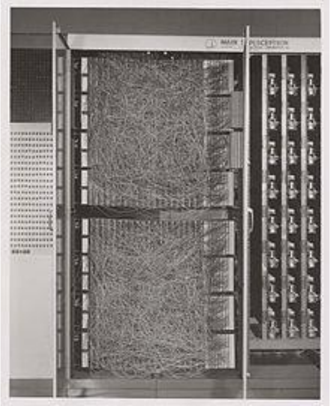
Introduction to Neural Networks

Perceptron, XOR Problem, Multi-layer Perceptron (MLP), Cost Functions, Activation functions and Output units

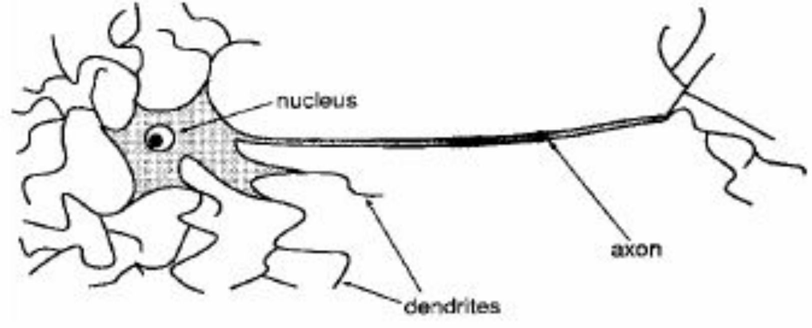
History

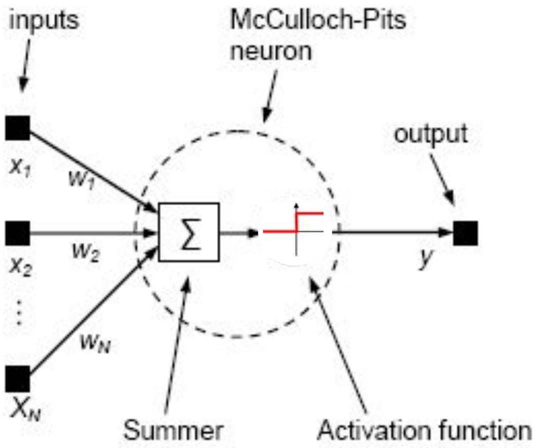
- 1932 - *The Integrative Action of the Nervous System*, **Sir Charles Scott Sherrington**
  - Nervous system - interconnection of individual entities (neuron)
- 1943 - *A Logical Calculus of Ideas Immanent in Nervous Activity*, **Warren McCulloch** and **Walter Pitts**
  - McCulloch and Pitt's model
- 1949 - *The Organization of Behavior,* **Donald Hebb**
  - Hebbian learning
- 1953 - *The Perceptron*, **Rosenblatt**
- 1969 - *Limitation of Perceptrons,* **Minsky** and **Papert**
- 1980's - *Connectionism*
  - *Error Back Propagation,* **Proposed simultaneously by Many**
- 20th century Deep learning
  - CNNs - LeNet, AlexNet, VGGNet, ResNet
  - Deep LSTMs,
- The **deep saga………** what followed is discussed in the last class



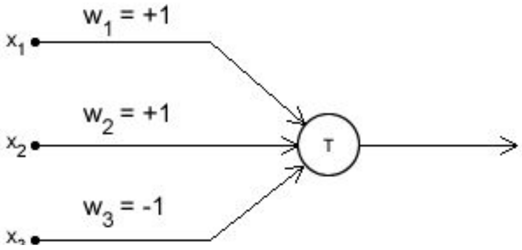
The Mark 1 Perceptron
By Rosenblat

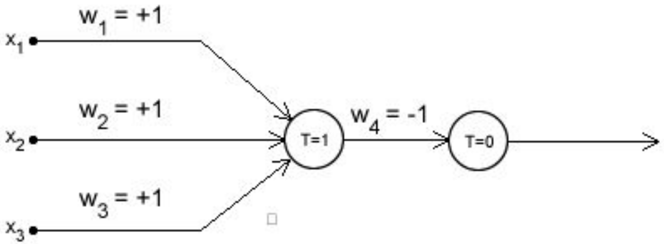
McCulloch - Pits model





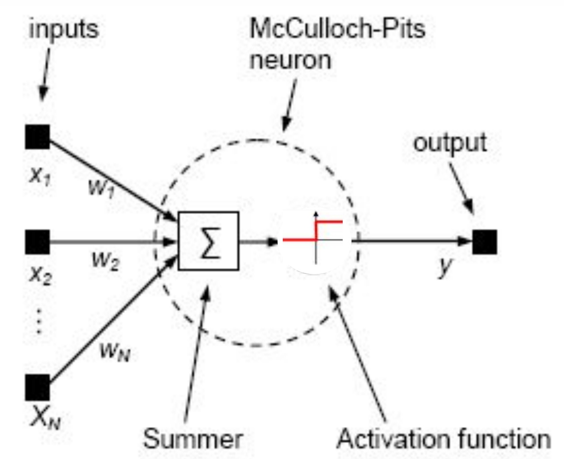
$$\sum_{i=1}^{n} w_i x_i > \mu$$



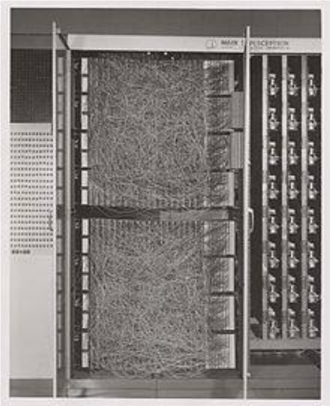


NOR gate

The Perceptron - Rosenblatt (1953)



