# Machine Learning
# DSECL ZG565

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# Lecture No. – 9 | Neural Network
# Date – 11/01/2020
# Time – 9:00 AM – 11:00 AM

These slides are prepared by the instructor, with grateful acknowledgement of Tom Mitchell, Andrew Ng and many others who made their course materials freely available online.

# Session Content

- Perceptron (Chapter 4 Tom Mitchell)
- Neural Network Architecture (Andrew Ng Notes and Chapter 4 Tom Mitchell)
- Back propagation Algorithm (Andrew Ng Notes)

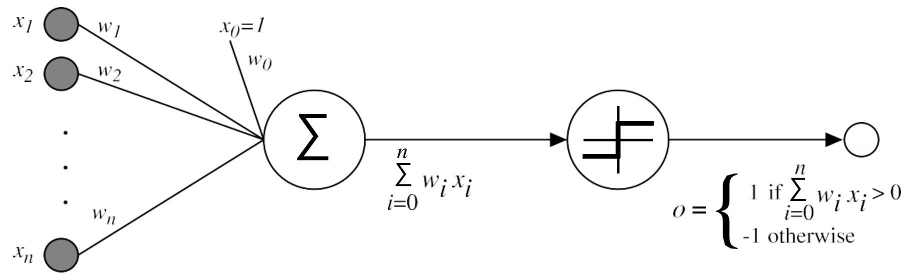
# When to Consider Neural Networks

- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant

Examples:

- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial predictio

# Perceptron

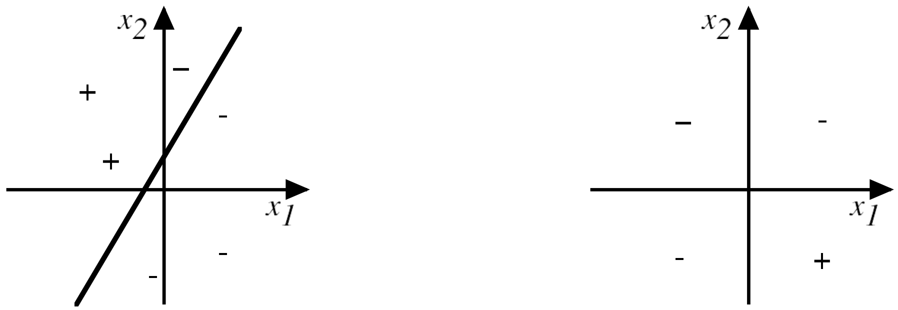



$$o(x_1, \ldots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Sometimes we'll use simpler vector notation:

$$o(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\ -1 & \text{otherwise.} \end{cases}$$

# Decision Surface of Perceptron




$(a)$ $(b)$

Represents some useful functions

- What weights represent
  $g(x_1, x_2) = AND(x_1, x_2)$?

But some functions not representable

- e.g., not linearly separable
- Therefore, we'll want networks of these...

# Perceptron Training rule

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

where

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

Where:

- $t = c(\vec{x})$ is target value
- $o$ is perceptron output
- $\eta$ is small constant (e.g., .1) called *learning rate*

# Gradient Descent

To understand, consider simpler *linear unit*, where

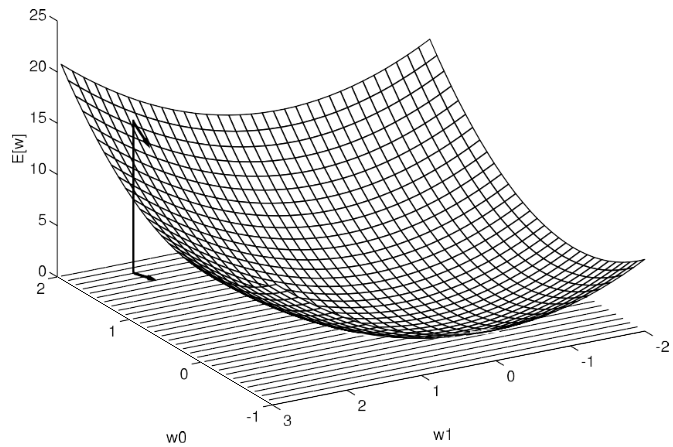
$$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$

Let's learn $w_i$'s that minimize the squared error

$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

Where $D$ is set of training examples

# Gradient Descent




Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

# Gradient Descent

$$
\begin{aligned}
\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\
&= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\
&= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\
&= \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \cdot \vec{x_d}) \\
\frac{\partial E}{\partial w_i} &= \sum_d (t_d - o_d)(-x_{i,d})
\end{aligned}
$$

# Gradient Descent

GRADIENT-DESCENT($training\_examples, \eta$)

*Each training example is a pair of the form $\langle \vec{x}, t \rangle$, where $\vec{x}$ is the vector of input values, and $t$ is the target output value. $\eta$ is the learning rate (e.g., .05).*

- Initialize each $w_i$ to some small random value
- Until the termination condition is met, Do
  - Initialize each $\Delta w_i$ to zero.
  - For each $\langle \vec{x}, t \rangle$ in $training\_examples$, Do
    - Input the instance $\vec{x}$ to the unit and compute the output $o$
    - For each linear unit weight $w_i$, Do

$$\Delta w_i \leftarrow \Delta w_i + \eta (t - o) x_i$$

  - For each linear unit weight $w_i$, Do

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

# Perceptron Training

Perceptron training rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate $\eta$

Linear unit training rule uses gradient descent

- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate $\eta$
- Even when training data contains noise
- Even when training data not separable by $H$

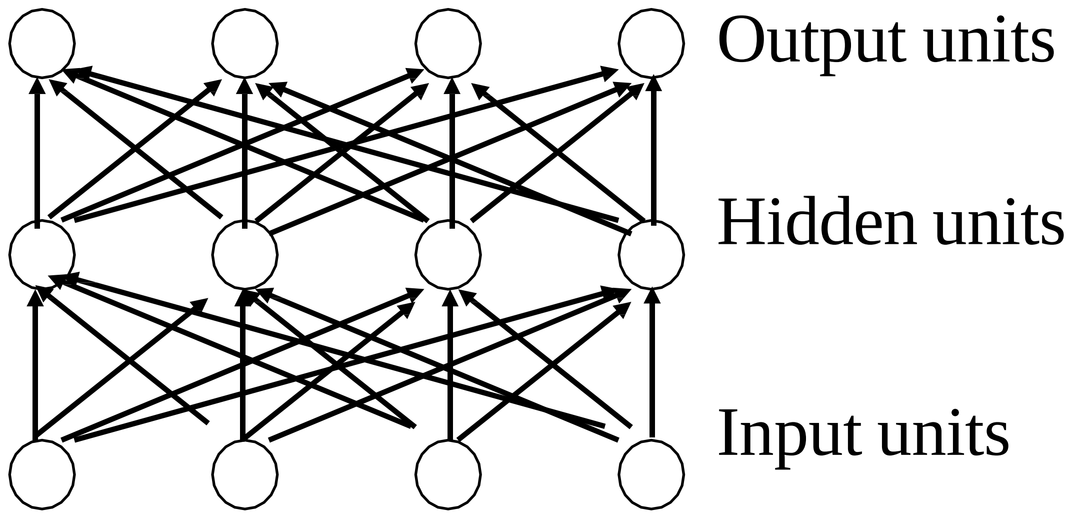
# Neural Networks

- Origins: Algorithms that try to mimic the brain.
- Very widely used in 80s and early 90s; popularity diminished in late 90s.
- Recent resurgence: State-of-the-art technique for many applications
- Artificial neural networks are not nearly as complex or intricate as the actual brain structure

# Multilayer network

- Single perceptrons can only express linear decision surfaces.
- In contrast, the kind of multilayer networks learned by the BACKPROPAGATION algorithm are capable of expressing a rich variety of nonlinear decision surfaces

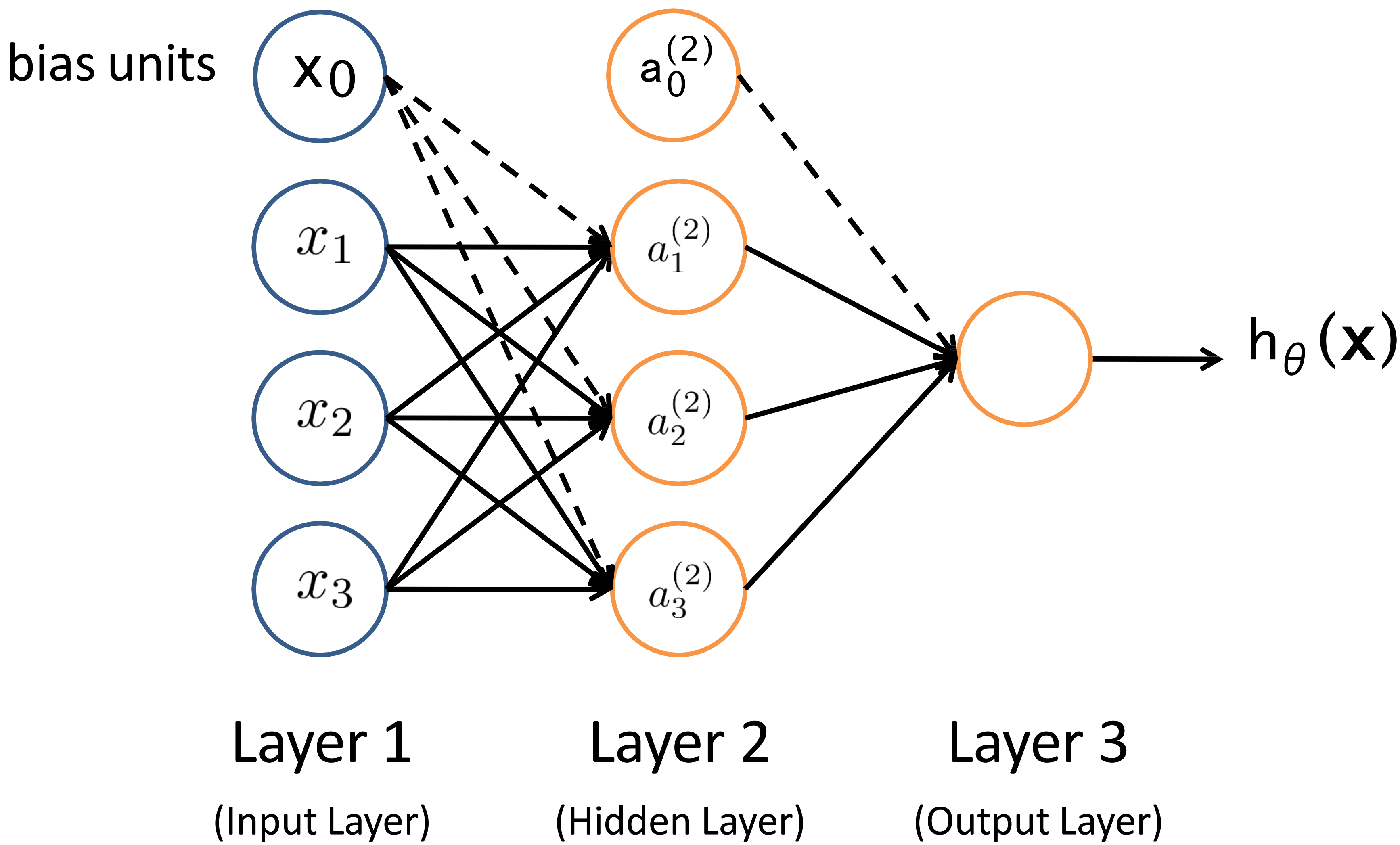
# Neural networks




Layered feed-forward network

- Neural networks are made up of **nodes** or **units**, connected by **links**
- Each link has an associated **weight** and **activation level**
- Each node has an **input function** (typically summing over weighted inputs), an **activation function**, and an **output**

