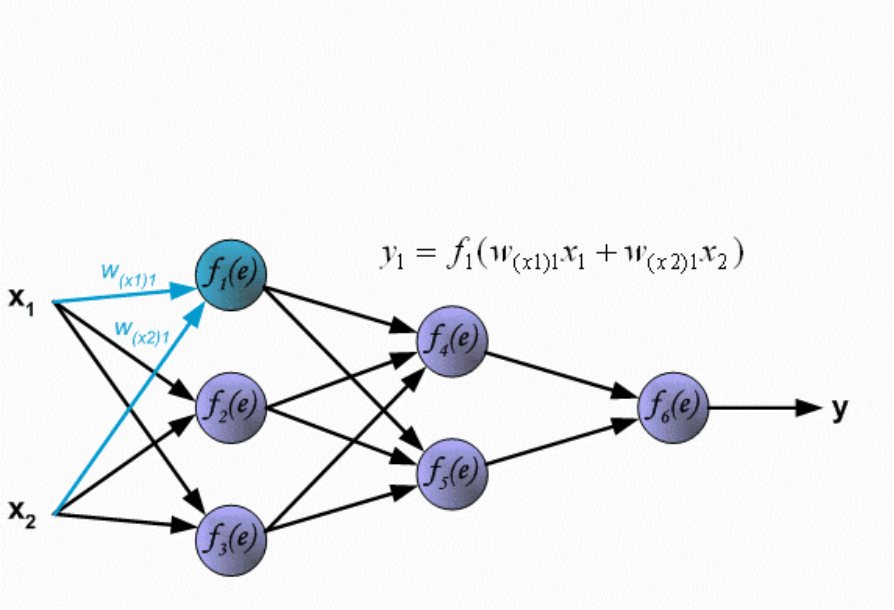
Where will We Converge?



3.3. Learning

Backpropagation

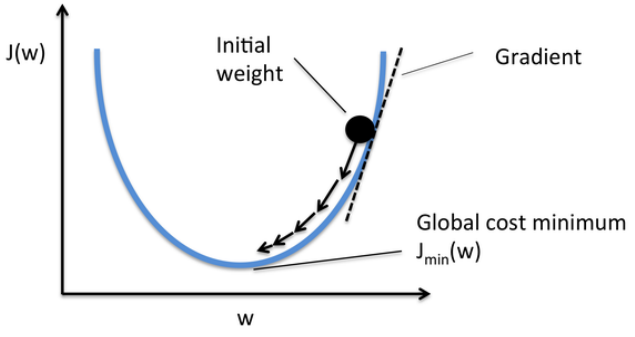
- Forward propagation
  - the initial information propagates up to the hidden units at each layer and finally produces output
- Backpropagation
  - allows the information from the cost to flow backwards through the network in order to compute the gradients

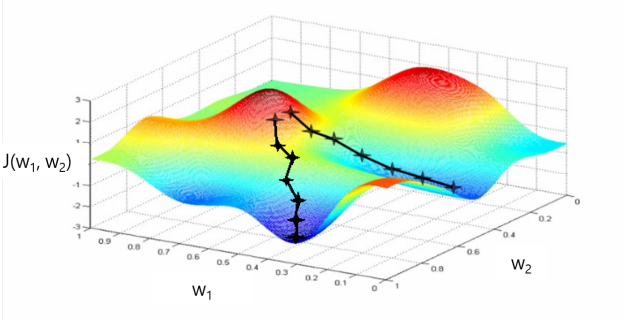


(Stochastic) Gradient Descent

- 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)

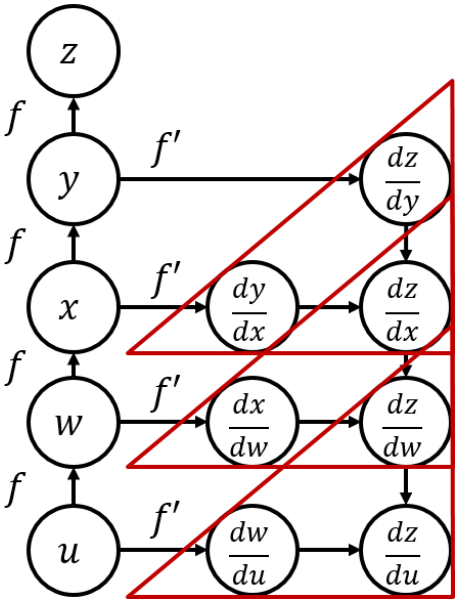
$$\theta := \theta - \alpha \nabla_\theta \left(h_\theta \left(x^{(i)} \right), y^{(i)} \right)$$