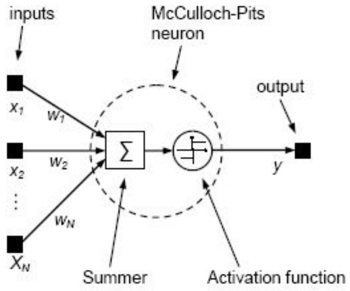
$$\sum_{i=1}^{n} w_i x_i > \mu$$



*Pic courtesy, wikipedia

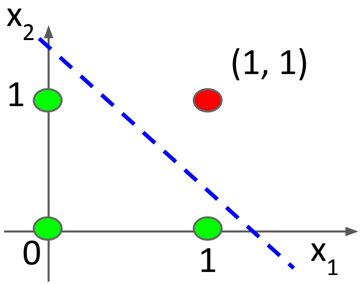
The Mark 1 Perceptron
By Rosenblat
for digit recognition

Perceptron - geometrical interpretation



$$\sum_{i=1}^{n} w_i x_i > \mu$$, What does this inequality imply in 2D case? Half plane

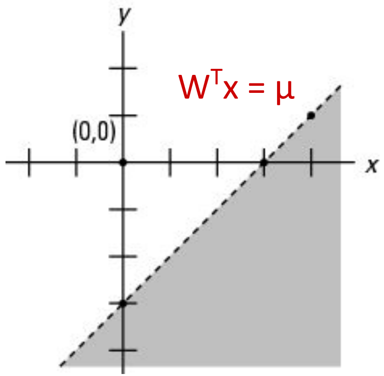
$\mathbb{X}$	*AND*
(0, 0)	0
(0, 1)	0
(1, 0)	0
(1, 1)	1



Solve for W, μ:

$$x_1 + x_2 > 1.5$$

$$w_1 = 1, w_2 = 1 \text{ and } \mu = 1.5$$



*Pic courtesy, cliffsnotes

Any function that is linearly separable can be computed by a perceptron

Perceptron Learning Algorithm (PLA)

How to learn the parameters {W} given only the input, output pairs

$$w_i \leftarrow w_i + \Delta w_i$$

where

$$\Delta w_i = \eta(t - o)x_i$$

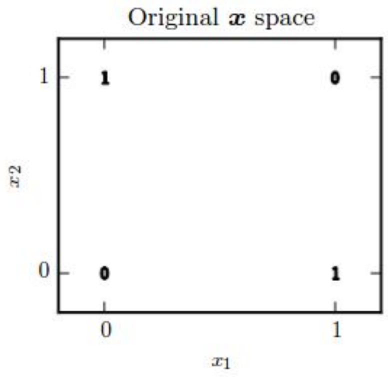
Where:

- $t = c(\vec{x})$ is target value
- o is perceptron output
- η is small constant (e.g., 0.1) called *learning rate*

Perceptron - Limitations

Goal: learn the XoR function (f^*)

$\mathbb{X}$	f^*
(0, 0)	0
(0, 1)	1
(1, 0)	1
(1, 1)	0



Task is adjust parameters θ, such that f is as close as to f^*

$$y = f(x,\theta) \qquad L = \sum_{\{x \in \mathbf{X}\}} \left(f^*(x) - f(x,\theta) \right)^2$$

Lets use our perceptron for f, $\theta = \{w,b\}$

$$f(x; w,b) = w^T x + b$$

Solve for {w,b}

W = 0, b = 0.5; output is 0.5 everywhere

Why this linear function can't model XoR**?**

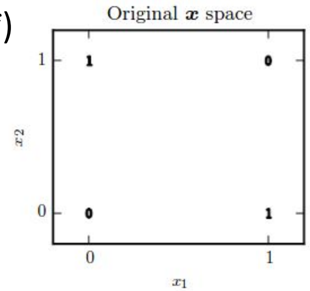
How to tackle this problem?

- Can we use more than one line?
- Yes, but how?

*Slide courtesy, Ian Goodfellow et al., deep learning book

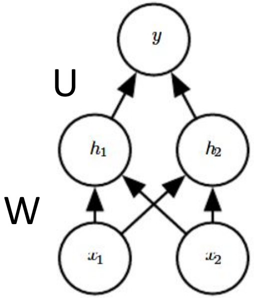
Perceptron - Limitations

Goal: learn the XoR function (f^*)



How to tackle this problem?

– Add a hidden layer with two units



$y = f^{(2)}(h; U, c)$

$y = f^{(2)}(\, f^{(1)}(x)\,)$

$h = f^{(1)}(x; W, b)$

What should $f^{(1)}$ compute?

– If its linear again the composition still remains linear

$f^{(2)}(h) = U^T h$; since $h = Wx$

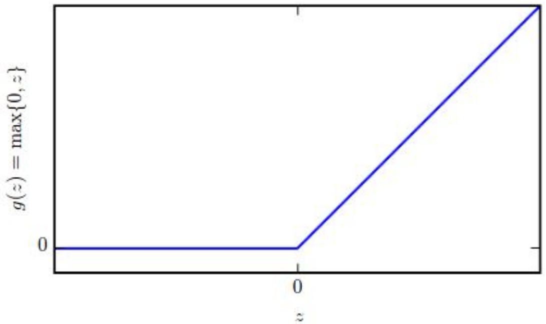
$y = U^T W x = W'x$

– $f^{(1)}$ should be nonlinear to extract useful features

$h = f^{(1)}(x; W, b) = g(Wx+b)$

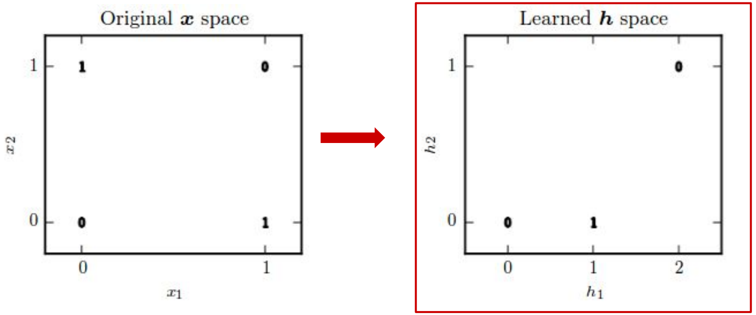
– g is referred as activation function commonly

– We will use ReLU here
  - Rectified Linear Unit (widely used)
  - $g(z) = \max\{0,z\}$



*Slide courtesy, Ian Goodfellow et al., deep learning book

Goal: learn the XoR function (f^*)



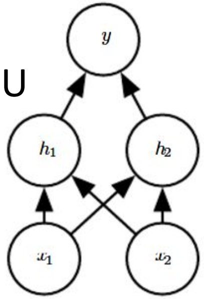
Perceptron - Limitations

How to tackle this problem?