# Neural Network

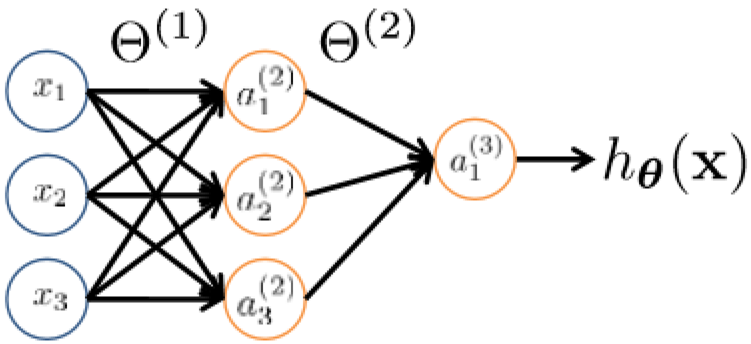


# Feed-Forward Process

- Input layer units are set by some exterior function (think of these as **sensors**), which causes their output links to be **activated** at the specified level
- Working forward through the network, the **input function** of each unit is applied to compute the input value
  - Usually this is just the weighted sum of the activation on the links feeding into this node
- The **activation function** transforms this input function into a final value
  - Typically this is a **nonlinear** function, often a **sigmoid** function corresponding to the "threshold" of that node

Based on slide by T. Finin, M. desJardins, L Getoor, R. Par

# Neural Network




$a_i^{(j)} =$ "activation" of unit $i$ in layer $j$

$\Theta^{(j)} =$ weight matrix controlling function mapping from layer $j$ to layer $j$ + 1

$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

If network has $s_j$ units in layer $j$ *and* $s_{j+1}$ units in layer $j+1$, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j+1)$ .

$$\Theta^{(1)} \in \mathbb{R}^{3\times 4} \qquad \Theta^{(2)} \in \mathbb{R}^{1\times 4}$$

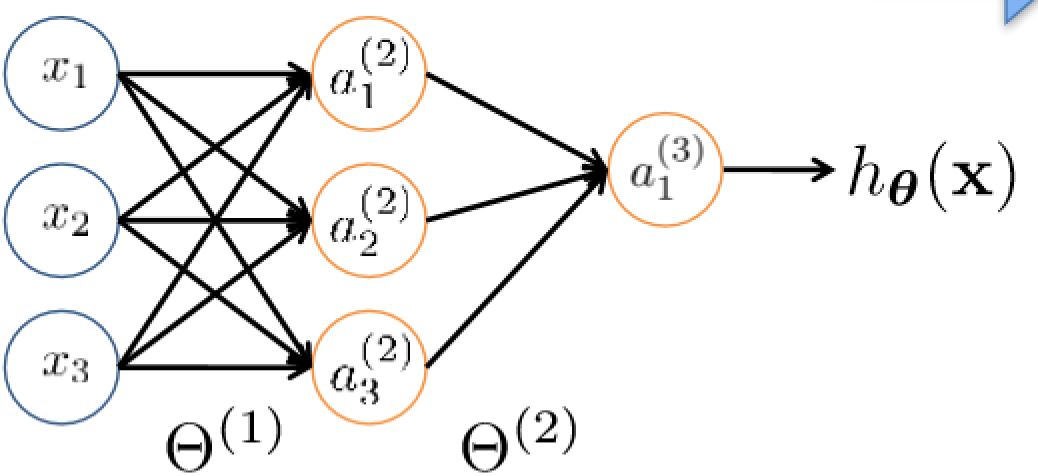
# Vectorization

$$a_1^{(2)} = g\left(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3\right) = g\left(z_1^{(2)}\right)$$

$$a_2^{(2)} = g\left(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3\right) = g\left(z_2^{(2)}\right)$$

$$a_3^{(2)} = g\left(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3\right) = g\left(z_3^{(2)}\right)$$

$$h_\Theta(\mathbf{x}) = g\left(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)}\right) = g\left(z_1^{(3)}\right)$$




**Feed-Forward Steps:**

$$\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{x}$$

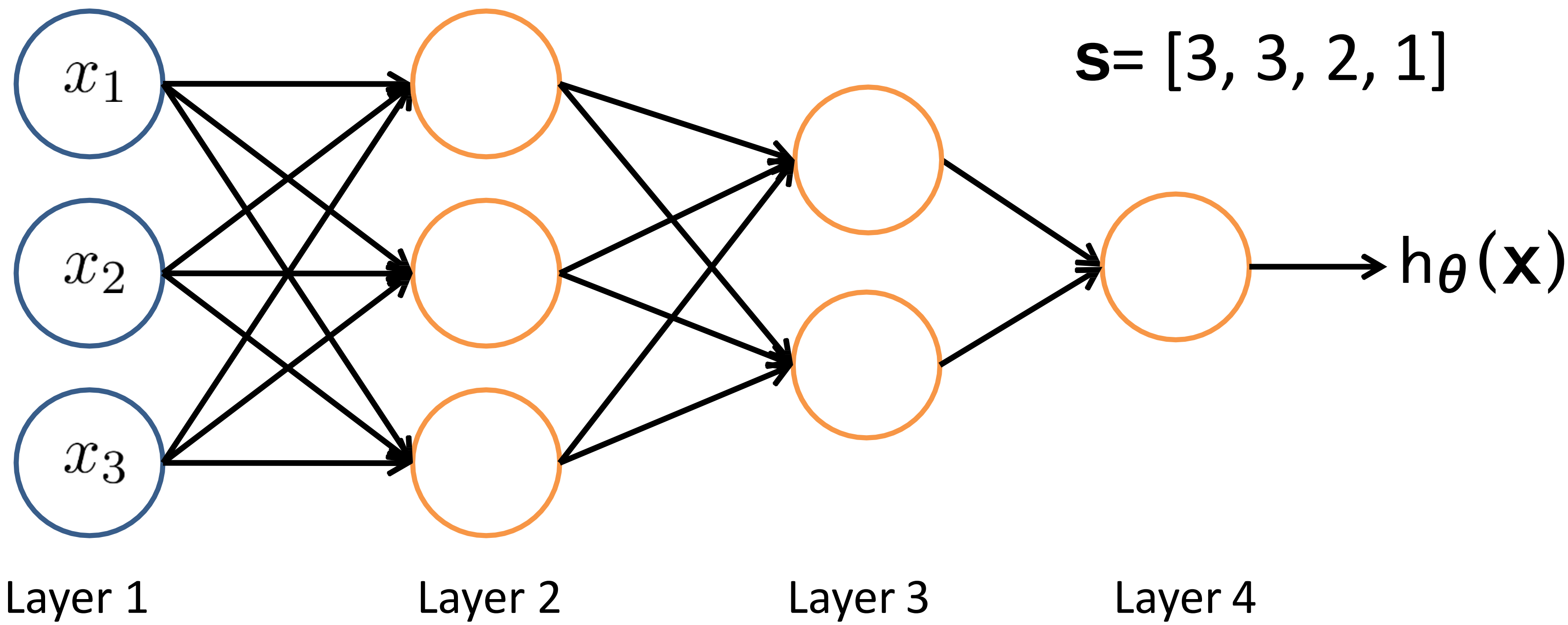
$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

$$\text{Add } a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$$

$$h_\Theta(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

# Other Network Architectures




$L$ denotes the number of layers

**s** $\in \mathbb{N}^{+L}$ contains the numbers of nodes at each layer

- Not counting bias units
- Typically, $s_0 = d$ (# input features) and $s_{L-1}=K$ (# classes)

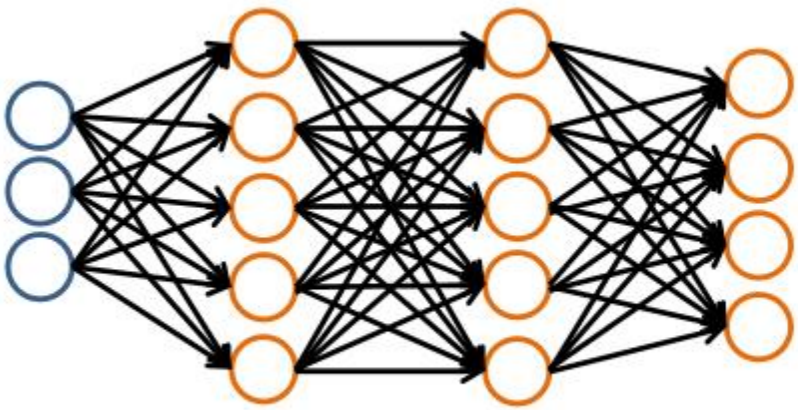
# Multiple Output Units:One-vs-Rest


Pedestrian


Car


Motorcycle


Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

We want:

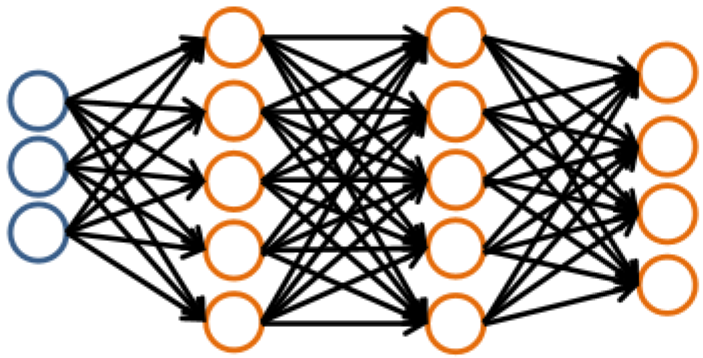
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$
when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$
when motorcycle

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
when truck

# Multiple Output Units: One-vs-Rest



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

We want:

$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ when pedestrian $\quad h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ when car $\quad h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when motorcycle $\quad h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ when truck

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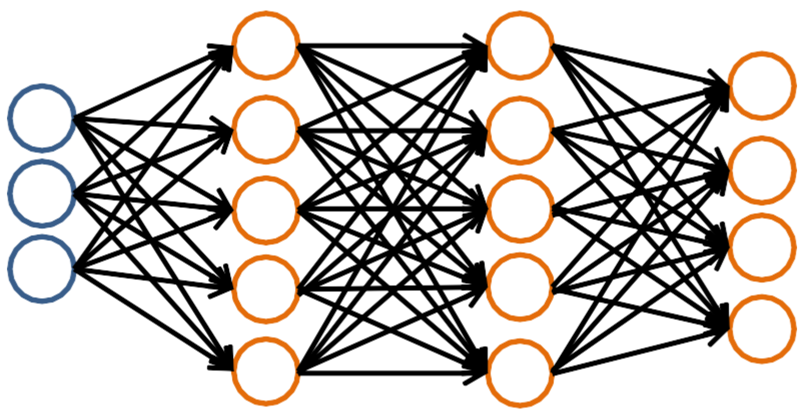
- Given $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)\}$
- Must convert labels to 1-of-$K$ representation
  - e.g., $\mathbf{y}_i = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when motorcycle, $\mathbf{y}_i = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ when car, etc.