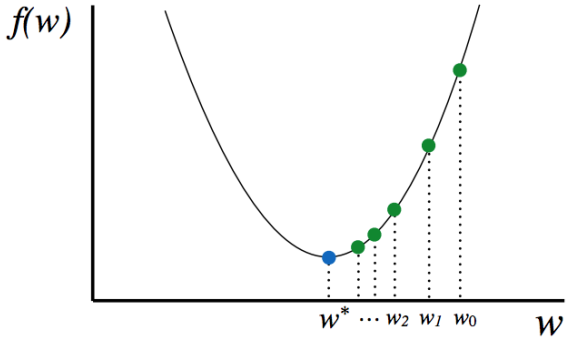
- Chain Rule
  - Computing the derivative of the composition of functions
    - $f(g(x))' = f'(g(x))g'(x)$
    - $\frac{dz}{dx} = \frac{dz}{dy} \bullet \frac{dy}{dx}$
    - $\frac{dz}{dw} = (\frac{dz}{dy} \bullet \frac{dy}{dx}) \bullet \frac{dx}{dw}$
    - $\frac{dz}{du} = (\frac{dz}{dy} \bullet \frac{dy}{dx}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

- Backpropagation
  - Update weights recursively



Optimization procedure

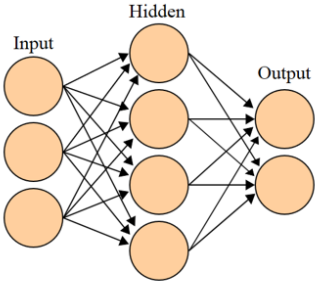
Start at a random point
Repeat
Determine a descent direction
Choose a step size
Update
Until stopping criterion is satisfied



- 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: $\mathrm{TensorFlow}$

Summary

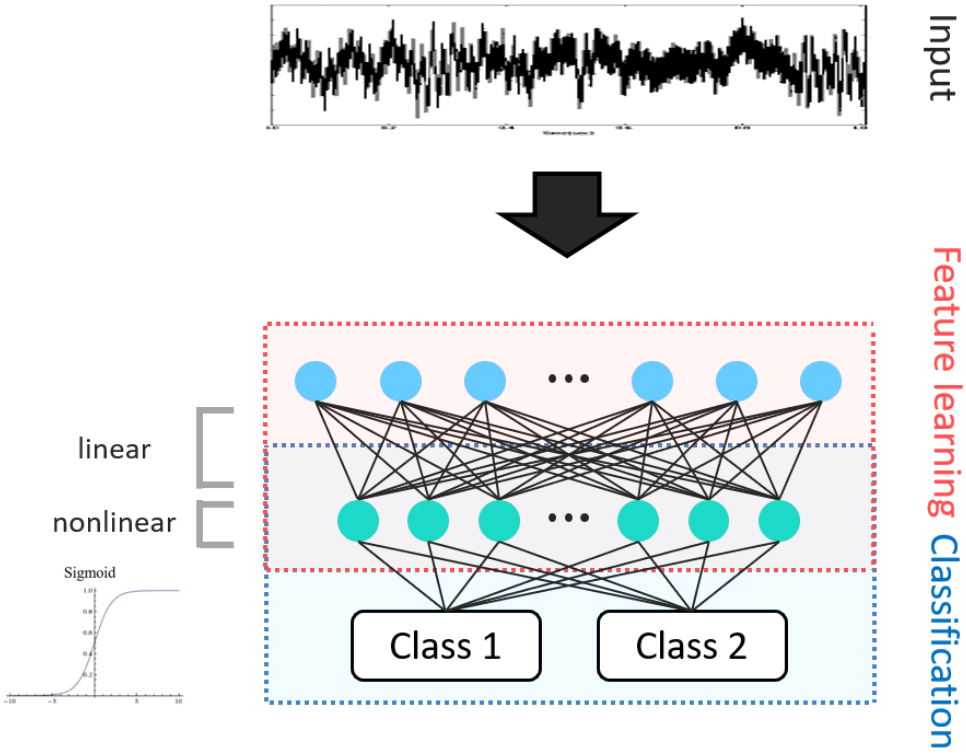
- Learning weights and biases from data using gradient descent