- Add a hidden layer with two units
- Use ReLU activation in 1st layer

U

W



$$y = U^T h + c\ ; \quad y = U^T \underbrace{\max\{0, Wx+b\}}_{\text{ReLU}} + c$$

$$h = g(Wx+b)$$

Let,

$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \quad U = \begin{bmatrix} 1 \\ -2 \end{bmatrix},$$

$$c = 0$$

$$X = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \qquad WX = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 1 & 1 & 2 \end{bmatrix}$$

$$WX + b = \begin{bmatrix} 0 & 1 & 1 & 2 \\ -1 & 0 & 0 & 1 \end{bmatrix} \qquad \boxed{h = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{Upon ReLU}}$$

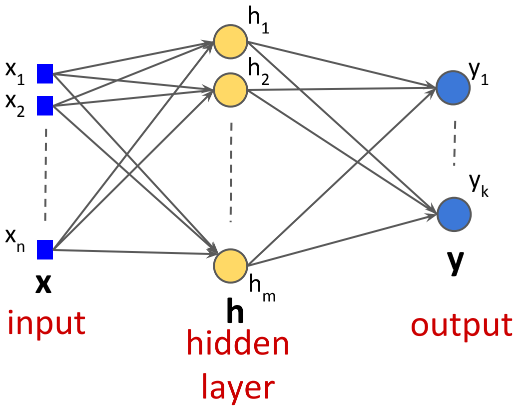
After layer2

$$[0\ 1\ 1\ 0]$$

*Slide courtesy, Ian Goodfellow et al., deep learning book

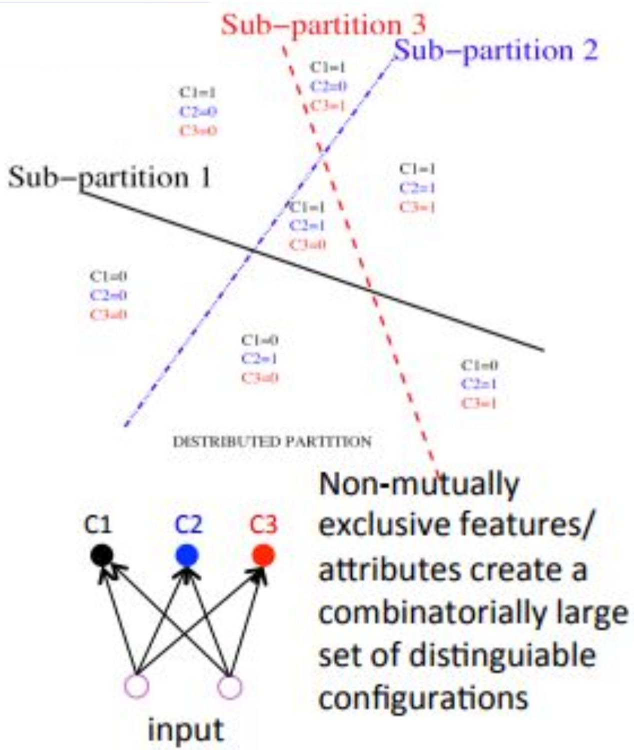
Multi-layer Perceptrons (MLP)

A typical feed forward neural network



$$\mathbf{h} = f(W\mathbf{x} + \mathbf{b}_1); \quad \mathbf{y} = g(U\mathbf{h} + \mathbf{b}_2)$$

With more hidden units network is more expressible



*Pic courtesy, Yoshua Bengio

Feedforward Neural Networks - Cost functions

For regression,

$$J(\theta) = \frac{1}{2}\mathbb{E}_{\mathbf{x},\mathbf{y}\sim\hat{p}_{\text{data}}} ||\boldsymbol{y} - f(\boldsymbol{x};\boldsymbol{\theta})||^2$$

$$\frac{1}{2}\sum_{\{x_i,y_i\}} ||y_i - f(x_i,\theta)||^2$$

For classification,

- Typically outputs a probability vector $q(c = k|x)\ \forall\ k$
- How do you compare two distributions?
  - KL divergence, KL(p // q)

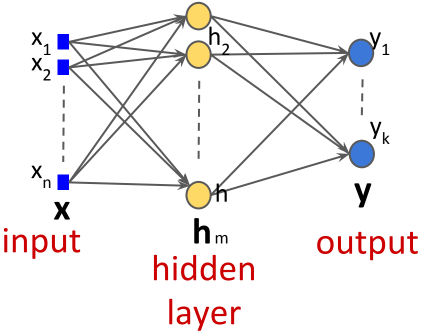
$$D_{KL}(p(x)||q(x)) = \sum_{x\in X} p(x) \ln \frac{p(x)}{q(x)}$$

$$= \sum p(x) \ln p(x) - p(x) \ln q(x)$$

$$= \underbrace{-H(p)}_{\text{entropy}} + \underbrace{H(p,q)}_{\text{cross-entropy}}$$