# Neural Network Classification



**Given:**

$\{(\mathbf{x}_1,y_1),\ (\mathbf{x}_2,y_2),\ \ldots,\ (\mathbf{x}_n,y_n)\}$

$\mathbf{S} \in \mathbb{N}^{+L}$ contains # nodes at each layer

- $s_0 = d$ (# features)

<u>Binary classification</u>

$y$ = 0 or 1

1 output unit ($s_{L-1} = 1$)

<u>Multi-class classification</u> ($K$ classes)

$\mathbf{y} \in \mathbb{R}^K$ e.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

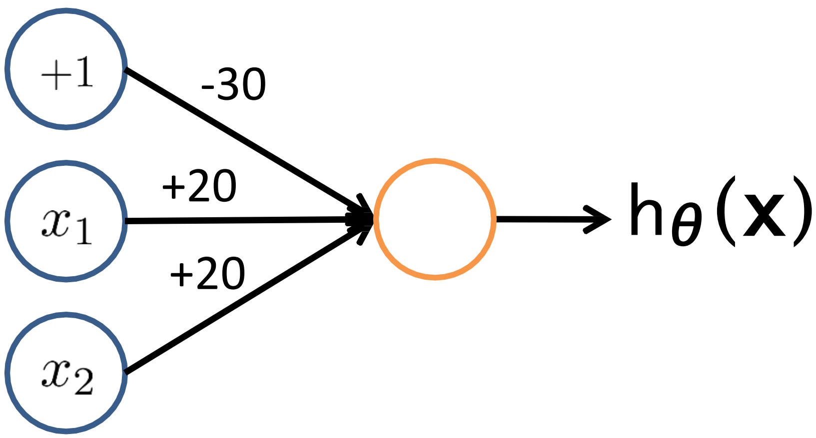
pedestrian car motorcycle truck

$K$ output units ($s_{L-1} = K$)

# Representing Boolean Functions

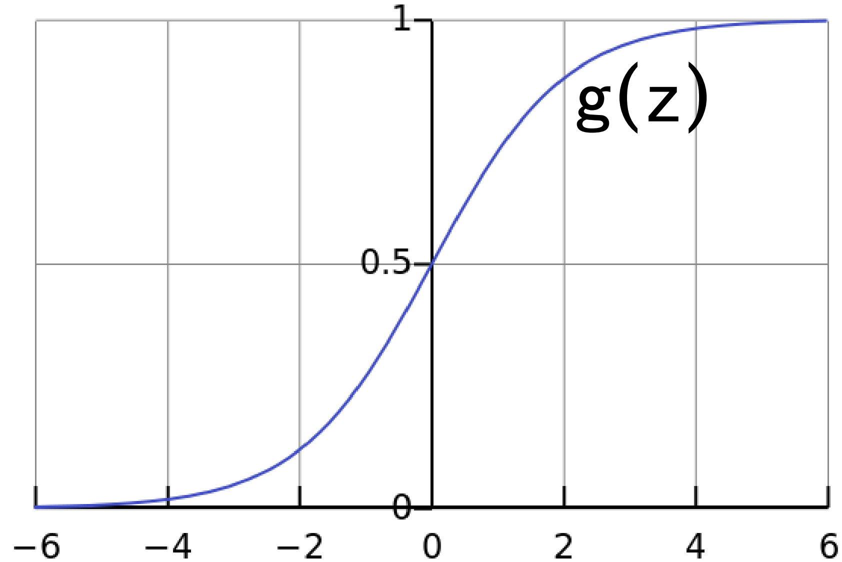
**Simple example: AND**

$$x_1, x_2 \in \{0, 1\}$$
$$y = x_1 \text{ AND } x_2$$




$$h_\Theta(\mathbf{x}) = g(-30 + 20x_1 + 20x_2)$$

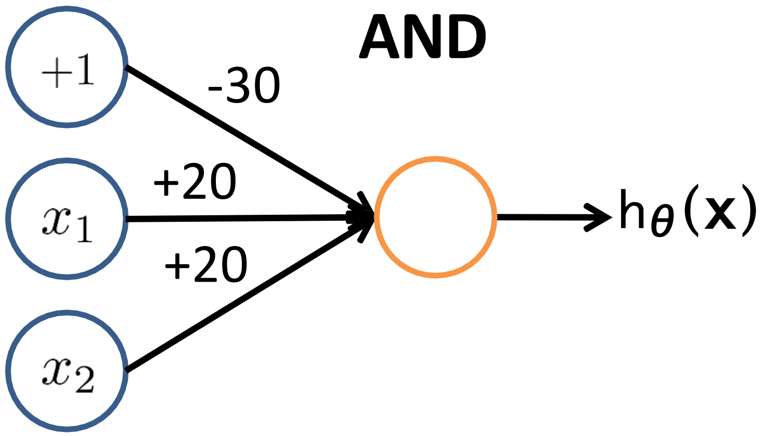
Logistic / Sigmoid Function



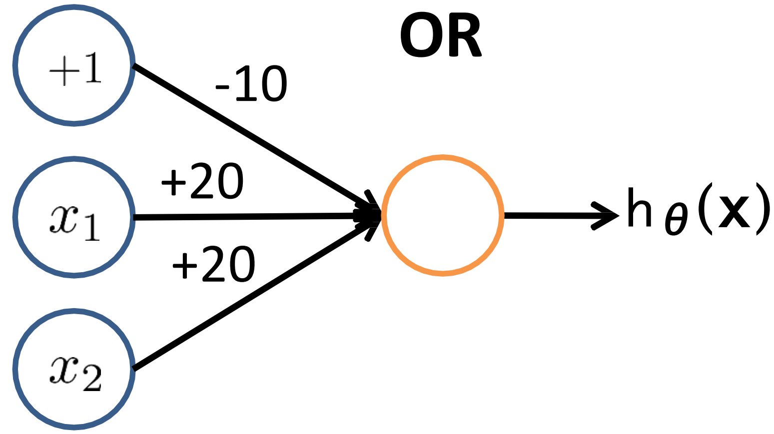

| $x_1$ | $x_2$ | $h_\Theta(\mathbf{x})$ |
|---|---|---|
| 0 | 0 | $g(-30) \approx 0$ |
| 0 | 1 | $g(-10) \approx 0$ |
| 1 | 0 | $g(-10) \approx 0$ |
| 1 | 1 | $g(10) \approx 1$ |