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

Artificial Neural Networks

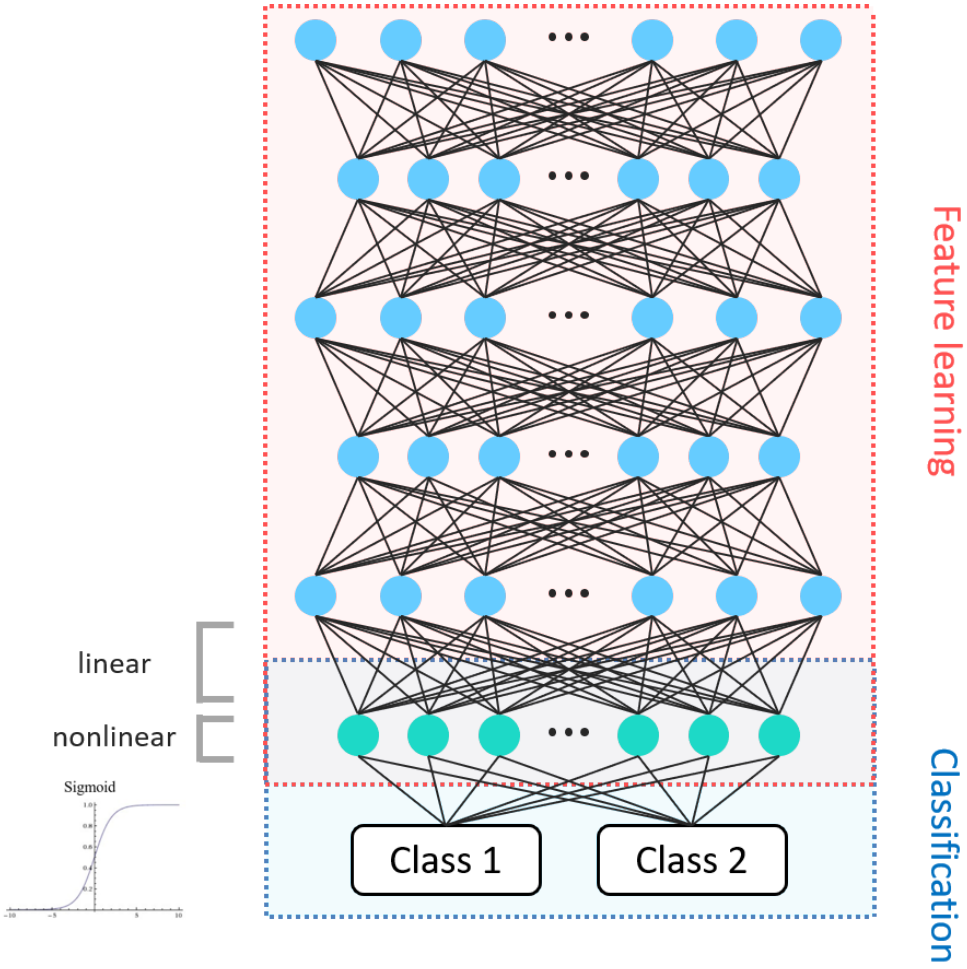
- Complex/Nonlinear function approximator
  - Linearly connected networks
  - Simple nonlinear neurons
- Hidden layers
  - Autonomous feature learning



Deep Artificial Neural Networks

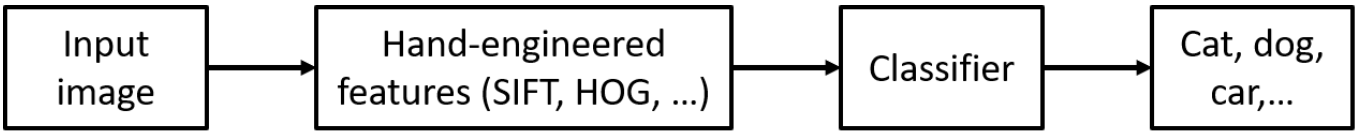
- Complex/Nonlinear function approximator
  - Linearly connected networks
  - Simple nonlinear neurons

- Hidden layers
  - Autonomous feature learning

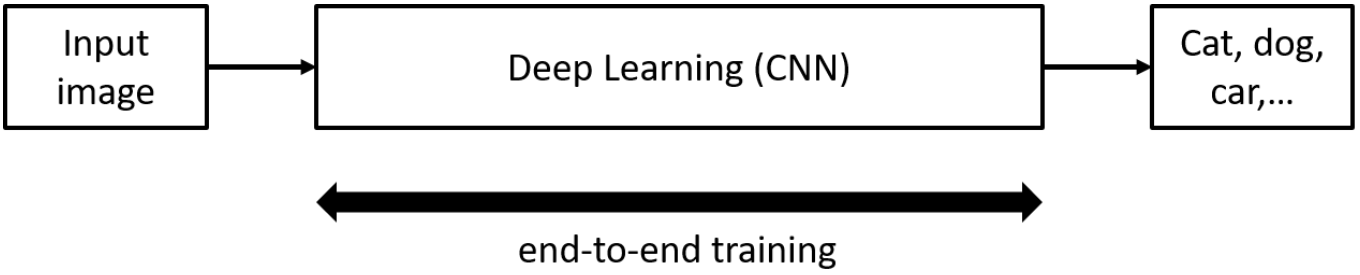


Machine Learning vs. Deep Learning

- State-of-the-art until 2012



- Deep supervised learning



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.