$$J(\theta) = \sum_{x_i,y_i} H(p(x_i),q(x_i))$$

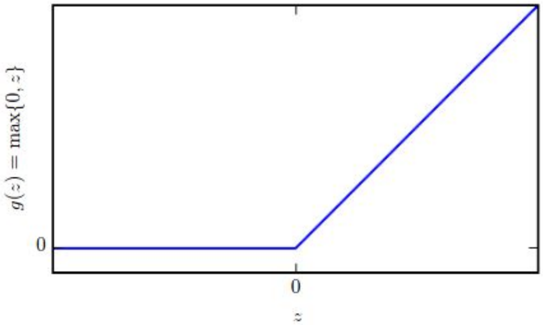
Activation functions



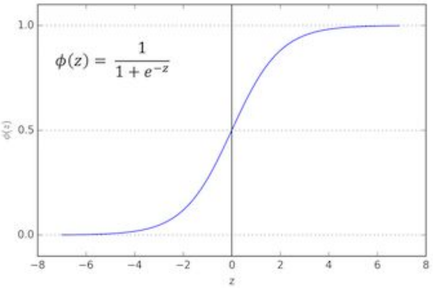
h = g(Wx+b); Affine transformation followed by activation function, g

– Very important factor in learning features

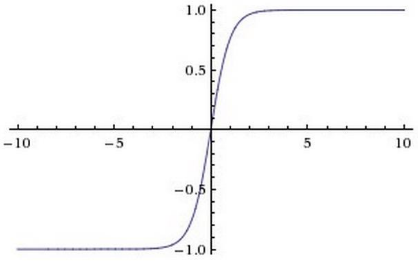
g(z) = max{0,z}, ReLU



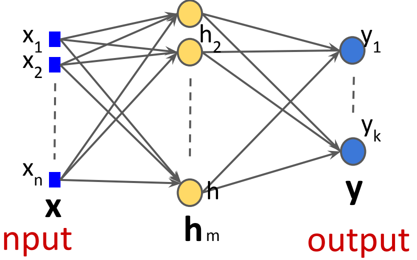
g(z) = σ(z), sigmoid



$tanh$(z) = 2σ(2z) - 1



Output units



- Linear units for real valued outputs
  - ❏ Activation function is left to be linear
  - ❏ Given features h,

    y’ = Wh+b

  - ❏ Most commonly used with regression tasks

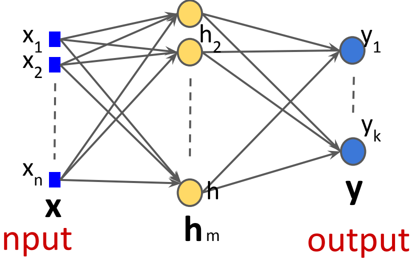
- Say you want to do binary classification
  - ❏ What kind of distribution describes output? **Bernouli**
  - ❏ How to constrain the output - valid probability? Can you use linear activation?

$$P(y=1 \mid \boldsymbol{x}) = \max\left\{0, \min\left\{1, \boldsymbol{w}^\top \boldsymbol{h} + b\right\}\right\}.$$

  - ❏ What is the problem? *Not amenable for gradient based learning*
  - ❏ Instead, use sigmoid unit - output ∈ [0,1]

$$\hat{y} = \sigma\left(\boldsymbol{w}^\top \boldsymbol{h} + b\right)$$

Output units

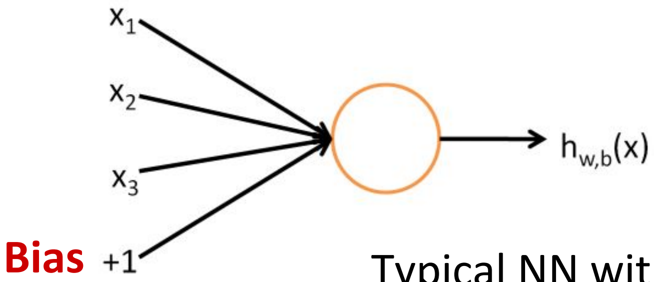


- Now, say we want to do multi-class classification (K classes)
  - ❑ Output should be K probabilities,
    $p_k = p(class = k|\mathrm{x})\ \forall\ k = 1$ to K
  - ❑ Can we use K sigmoid units?
    Won't be sufficient, since probabilities are not constrained to sum to 1
    $\sum_k p_k = 1$
  - ❑ We will look at softmax unit for this
    Idea is to convert a vector of real values to valid probabilities, How?
    - ❑ Make all the elements positive
    - ❑ Normalize the values

- Let, $\mathbf{z} = [z_1, \ldots, z_K]^T$; $\mathbf{z} = W\mathbf{h} + \mathbf{b}$

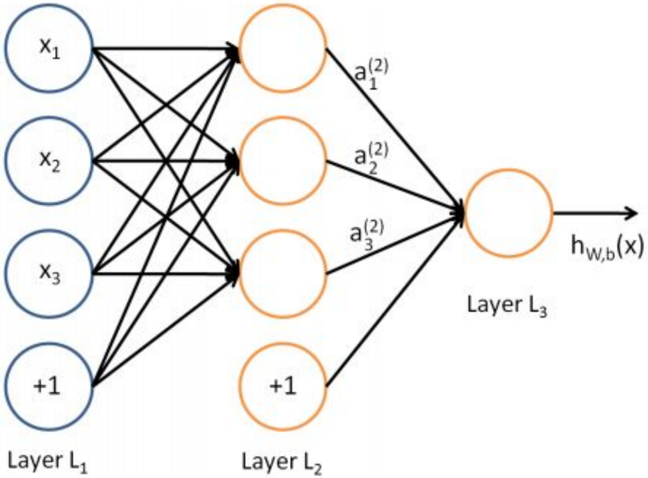
$$\text{softmax}(\boldsymbol{z})_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}.$$

How to learn the parameters?