# Representing Boolean Functions

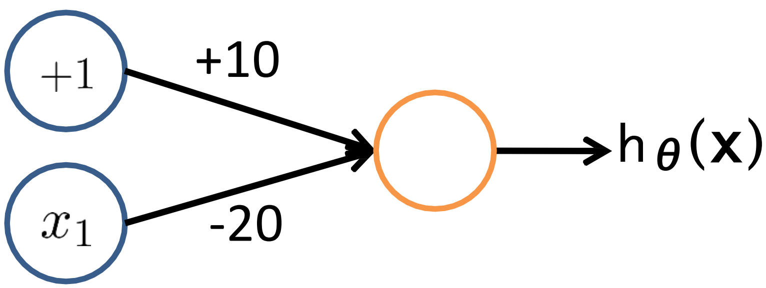
**AND**



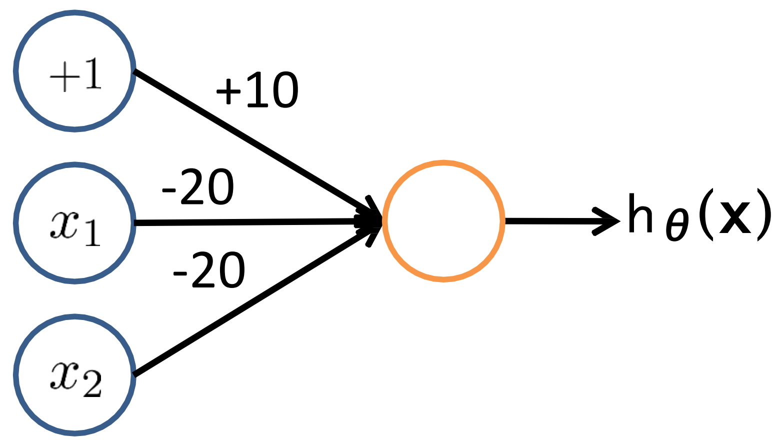

**OR**



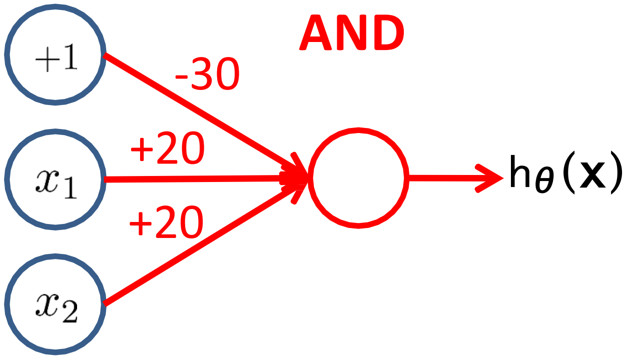

**NOT**

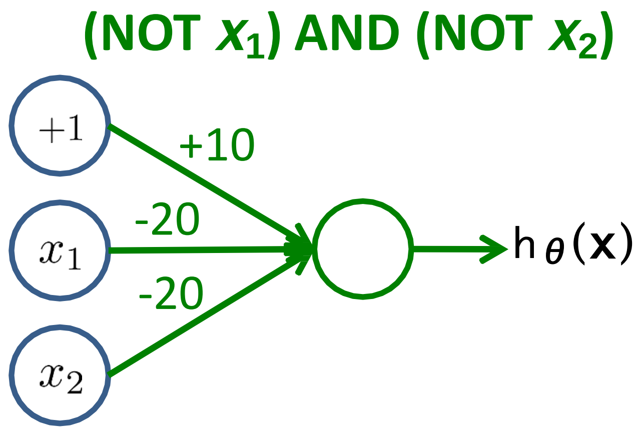


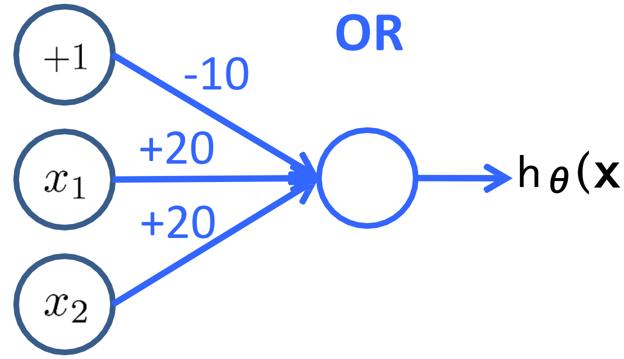

**(NOT $x_1$) AND (NOT $x_2$)**



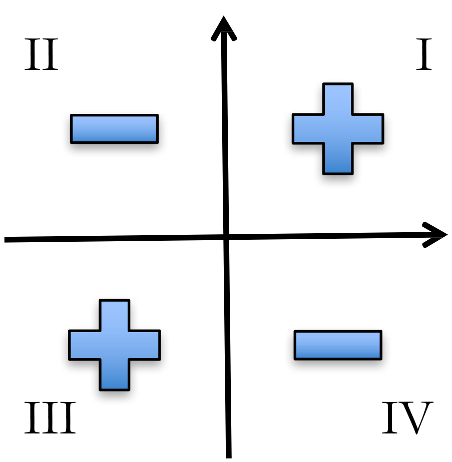
# Combining Representations to Create Non-Linear Functions