4.1. Computational Graph

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

In [3]:
```
import tensorflow as tf

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

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

```
C:\ProgramData\Anaconda3\lib\site-packages\h5py\__init__.py:34: FutureWarni
ng: Conversion of the second argument of issubdtype from `float` to `np.flo
ating` is deprecated. In future, it will be treated as `np.float64 == np.dt
ype(float).type`.
  from ._conv import register_converters as _register_converters
```

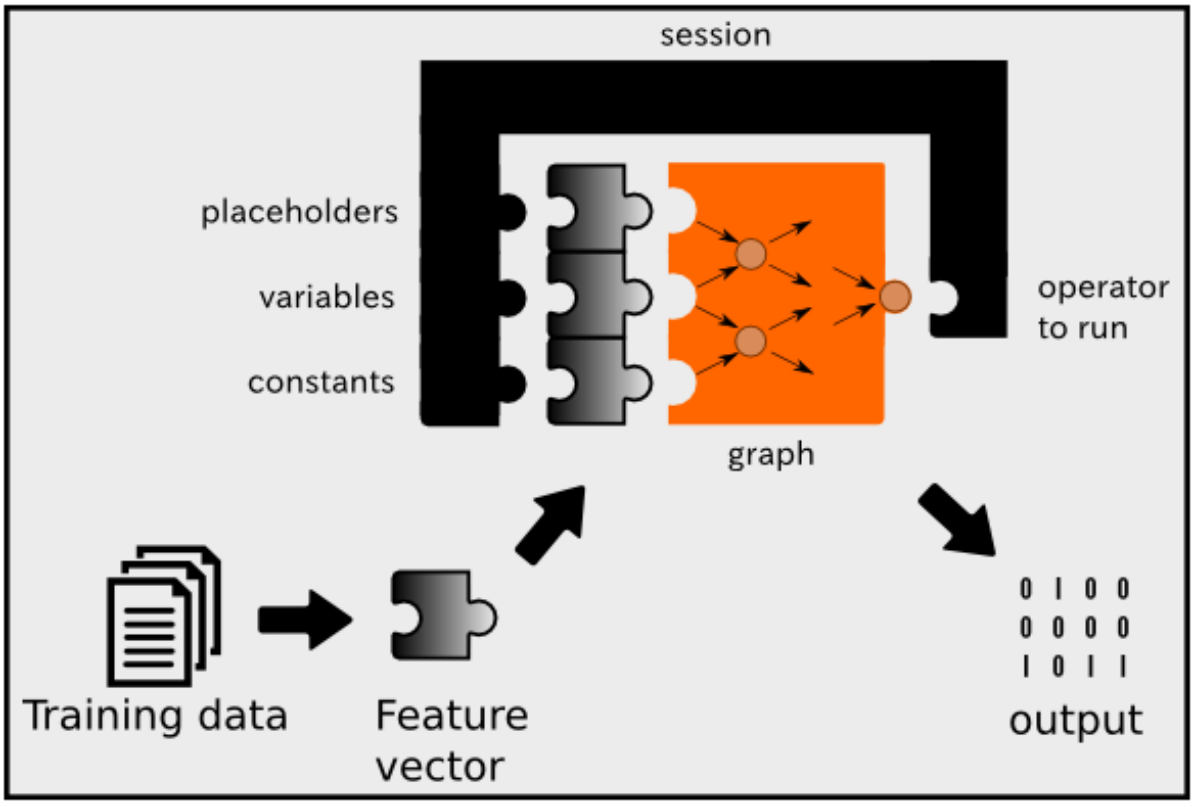
In [4]:
```
A
```

Out[4]:
```
<tf.Tensor 'add:0' shape=(3,) dtype=int32>
```

In [5]:
```
B
```

Out[5]:
```
<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 [6]:
```
sess = tf.Session()
sess.run(A)
```

Out[6]:
```
array([5, 7, 9])
```

In [7]:
```
sess.run(B)
```

Out[7]:
```
array([ 4, 10, 18])
```

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

```
In [8]: w = tf.Variable([1, 1])
```

```
In [9]: init = tf.global_variables_initializer()
        sess.run(init)
```

```
In [10]: sess.run(w)
```

```
Out[10]: array([1, 1])
```