$$h_{W,b}(x) = f(W^T x) = f(\sum_{i=1}^{3} W_i x_i + b)$$

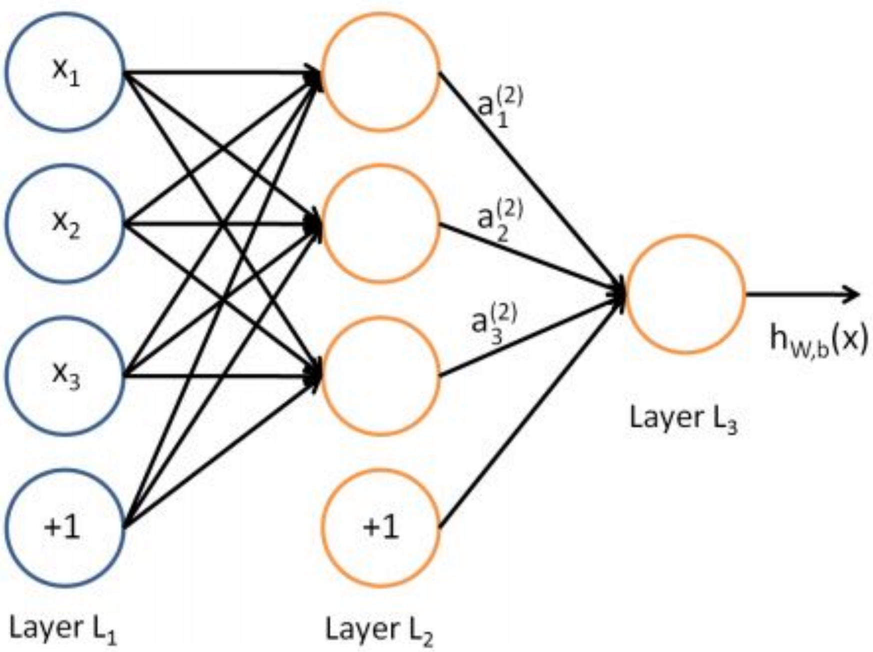
Typical NN with many such units



- One hidden layer
  - 3 neuron units
- One output

*Slide courtesy, [sparse autoencoder by Andrew Ng]

How to learn the parameters?



L_l – Layer l

$a_i^{(l)}$ – activation of unit i in layer l

$W_{ij}^{(l)}$ – Weight from j^{th} unit in l to i^{th} unit in $l+1$

$b_i^{(l)}$ – bias to unit i in layer $l+1$

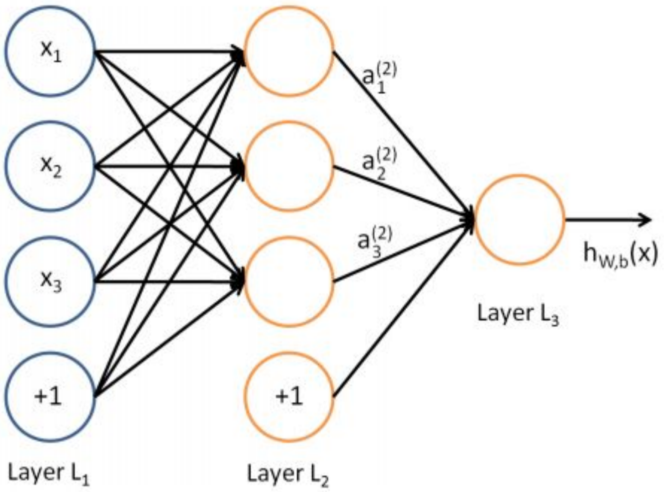
Parameters:

$$(W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$$

$$W^{(1)} \in \mathbb{R}^{3\times3}, W^{(2)} \in \mathbb{R}^{1\times3}$$

*Slide courtesy, sparse autoencoder by Andrew Ng

How to learn the parameters?



Layer 2,

$$
\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)}) \\
a_2^{(2)} &= f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)}) \\
a_3^{(2)} &= f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)})
\end{aligned}
$$

Layer 3,

$$
h_{W,b}(x) = a_1^{(3)} = f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)})
$$

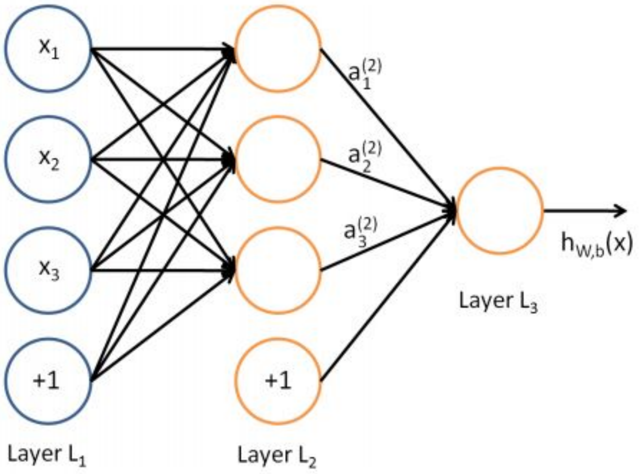
Simplification

Let, $z_i^{(l)}$ denote weighted sum for the activation $a_i^{(l)}$

$a_i^{(l)} = f(z_i^{(l)})$ *f*(.) applies the function point wise

*Slide courtesy, [sparse autoencoder by Andrew Ng]

How to learn the parameters?