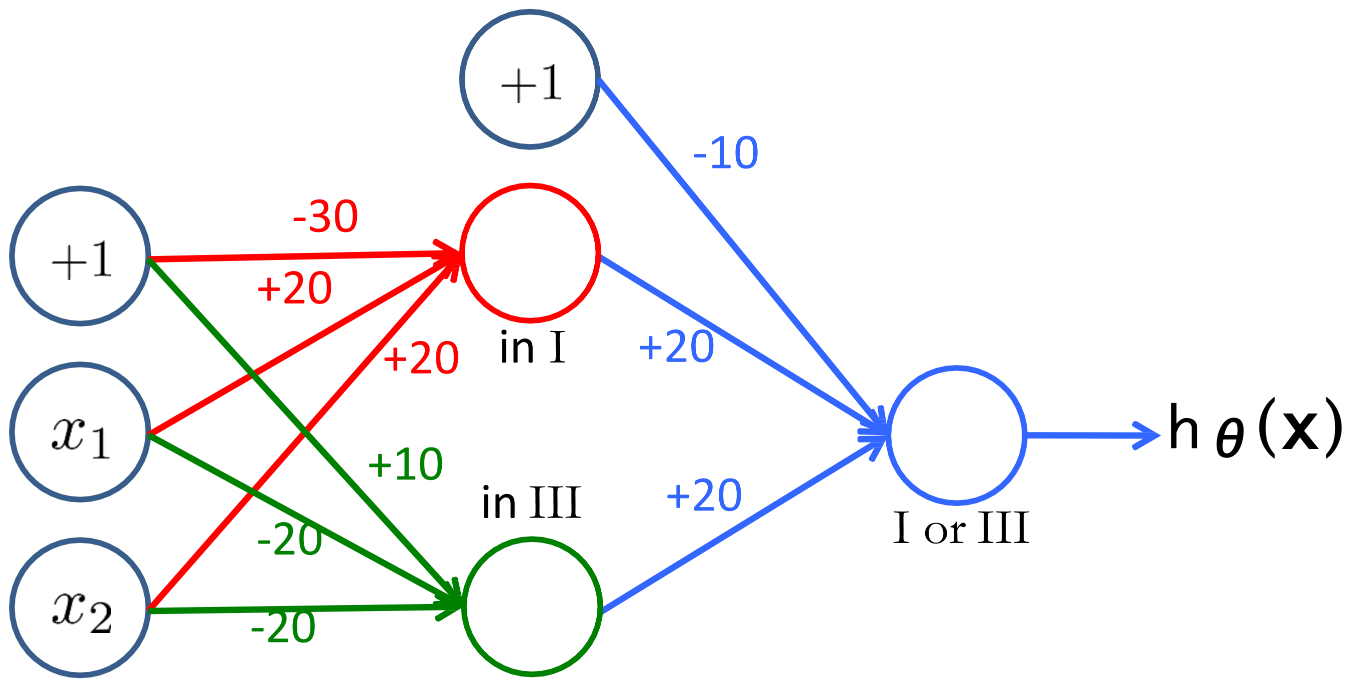


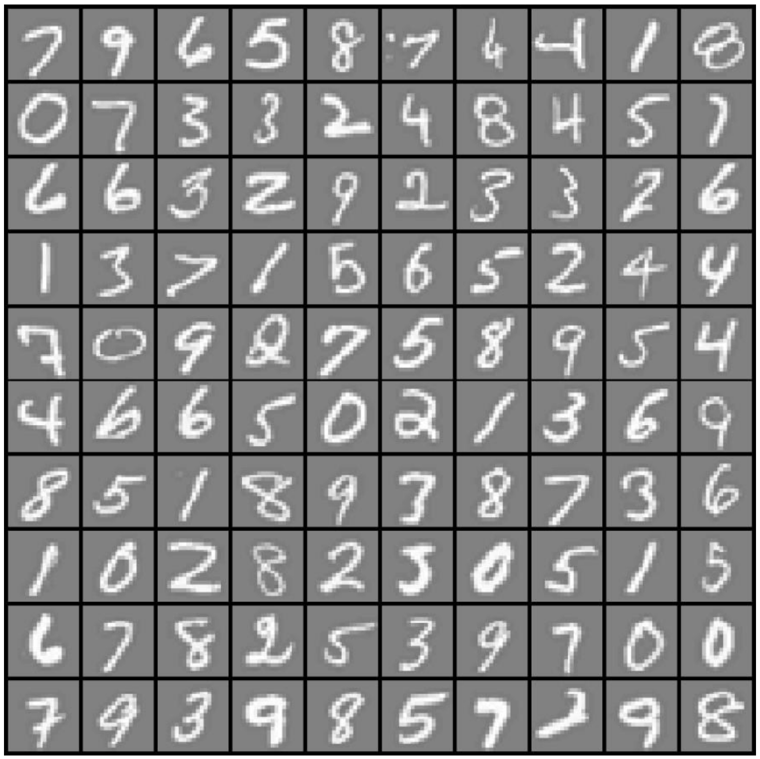

**not(XOR)**



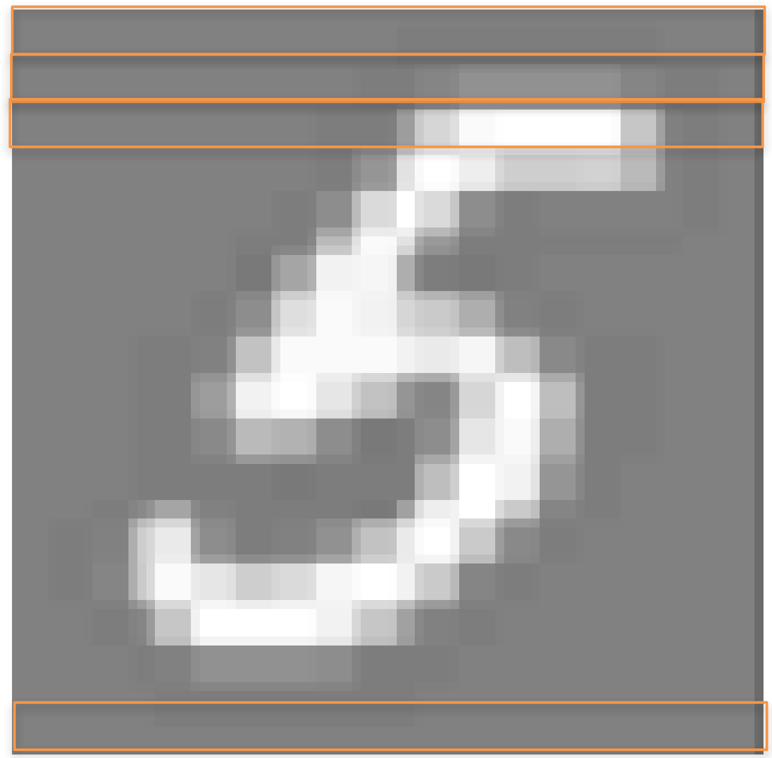

Based on example by Andrew Ng

# Layering Representations



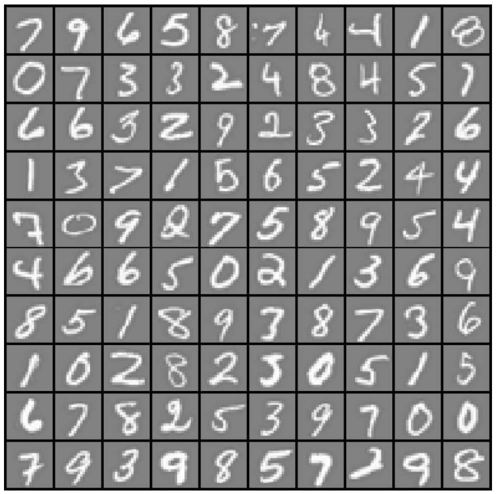
$20 \times 20$ pixel images

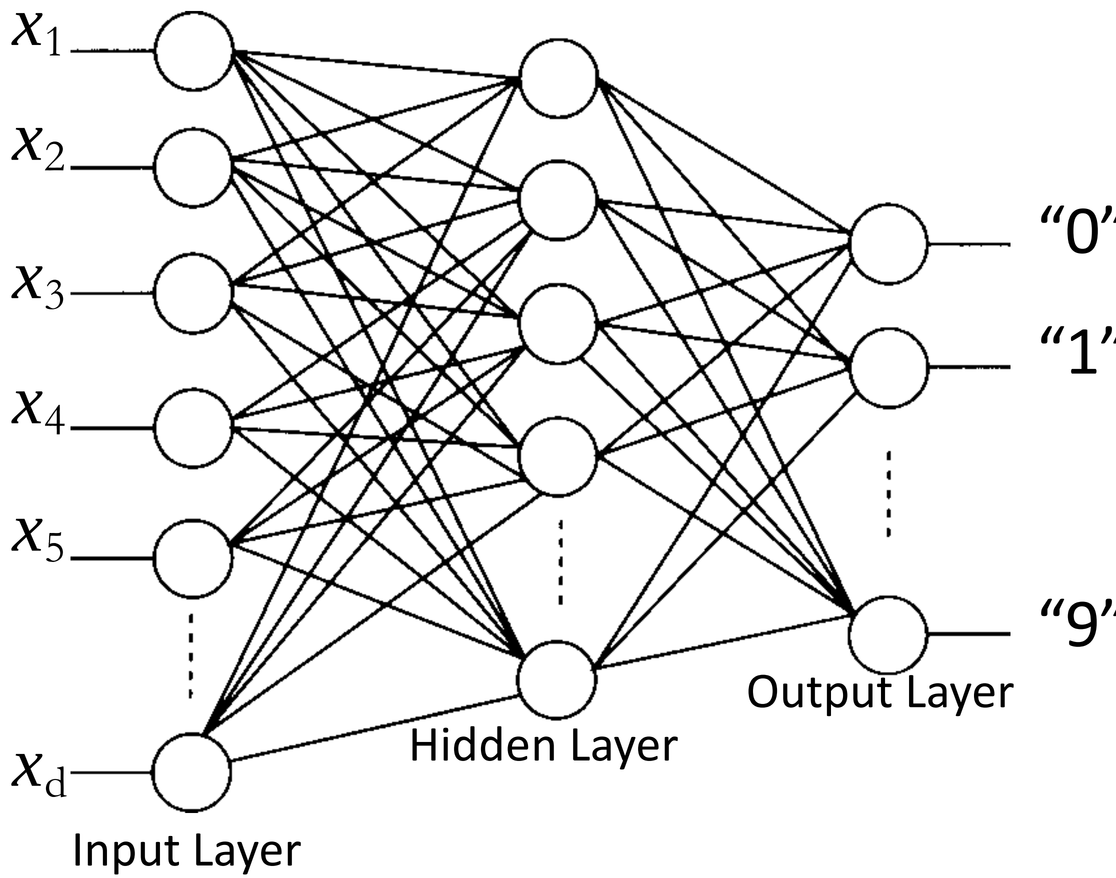
$d = 400$ 10 classes

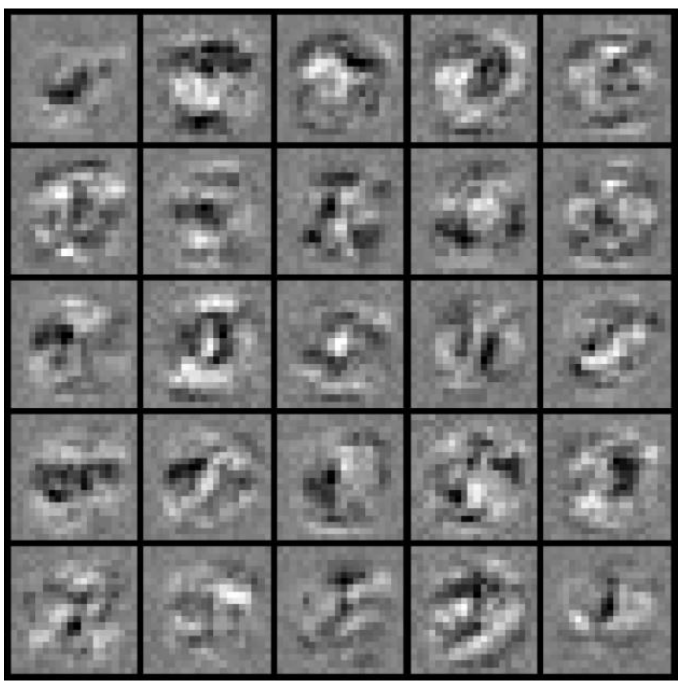



Each image is “unrolled” into a vector **x** of pixel intensities

# Layering Representations

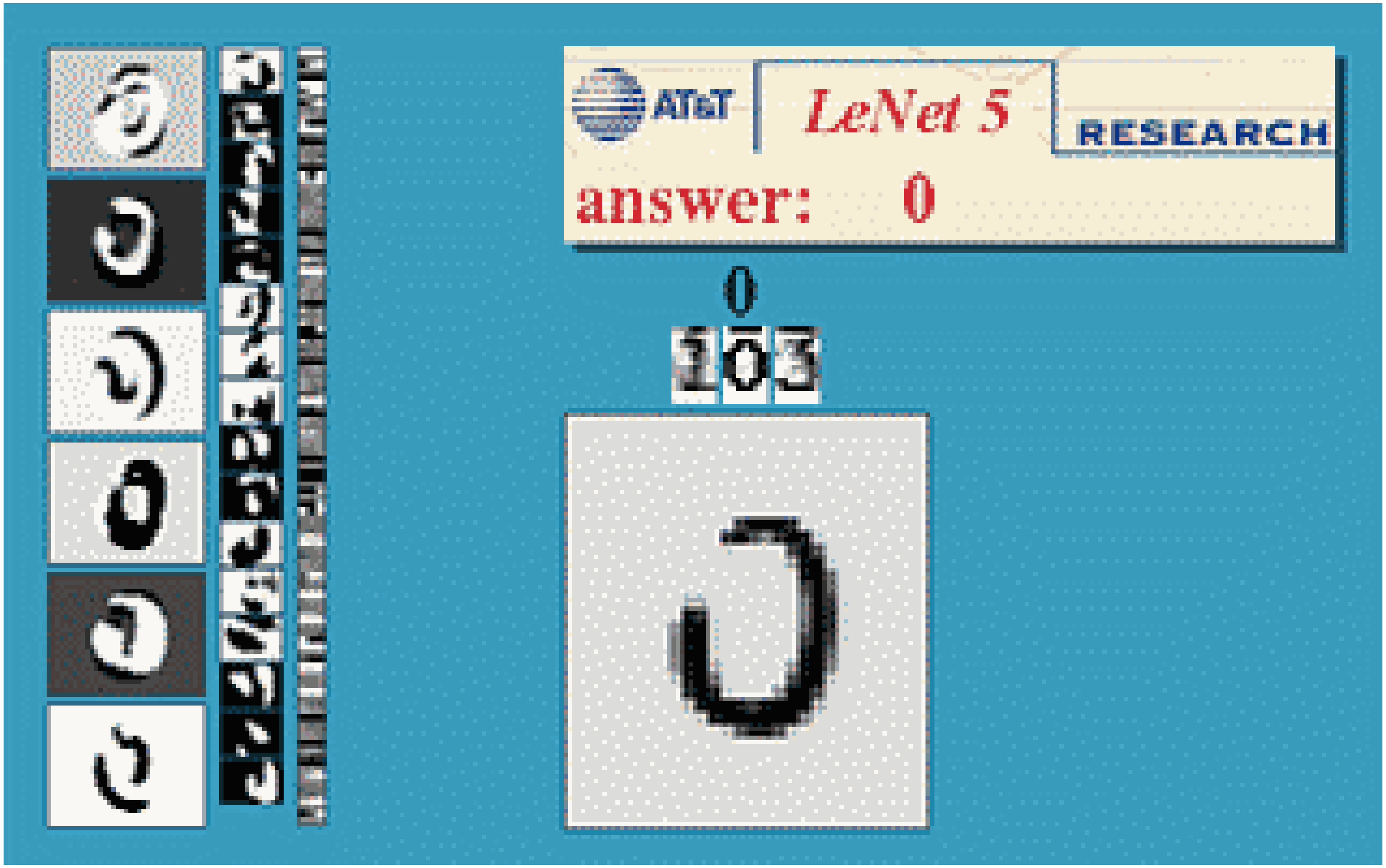




Visualization of Hidden Layer

# Digit Recognition



# Handwriting Recognition

LeNet 5 Demonstration:

http://yann.lecun.com/exdb/lenet/

http://yann.lecun.com/exdb/lenet/weirdos.html

# Perceptron learning rule

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha(y - h(\mathbf{x}))\mathbf{x}$$

Equivalent to the intuitive rules:

- If output is correct, don't change the weights
- If output is low ($h(\mathbf{x})$ = 0, $y$ = 1), increment weights for all the inputs which are 1
- If output is high ($h(\mathbf{x})$ = 1, $y$ = 0), decrement weights for all inputs which are 1

**Perceptron Convergence Theorem**:

- If there is a set of weights that is consistent with the training data (i.e., the data is linearly separable), the perceptron learning algorithm will converge [Minicksy & Papert, 1969]

# Learning in NN: Backpropagation

- Similar to the perceptron learning algorithm, we cycle through our examples
  - If the output of the network is correct, no changes are made
  - If there is an error, weights are adjusted to reduce the error

- The trick is to assess the blame for the error and divide it among the contributing weights

Based on slide by T. Finin, M. desJardins, L Getoor, R. Par

# Cost Function

(9.1 NN video of Andrew Ng)

## Logistic Regression:

$$J(\theta) = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log h_{\boldsymbol{\theta}}(\mathbf{x}_i) + (1-y_i)\log(1-h_{\boldsymbol{\theta}}(\mathbf{x}_i))] + \frac{\lambda}{2n}\sum_{j=1}^{d}\theta_j^2$$

## Neural Network:

$$h_\Theta \in \mathbb{R}^K \qquad (h_\Theta(\mathbf{x}))_i = i^{th}\text{output}$$

$$J(\Theta) = -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{k=1}^{K} y_{ik}\log(h_\Theta(\mathbf{x}_i))_k + (1-y_{ik})\log\left(1-(h_\Theta(\mathbf{x}_i))_k\right)\right]$$

$$+\frac{\lambda}{2n}\sum_{l=1}^{L-1}\sum_{i=1}^{s_{l-1}}\sum_{j=1}^{s_l}\left(\Theta_{ji}^{(l)}\right)^2$$

$k^{\text{th}}$ class: true, predicted
not $k^{\text{th}}$ class: true, predicted

# Optimizing the Neural Network

$$J(\Theta) = -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{k=1}^{K} y_{ik}\log(h_\Theta(\mathbf{x}_i))_k + (1-y_{ik})\log\left(1-(h_\Theta(\mathbf{x}_i))_k\right)\right]$$
$$+\frac{\lambda}{2n}\sum_{l=1}^{L-1}\sum_{i=1}^{s_{l-1}}\sum_{j=1}^{s_l}\left(\Theta_{ji}^{(l)}\right)^2$$

Solve via: $\min_{\Theta} J(\Theta)$

$J(\Theta)$ is not convex, so GD on a neural net yields a local optimum

- But, tends to work well in practice

Need code to compute:

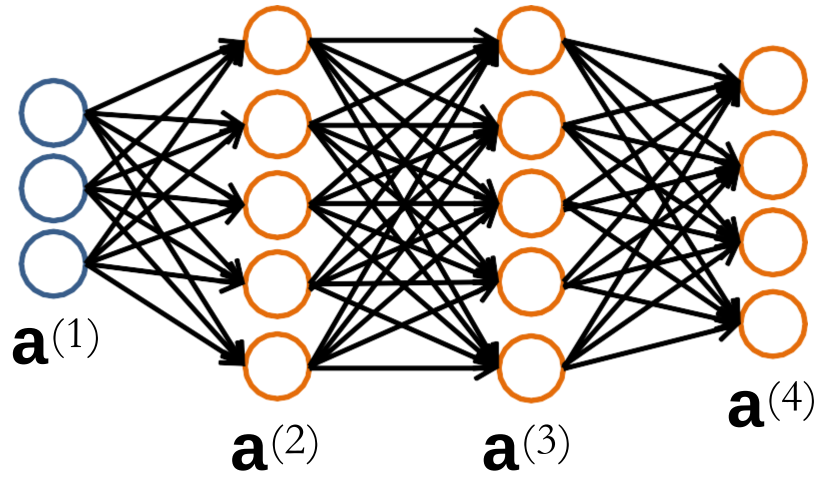
- $J(\Theta)$
- $\frac{\partial}{\partial\Theta_{ij}^{(l)}} J(\Theta)$

# Forward Propagation

- Given one labeled training instance $(\mathbf{x}, y)$:

<u>Forward Propagation</u>

- $\mathbf{a}^{(1)} = \mathbf{x}$
- $\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{a}^{(1)}$
- $\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$ [add $\mathrm{a}_0{}^{(2)}$]
- $\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$
- $\mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$ [add $\mathrm{a}_0{}^{(3)}$]
- $\mathbf{z}^{(4)} = \Theta^{(3)}\mathbf{a}^{(3)}$
- $\mathbf{a}^{(4)} = \mathrm{h}_\Theta(\mathbf{x}) = g(\mathbf{z}^{(4)})$



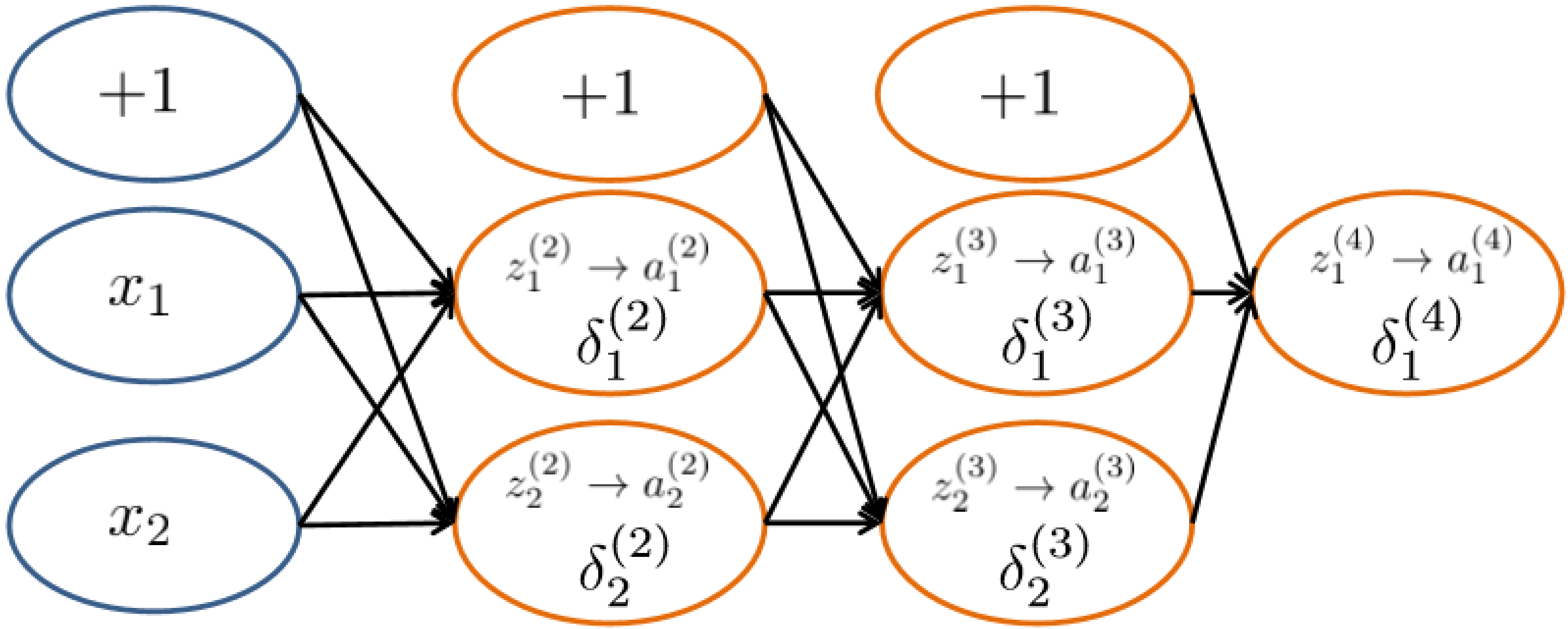
# Backpropagation Intuition

- Each hidden node $j$ is "responsible" for some fraction of the error $\delta_j^{(l)}$ in each of the output nodes to which it connects

- $\delta_j^{(l)}$ is divided according to the strength of the connection between hidden node and the output node

- Then, the "blame" is propagated back to provide the error values for the hidden layer

# Backpropagation Intuition

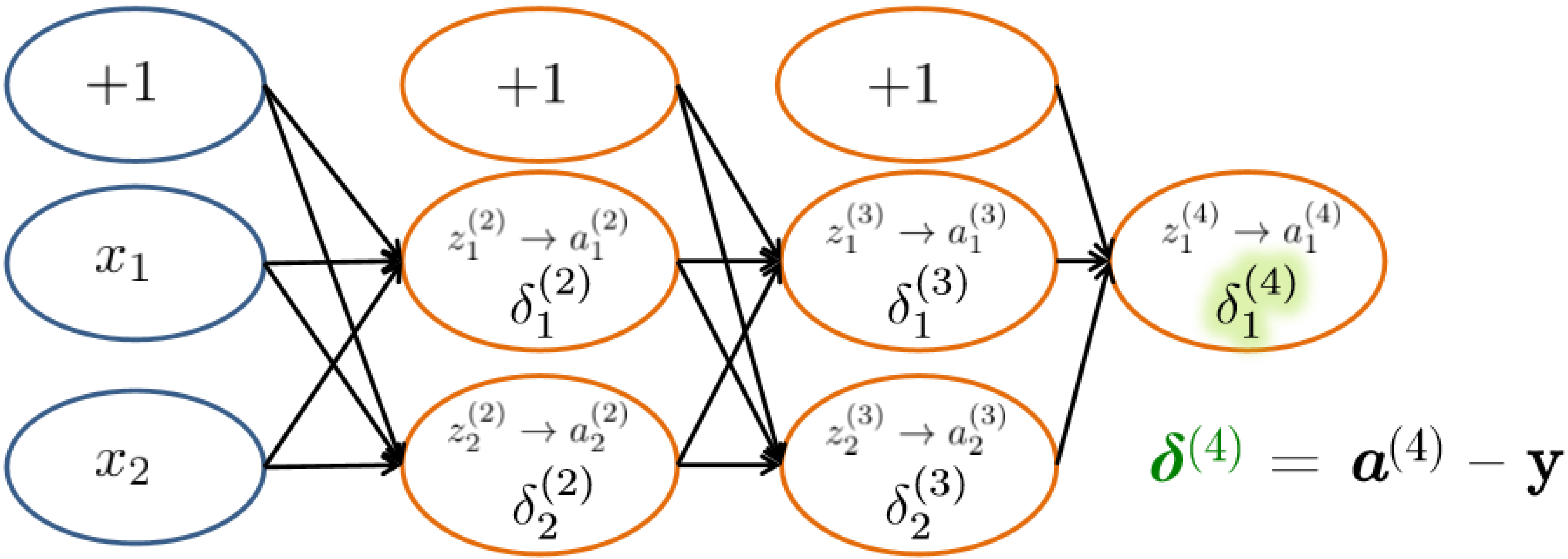



$\delta_j^{(l)} =$ "error" of node $j$ in layer $l$

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

$$\text{where } \text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

# Backpropagation Intuition

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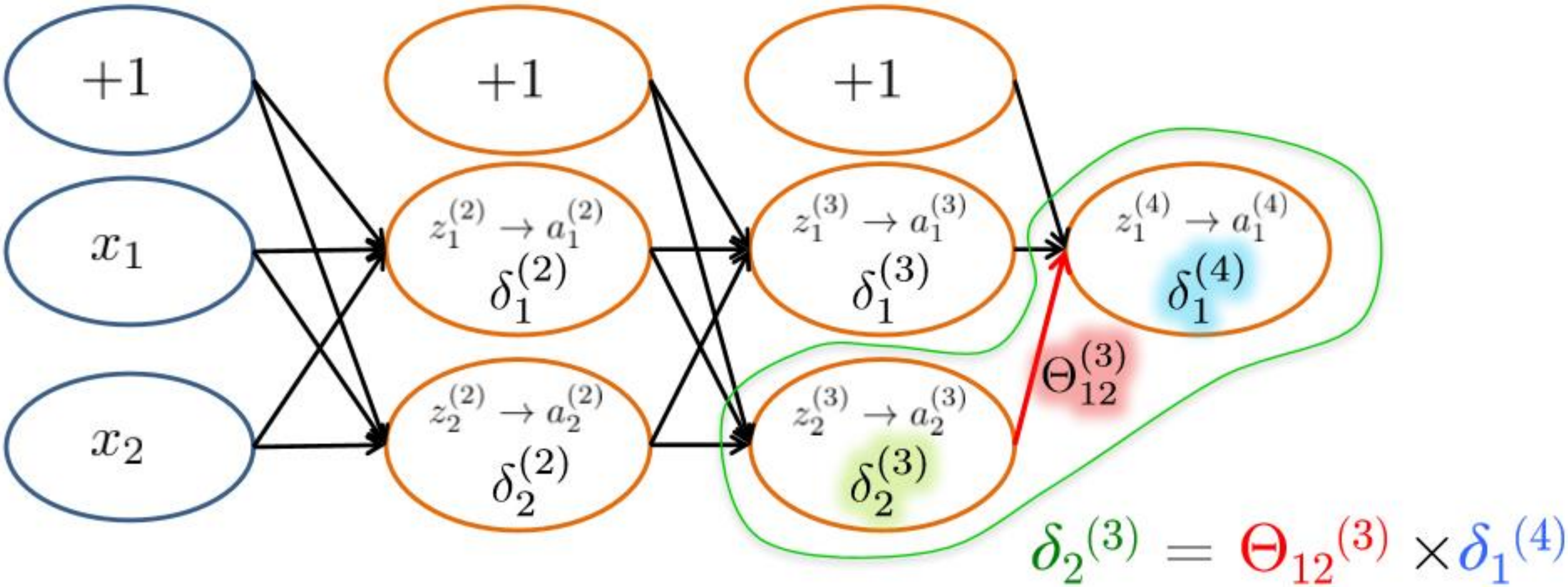
# Backpropagation Intuition