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

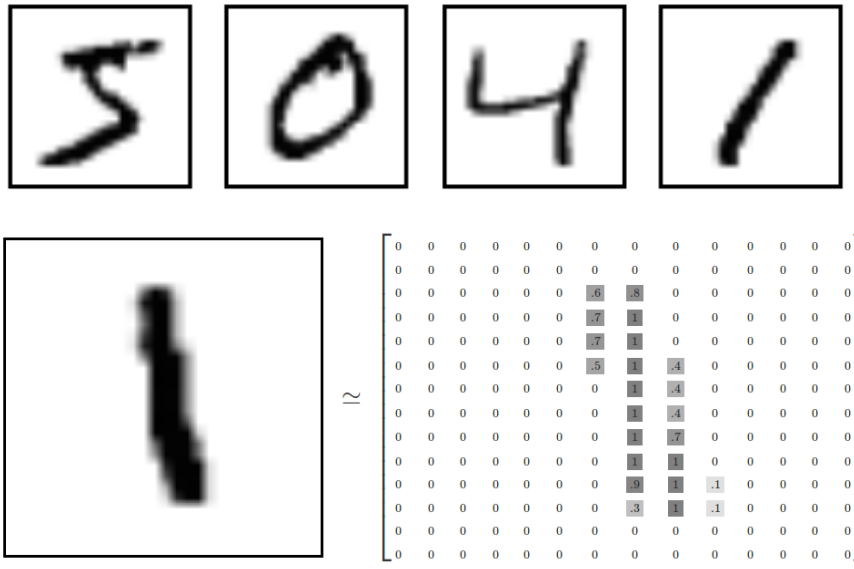
```
In [11]: x = tf.placeholder(tf.float32, [2, 2])
```

```
In [12]: sess.run(x, feed_dict={x : [[1,2],[3,4]]})
```

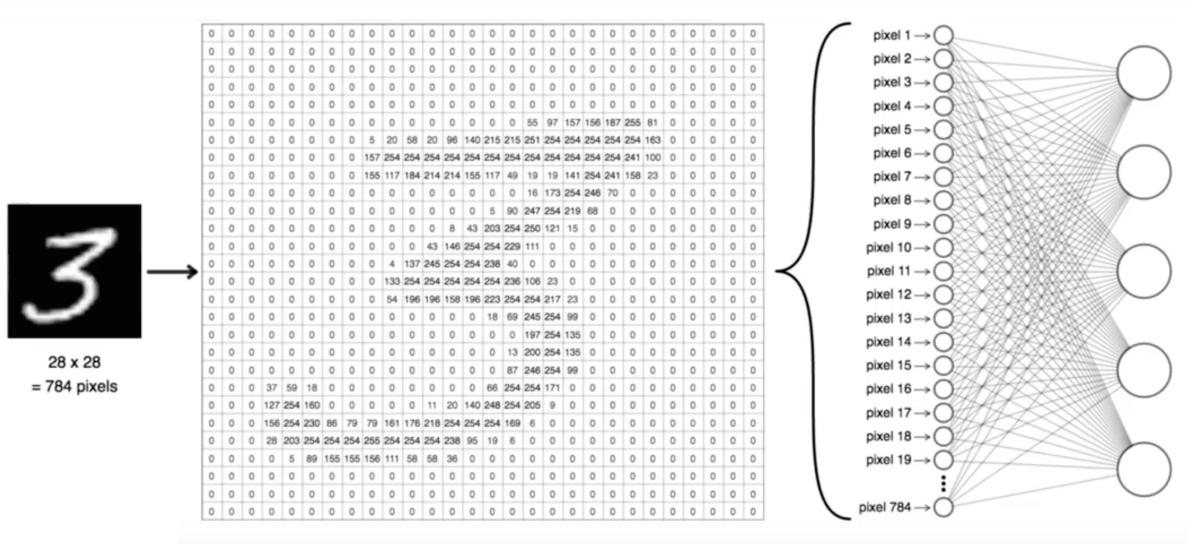
```
Out[12]: array([[1., 2.],
                [3., 4.]], dtype=float32)
```

7. ANN with TensorFlow

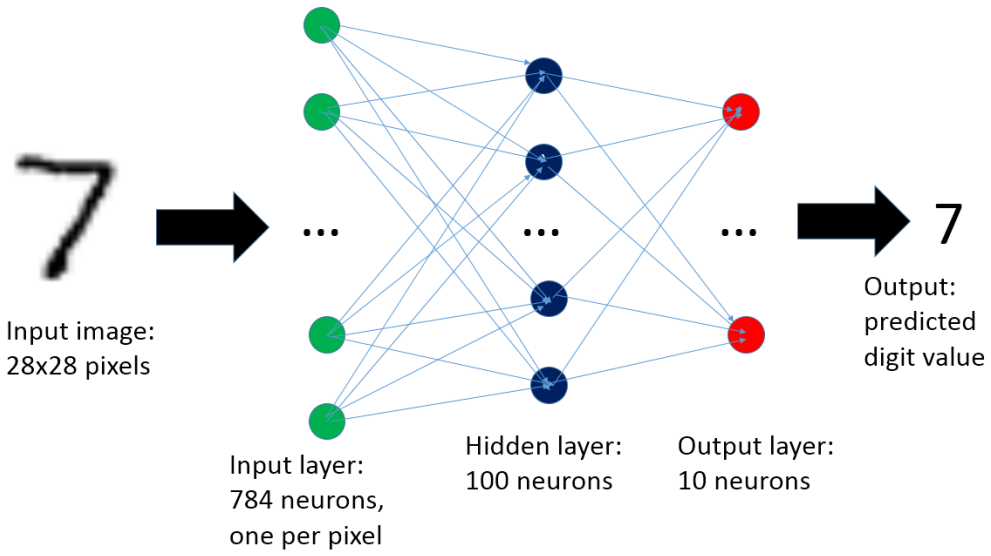
- MNIST (Mixed National Institute of Standards and Technology database) database
  - Handwritten digit database
  - 28×28 gray scaled image
  - Flattened matrix into a vector of $28 \times 28 = 784$