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\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)}) \\
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\end{aligned}
$$

$$
h_{W,b}(x) = a_1^{(3)} = f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)})
$$

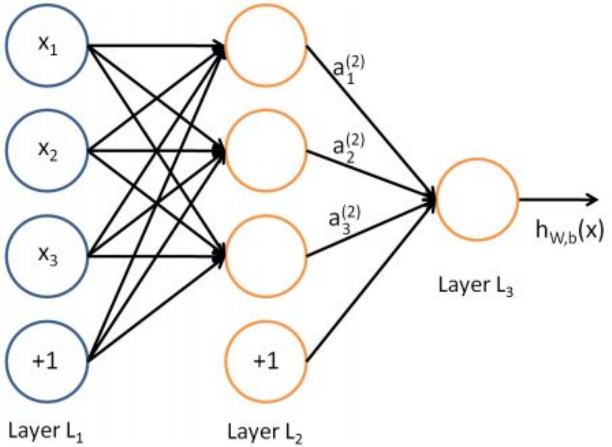
Let, $z_i^{(l)}$ denote weighted sum for the activation $a_i^{(l)}$

$$
\begin{aligned}
z^{(2)} &= W^{(1)}x + b^{(1)} \\
a^{(2)} &= f(z^{(2)}) \\
z^{(3)} &= W^{(2)}a^{(2)} + b^{(2)} \\
h_{W,b}(x) &= a^{(3)} = f(z^{(3)})
\end{aligned}
$$

$$
\begin{aligned}
z^{(l+1)} &= W^{(l)}a^{(l)} + b^{(l)} \\
a^{(l+1)} &= f(z^{(l+1)})
\end{aligned}
$$

*Slide courtesy, sparse autoencoder by Andrew Ng

How to learn the parameters?



Given *m* training examples

$$\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$$

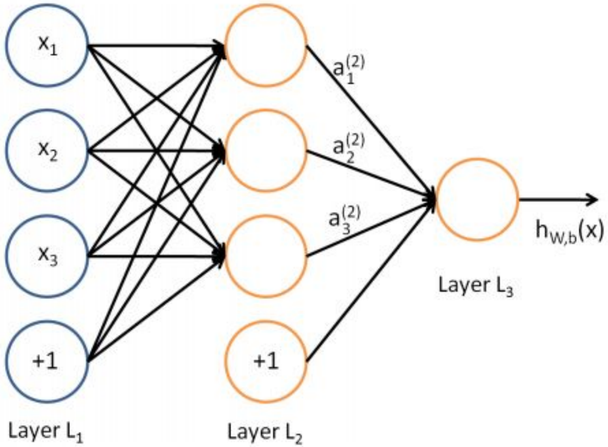
Minimize:

$$J(W,b;x,y) = \frac{1}{2}\left\|h_{W,b}(x) - y\right\|^2$$

$$\begin{aligned} J(W,b) &= \left[\frac{1}{m}\sum_{i=1}^{m} J(W,b;x^{(i)},y^{(i)})\right] + \frac{\lambda}{2}\sum_{l=1}^{n_l-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}\left(W_{ji}^{(l)}\right)^2 \qquad (8 \\ &= \left[\frac{1}{m}\sum_{i=1}^{m}\left(\frac{1}{2}\left\|h_{W,b}(x^{(i)}) - y^{(i)}\right\|^2\right)\right] + \frac{\lambda}{2}\sum_{l=1}^{n_l-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}\left(W_{ji}^{(l)}\right)^2 \end{aligned}$$

*Slide courtesy, [sparse autoencoder by Andrew Ng]

How to learn the parameters?



Minimize:

$$J(W,b;x,y) = \frac{1}{2}\left\|h_{W,b}(x) - y\right\|^2$$

Gradient descent:

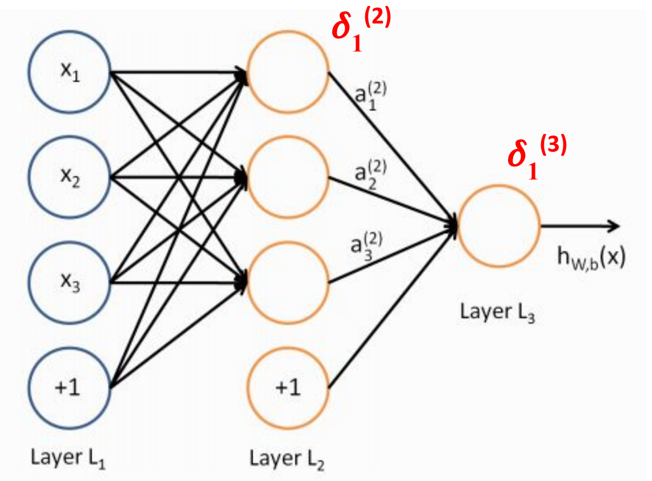
$$\begin{aligned} W_{ij}^{(l)} &:= W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b) \\ b_i^{(l)} &:= b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W,b) \end{aligned}$$

How to evaluate these partial derivatives?

Error back-propagation

*Slide courtesy, sparse autoencoder by Andrew Ng

Back-propagation algorithm



Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b)$$

Idea:

First, forward pass the data to calc. all responses

In backward pass, for each unit i in layer l calculate **error** term $\delta_i^{(l)}$ - measures how much unit i is responsible for output error

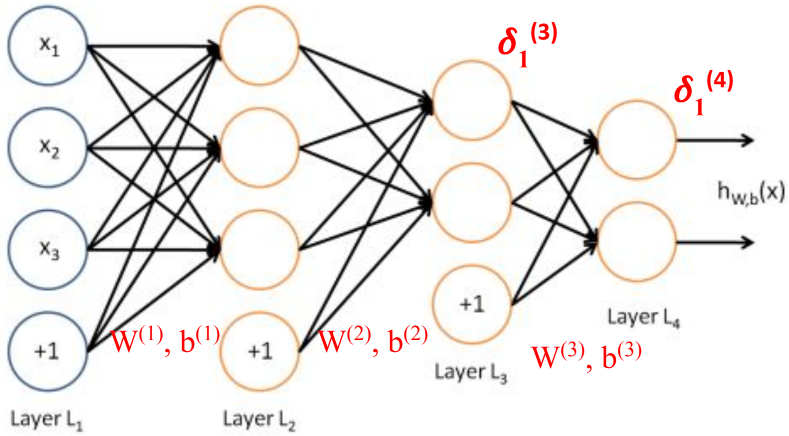
– For output unit in last layer (n_l), this is easy

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z_i^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$

– How to measure $\delta_i^{(l)}$ for hidden units?