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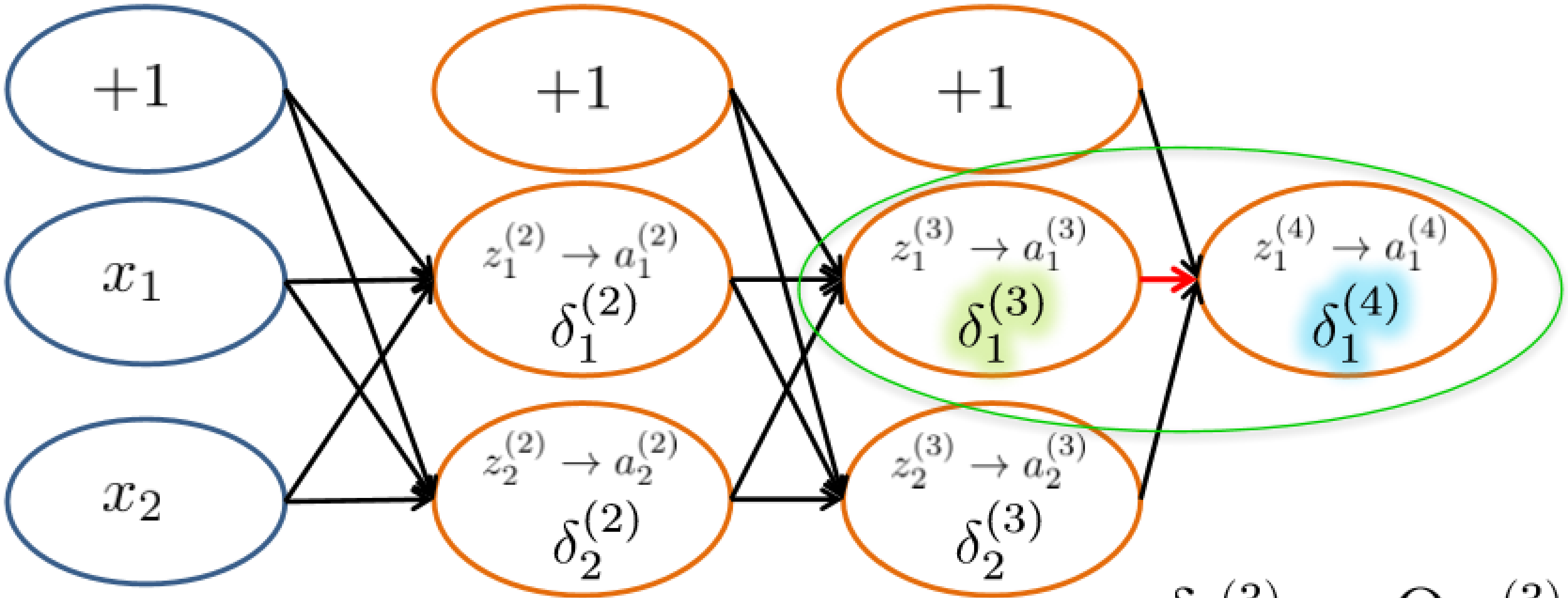
Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \mathrm{cost}(\mathbf{x}_i)$

$$\text{where } \mathrm{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

# Backpropagation Intuition




$$\delta_2^{(3)} = \Theta_{12}^{(3)} \times \delta_1^{(4)}$$

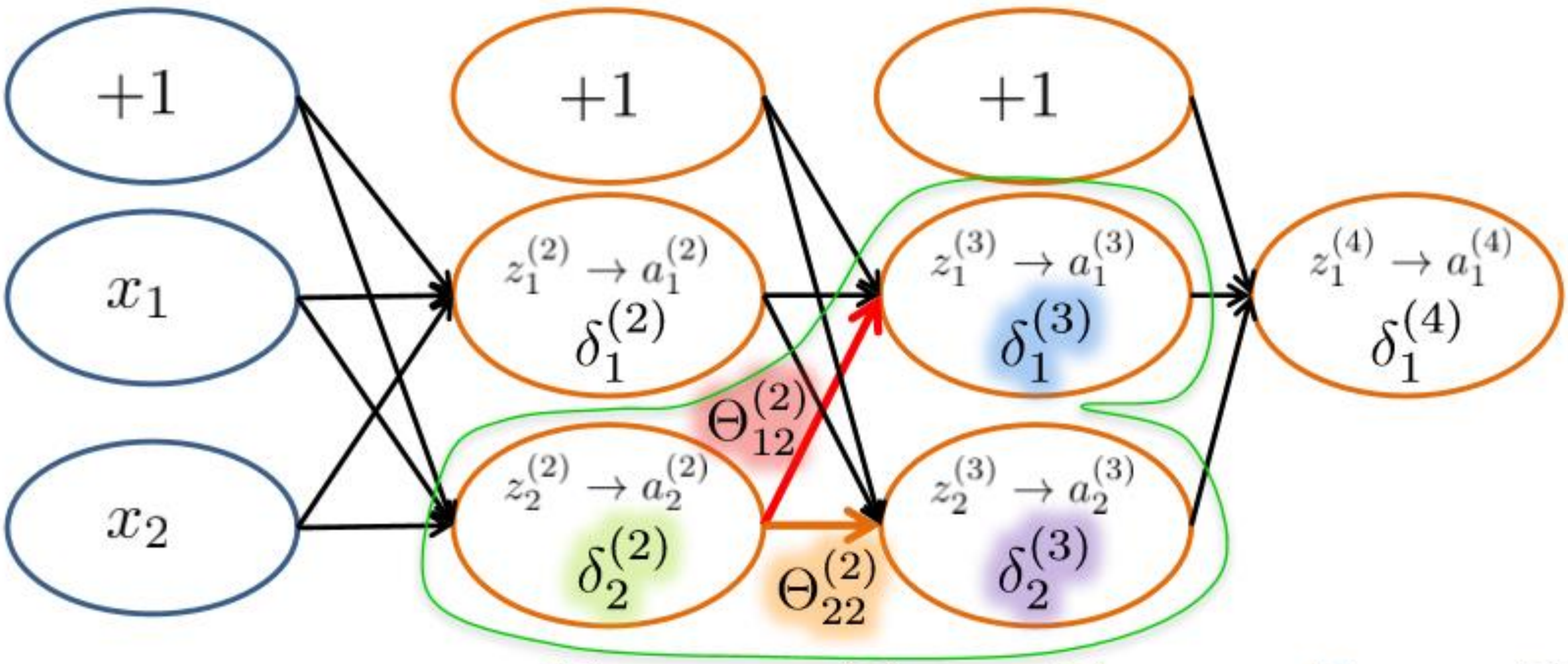
$$\delta_1^{(3)} = \Theta_{11}^{(3)} \times \delta_1^{(4)}$$

$\delta_j^{(l)} =$ "error" of node $j$ in layer $l$

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

$$\text{where cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

# Backpropagation Intuition




$$\delta_2^{(2)} = \Theta_{12}^{(2)} \times \delta_1^{(3)} + \Theta_{22}^{(2)} \times \delta_2^{(3)}$$

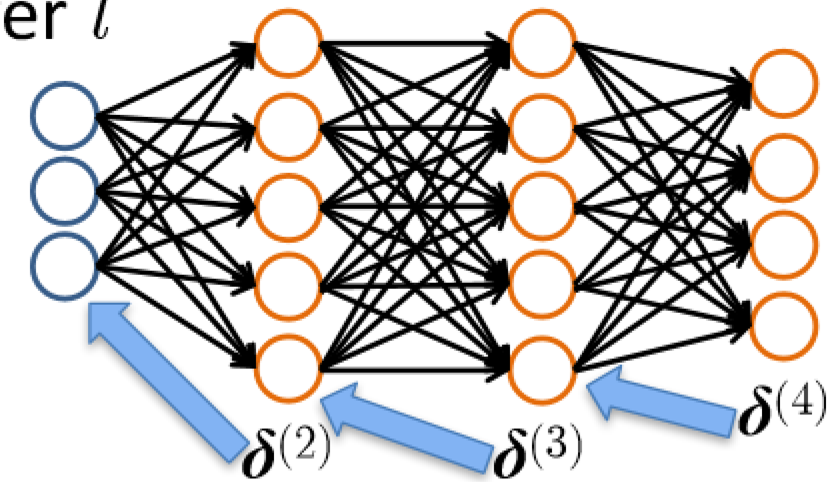
$\delta_j^{(l)} =$ "error" of node $j$ in layer $l$

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \mathrm{cost}(\mathbf{x}_i)$

$$\text{where } \mathrm{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

# Backpropagation: Gradient Computation

Let $\delta_j^{(l)}$ = "error" of node $j$ in layer $l$




(#layers $L$ = 4)

Element-wise product .*

<u>Backpropagation</u>

- $\boldsymbol{\delta}^{(4)} = \boldsymbol{a}^{(4)} - \mathbf{y}$
- $\boldsymbol{\delta}^{(3)} = (\Theta^{(3)})^\mathsf{T}\boldsymbol{\delta}^{(4)} \;.\!*\; \boxed{g'(\mathbf{z}^{(3)})}$
- $\boldsymbol{\delta}^{(2)} = (\Theta^{(2)})^\mathsf{T}\boldsymbol{\delta}^{(3)} \;.\!*\; \boxed{g'(\mathbf{z}^{(2)})}$
- (No $\boldsymbol{\delta}^{(1)}$)

$g'(\mathbf{z}^{(3)}) = \mathbf{a}^{(3)} \;.\!*\; (1 - \mathbf{a}^{(3)})$

$g'(\mathbf{z}^{(2)}) = \mathbf{a}^{(2)} \;.\!*\; (1 - \mathbf{a}^{(2)})$

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$$ (ignoring λ; if $\lambda = 0$)

# Backpropagation

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)

For each training instance $(\mathbf{x}_i, y_i)$:

Set $\mathbf{a}^{(1)} = \mathbf{x}_i$

Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation

Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_i$

Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \ldots, \boldsymbol{\delta}^{(2)}\}$

Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

$\boldsymbol{D}^{(l)}$ is the matrix of partial derivatives of $J(\Theta)$

Note: Can vectorize $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ as $\boldsymbol{\Delta}^{(l)} = \boldsymbol{\Delta}^{(l)} + \boldsymbol{\delta}^{(l+1)} \mathbf{a}^{(l)\mathsf{T}}$

# Backpropagation

Given: training set $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
Initialize all $\Theta^{(l)}$ randomly (NOT to 0!)
Loop // each iteration is called an epoch

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)
For each training instance $(\mathbf{x}_i, y_i)$:
Set $\mathbf{a}^{(1)} = \mathbf{x}_i$
Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation
Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_i$
Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \ldots, \boldsymbol{\delta}^{(2)}\}$
Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$
Until weights converge or max #epochs is reached

Backpropagation

# Backprop Issues

“Backprop is the cockroach of machine learning. It’s ugly, and annoying, but you just can’t get rid of it.”