- feed a gray image to ANN

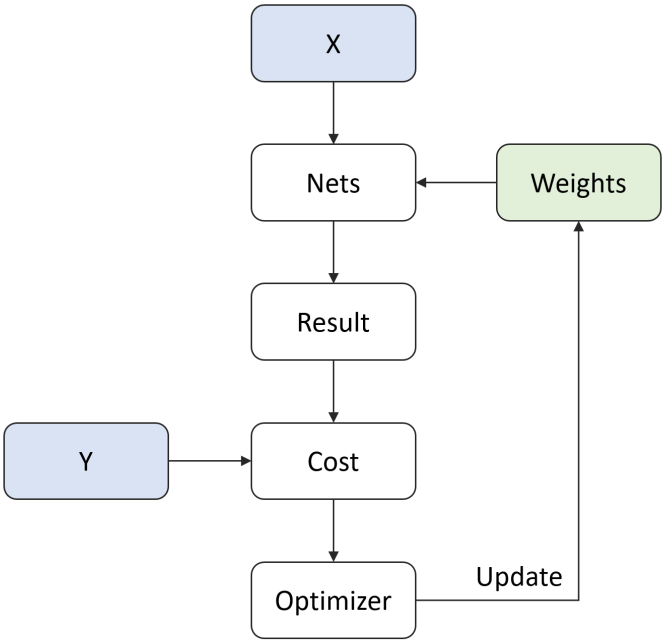


- our network model



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

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



Mini-batch Gradient Descent

① Linear Regression Cost function $J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (\hat{y}^i - y^i)^2$

m training data

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (\hat{y}^i - y^i) \cdot x_j^i$$

② Vanilla (Batch) G.D.

$$\theta_j := \theta_j - \alpha \cdot \frac{\partial}{\partial \theta_j} J(\theta)$$

$$\frac{1}{m} \sum_{i=1}^{m} (\hat{y}^i - y^i) x_j^i$$

③ Stochastic G.D.

```
for i in range(m):
    θj := θj − α · (ŷ^i − y^i) x_j^i   # only one example
```

4.1. Import Library

In [13]:
```
# Import Library
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
```