*Slide courtesy, sparse autoencoder by Andrew Ng

Back-propagation algorithm



Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b)$$

$$J(W,b;x,y) = \frac{1}{2} \left\| h_{W,b}(x) - y \right\|^2$$

$$h_{W,b}(x) = a^{(4)} = f(z^{(4)});\; z^{(4)} = W^{(3)} a^{(3)} + b^{(3)}$$

For last layer:

$$\frac{\partial J}{\partial W_{ij}^{(3)}} = \boxed{\frac{\partial J}{\partial z_i^4}} \boxed{\frac{\partial z_i^4}{\partial W_{ij}^{(3)}}}$$

$$\boxed{\frac{\partial J}{\partial z_i{}^4} = -(y_i - a_i^{(4)})\ .f'(z_i^4)}$$

$\delta_i^{(4)}$ **error term**

$$\boxed{\frac{\partial z_i^4}{\partial W_{ij}^3} = a_j^{(3)}}$$

$$\frac{\partial J}{\partial W_{ij}^{(l)}} = \delta_i^{(l+1)} a_j^{(l)} \qquad \frac{\partial J}{\partial b_i^{(l)}} = \delta_i^{(l+1)}$$

*Slide courtesy, sparse autoencoder by Andrew Ng

Back-propagation algorithm

Gradient descent:

$$W_{ij}^{(l)} \;:=\; W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b)$$

$$J(W,b;x,y) = \frac{1}{2}\left\|h_{W,b}(x) - y\right\|^2$$

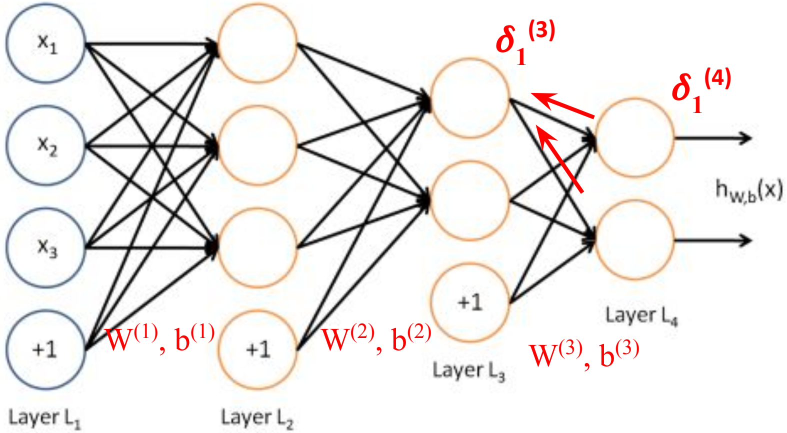
For layers other than last:

$$\frac{\partial J}{\partial W_{ij}^{(2)}} = \boxed{\frac{\partial J}{\partial z_i^{(3)}}}\,\boxed{\frac{\partial z_i^{(3)}}{\partial W_{ij}^{(2)}}}$$

$a_j^{(2)}$

$$\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)}\right) f'(z_i^{(l)})$$

$$\frac{\partial J}{\partial W_{ij}^{(l)}} = \delta_i^{(l+1)} a_j^{(l)} \qquad \frac{\partial J}{\partial b_i^{(l)}} = \delta_i^{(l+1)}$$



$$h_{W,b}(x) = a^{(4)} = f(z^{(4)}); \quad z^{(4)} = W^{(3)}a^{(3)} + b^{(3)}$$

$$a^{(3)} = f(z^{(3)}); \quad z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$

$\delta_i^{(3)}$
error term

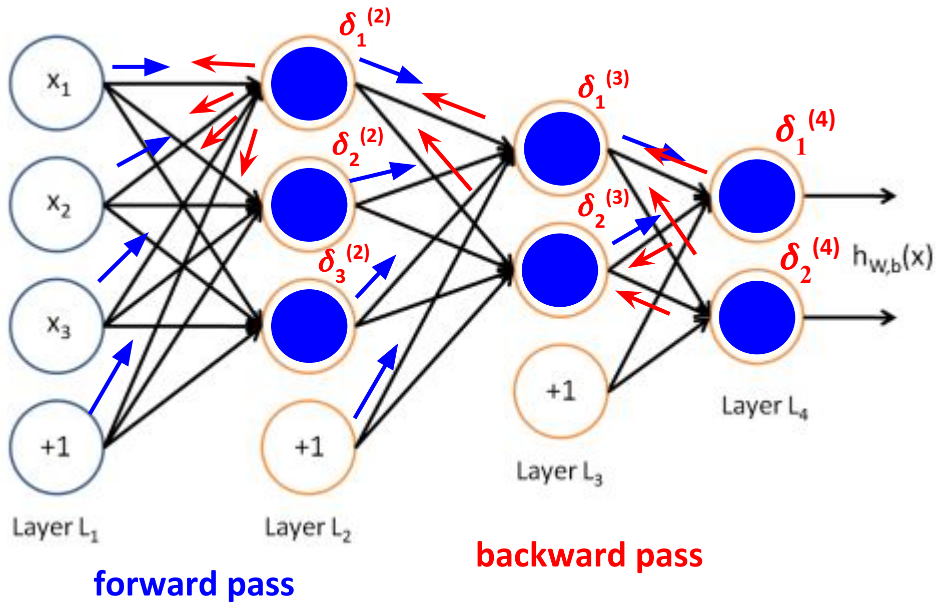
$$\boxed{\begin{aligned}\frac{\partial J}{\partial z_i^{(3)}} &= \frac{\partial J}{\partial a_i^{(3)}} \frac{\partial a_i^{(3)}}{\partial z_i^{(3)}} \\ &= \left(\sum_j \frac{\partial J}{\partial z_j^{(4)}} \frac{\partial z_j^{(4)}}{\partial a_i^{(3)}}\right) f'(z_i^{(3)})\end{aligned}}$$