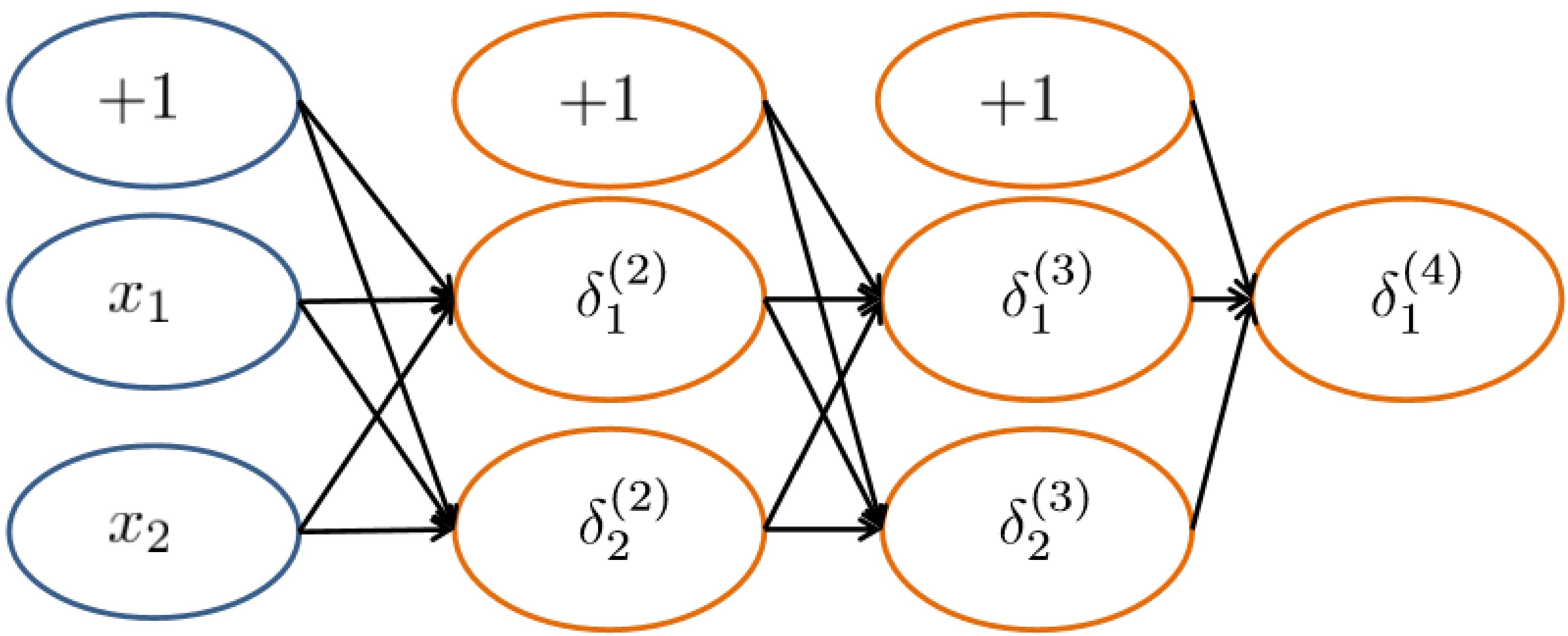
–Geoff Hinton

Problems:

- black box
- local minima

# Random Initialization

- Important to randomize initial weight matrices
- Can't have uniform initial weights, as in logistic regression
  - Otherwise, all updates will be identical & the net won't learn



# Implementation Details

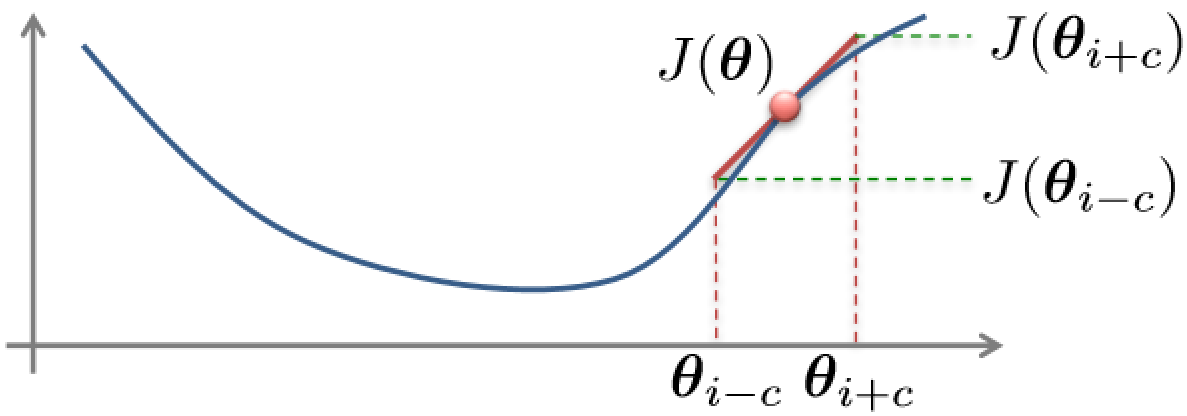
- For convenience, compress all parameters into $\boldsymbol{\theta}$
  - "unroll" $\Theta^{(1)}$, $\Theta^{(2)}$,... , $\Theta^{(\text{L-1})}$ into one long vector $\boldsymbol{\theta}$
    - E.g., if $\Theta^{(1)}$ is 10 x 10, then the first 100 entries of $\boldsymbol{\theta}$ contain the value in $\Theta^{(1)}$
  - Use the `reshape` command to recover the original matrices
    - E.g., if $\Theta^{(1)}$ is 10 x 10, then

```
theta1 = reshape(theta[0:100], (10, 10))
```

- Each step, check to make sure that $J(\boldsymbol{\theta})$ decreases
- Implement a gradient-checking procedure to ensure that the gradient is correct...

# Gradient Checking

**Idea:** estimate gradient numerically to verify implementation, then turn off gradient checking




$$\frac{\partial}{\partial \theta_i} J(\boldsymbol{\theta}) \approx \frac{J(\boldsymbol{\theta}_{i+c}) - J(\boldsymbol{\theta}_{i-c})}{2c} \qquad c \approx 1\text{E-4}$$

$$\boldsymbol{\theta}_{i+c} = [\theta_1,\ \theta_2,\ \ldots,\ \theta_{i-1},\ \theta_i + c,\ \theta_{i+1},\ \ldots]$$

Change ONLY the $i$ th entry in $\boldsymbol{\theta}$, increasing (or decreasing) it by $c$

# Gradient Checking

$$\boldsymbol{\theta} \in \mathbb{R}^m \qquad \boldsymbol{\theta} \text{ is an "unrolled" version of } \Theta^{(1)}, \Theta^{(2)}, \ldots$$

$$\boldsymbol{\theta} = [\theta_1, \theta_2, \theta_3, \ldots, \theta_m]$$

Put in vector called `gradApprox`

$$\frac{\partial}{\partial \theta_1} J(\boldsymbol{\theta}) \approx \frac{J([\theta_1 + c, \theta_2, \theta_3, \ldots, \theta_m]) - J([\theta_1 - c, \theta_2, \theta_3, \ldots, \theta_m])}{2c}$$

$$\frac{\partial}{\partial \theta_2} J(\boldsymbol{\theta}) \approx \frac{J([\theta_1, \theta_2 + c, \theta_3, \ldots, \theta_m]) - J([\theta_1, \theta_2 - c, \theta_3, \ldots, \theta_m])}{2c}$$

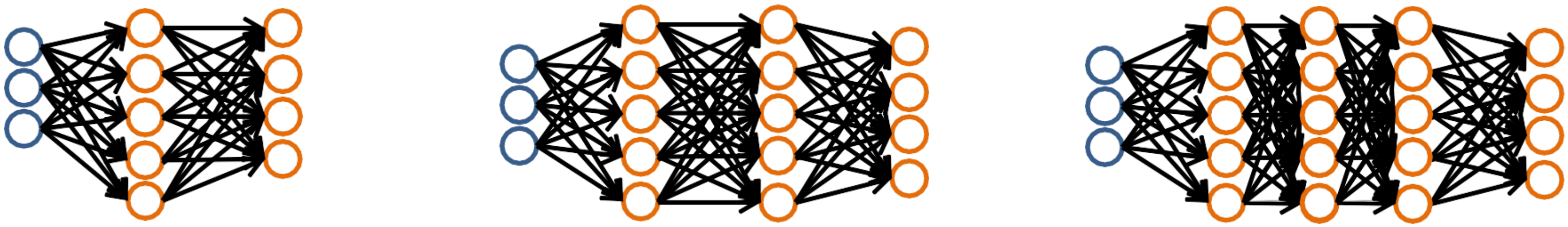
$$\vdots$$

$$\frac{\partial}{\partial \theta_m} J(\boldsymbol{\theta}) \approx \frac{J([\theta_1, \theta_2, \theta_3, \ldots, \theta_m + c]) - J([\theta_1, \theta_2, \theta_3, \ldots, \theta_m - c])}{2c}$$

Check that the approximate numerical gradient matches the entries in the $D$ matrices

# Training a Neural Network

Pick a network architecture (connectivity pattern between nodes)



- # input units = # of features in dataset
- # output units = # classes

**Reasonable default:** 1 hidden layer

- or if >1 hidden layer, have same # hidden units in every layer (usually the more the better)

Based on slide by Andrew Ng

# Training a Neural Network

1. Randomly initialize weights
2. Implement forward propagation to get $h_\Theta(\mathbf{x}_i)$ for any instance $\mathbf{x}_i$
3. Implement code to compute cost function $J(\Theta)$
4. Implement backprop to compute partial derivatives $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$
5. Use gradient checking to compare $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$ computed using backpropagation vs. the numerical gradient estimate.
   - Then, disable gradient checking code
6. Use gradient descent with backprop to fit the network

# Good References for understanding Neural Network

Andrew Ng videos on neural network

https://www.youtube.com/watch?v=EVeqrPGfuCY&list=PLLssT5z_DsK-h9vYZkQkYNWcItqhlRJLN&index=45

Autonomous driving using neural network

https://www.youtube.com/watch?v=ppFyPUx9RIU&list=PLLssT5z_DsK-h9vYZkQkYNWcItqhlRJLN&index=57