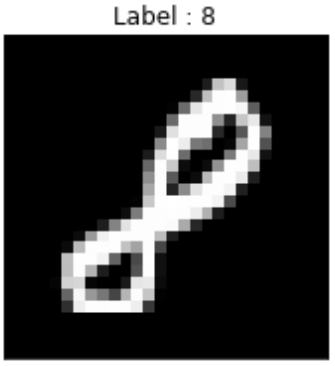
4.2. Load MNIST Data

- Download MNIST data from tensorflow tutorial example

In [14]:
```
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 [15]:
```
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()
```



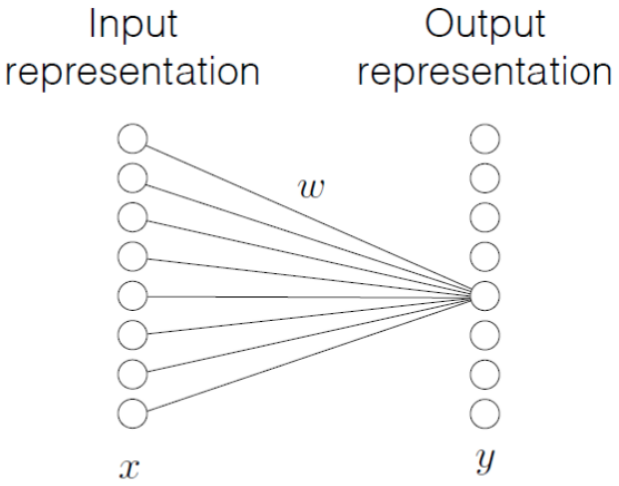
One hot encoding

In [16]:
```
print ('Train labels : {}'.format(train_y[3, :]))
```

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

4.3. Build a Model

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

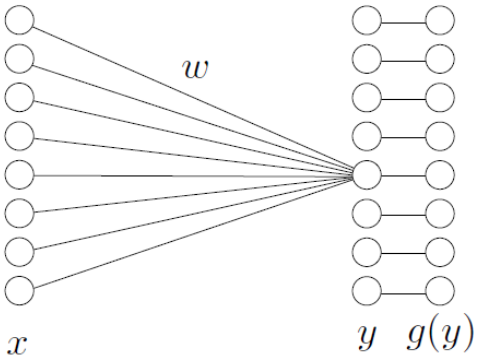


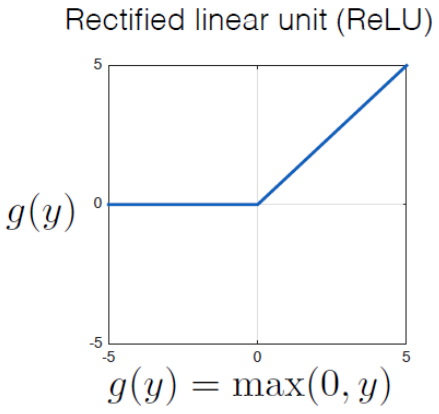
$$y_j = \left(\sum_i \omega_{ij} x_i \right) + b_j$$

$$y = \omega^T x + b$$

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

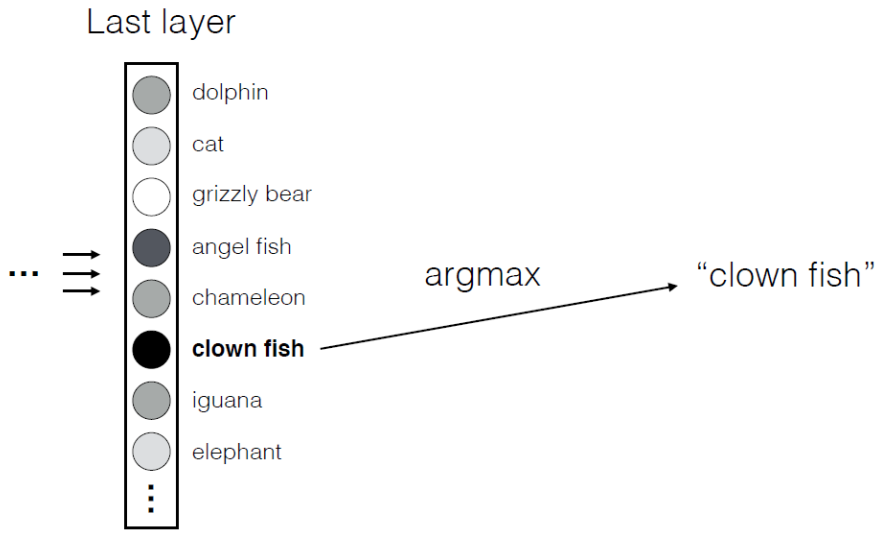
Second, each linear activation is running through a nonlinear activation function






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

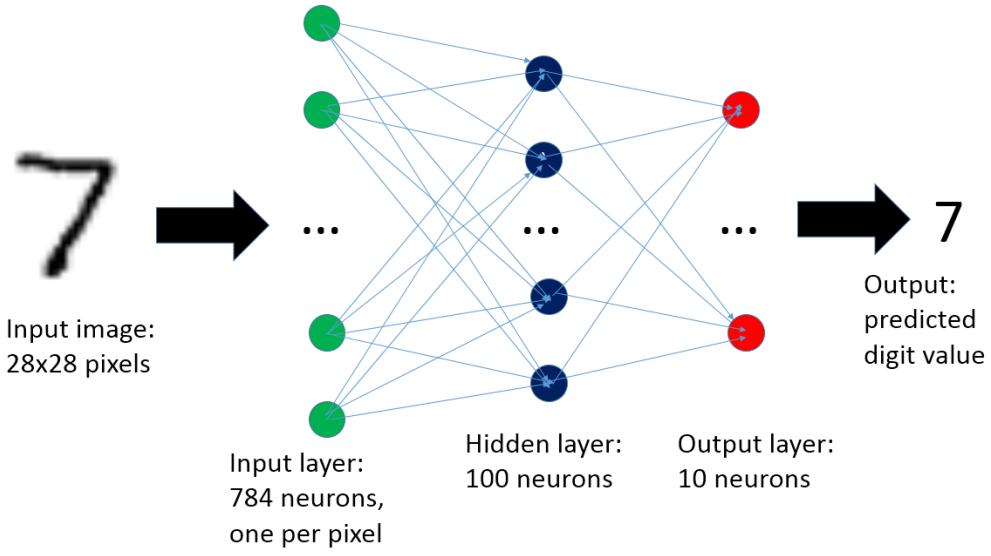
Third, predict values with an affine transformation