$\delta_j^{(4)}$
Layer - (l+1)

$W_{ji}^{(3)}$

*Slide courtesy, sparse autoencoder by Andrew Ng

Back-propagation algorithm



1. Perform a feedforward pass
   - Computing activations L_1, L_2 and so on ...

2. For each output unit i in layer L_4 (output layer), set

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z_i^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$

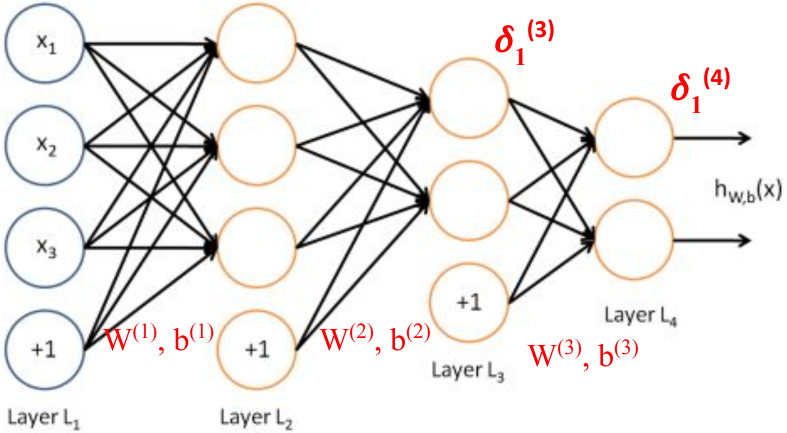
3. Starting from last but one layer to 2nd layer;
   $l = n_l - 1, n_l - 2, \ldots, 2$
   - For each node i in layer l, set $\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)} \right) f'(z_i^{(l)})$

4. Compute the desired partial derivatives, as:

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x, y) = a_j^{(l)} \delta_i^{(l+1)} \qquad \frac{\partial}{\partial b_i^{(l)}} J(W, b; x, y) = \delta_i^{(l+1)}.$$

*Slide courtesy, sparse autoencoder by Andrew Ng

Back-propagation algorithm



$$h_{W,b}(x) = a^{(4)} = f(z^{(4)}); \;\; z^{(4)} = W^{(3)}a^{(3)} + b^{(3)}$$

Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b)$$

$$J(W,b;x,y) = \frac{1}{2} \left\| h_{W,b}(x) - y \right\|^2$$

Partial derivatives:

$$\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)} \right) f'(z_i^{(l)})$$

$$\frac{\partial J}{\partial W_{ij}^{(l)}} = \delta_i^{(l+1)} a_j^{(l)} \qquad \frac{\partial J}{\partial b_i^{(l)}} = \delta_i^{(l+1)}$$

Matrix notation:

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)} \right) \bullet f'(z^{(l)})$$

$$\frac{\partial J}{\partial W^{(l)}} = \delta^{(l+1)} (a^{(l)})^T \qquad \frac{\partial J}{\partial b^{(l)}} = \delta^{(l+1)}$$

*Slide courtesy, [sparse autoencoder by Andrew Ng]

Back-propagation algorithm

1. Perform a feedforward pass
   - Computing activations L_1, L_2 and so on ...

2. For each output unit i in layer L_4 (output layer), set

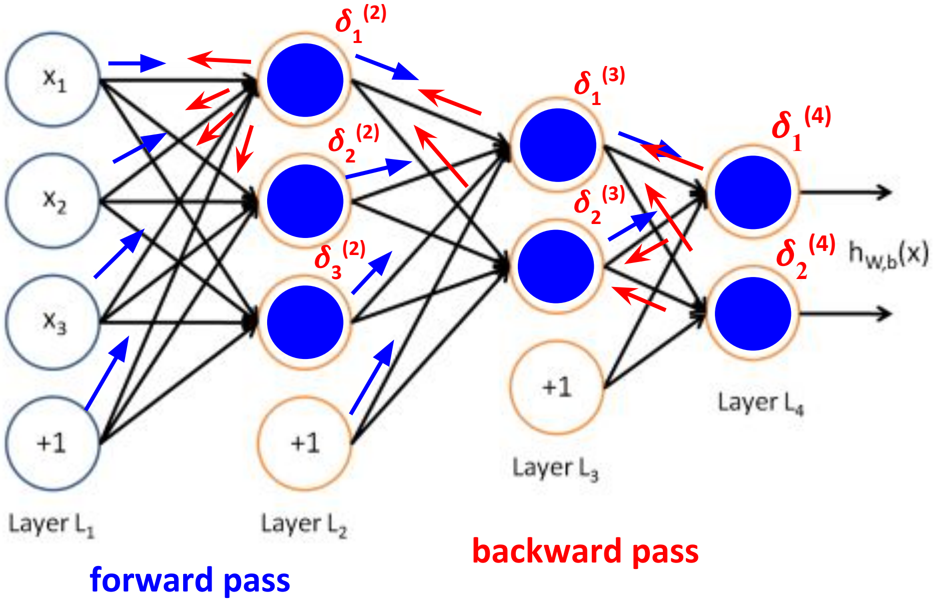
$$\delta^{(n_l)} = -(y - a^{(n_l)}) \bullet f'(z^{(n)})$$

3. Starting from last but one layer to 2nd layer; $l = n_l\text{-}1, n_l\text{-}2, \ldots\ldots, 2$

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)}\right) \bullet f'(z^{(l)})$$

4. Compute the desired partial derivatives, as:

$$\begin{aligned} \nabla_{W^{(l)}} J(W,b;x,y) &= \delta^{(l+1)} (a^{(l)})^T, \\ \nabla_{b^{(l)}} J(W,b;x,y) &= \delta^{(l+1)}. \end{aligned}$$



*Slide courtesy, sparse autoencoder by Andrew Ng

END