```
# 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 [17]:
```
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 [18]:
```
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 [19]:
```
# 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

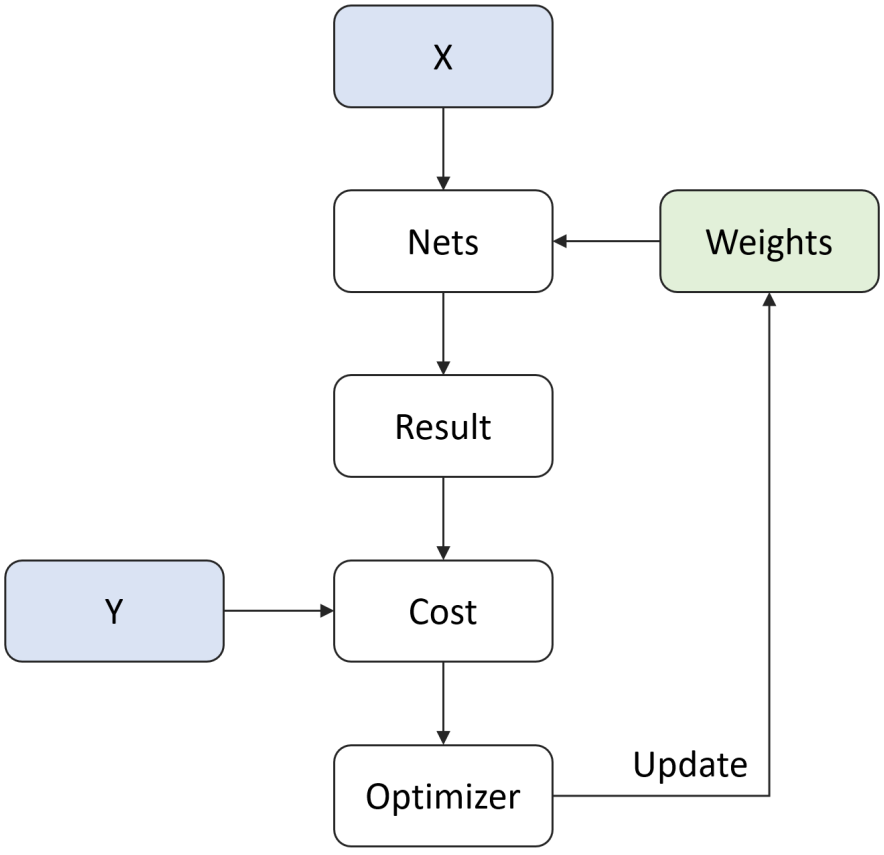
Optimizer

- AdamOptimizer: the most popular optimizer

In [20]:
```
# 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(cos
t)
LR = 0.0001
optm = tf.train.AdamOptimizer(LR).minimize(loss)

init = tf.global_variables_initializer()
```

```
WARNING:tensorflow:From <ipython-input-20-f59549b55e1c>:3: softmax_cross_en
tropy_with_logits (from tensorflow.python.ops.nn_ops) is deprecated and wil
l be removed in a future version.
Instructions for updating:

Future major versions of TensorFlow will allow gradients to flow
into the labels input on backprop by default.

See tf.nn.softmax_cross_entropy_with_logits_v2.
```

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 [21]:
```
n_batch = 50     # Batch Size
n_iter = 2500    # Learning Iteration
n_prt = 250      # Print Cycle
```

4.9. Optimization

In [22]:
```
# Run initialize
# config = tf.ConfigProto(allow_soft_placement=True)  # GPU Allocating polic
y
# 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))
```

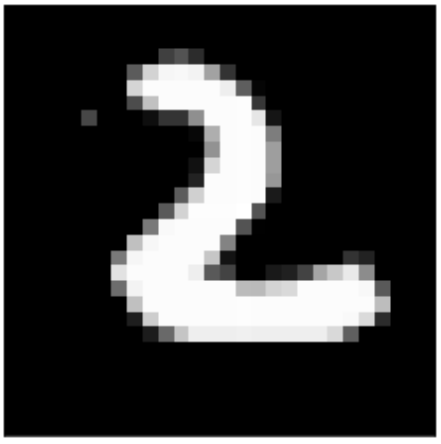
```
Iter : 0
Cost : 2.8692855834960938
Iter : 250
Cost : 1.202142357826233
Iter : 500
Cost : 0.8901556134223938
Iter : 750
Cost : 0.5407989621162415
Iter : 1000
Cost : 0.3589915931224823
Iter : 1250
Cost : 0.28060182929039
Iter : 1500
Cost : 0.37031352519989014
Iter : 1750
Cost : 0.6127738952636719
Iter : 2000
Cost : 0.47615474462509155
Iter : 2250
Cost : 0.3511289358139038
```

4.10. Test

In [23]:
```
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 : 93.0%
```

In [24]:
```
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 : 2
Probability : [0.   0.   0.93 0.01 0.   0.   0.06 0.   0.   0.  ]
```

In [25]:
```
%%javascript
$.getScript('https://kmahelona.github.io/ipython_notebook_goodies/ipython_notebook_toc.js')
```