Machine Learning
DSECL ZG565

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Lecture No. – 9 | Neural Network

Date – 29/11/2020

Time – 1:55 PM – 04:05 PM

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)

Artificial Neural Network

- Artificial neural networks (ANNs) provide a general, practical method for learning real-valued, discrete-valued, and vector-valued functions from examples.
- Successfully applied to problems
  - Interpreting visual scenes
  - Speech recognition
  - Recognize handwritten character
  - Face recognition

Rumelhart, D., Widrow, B., & Lehr, M. (1994). The basic ideas in neural networks. Communications of the ACM, 37(3), 87-92.

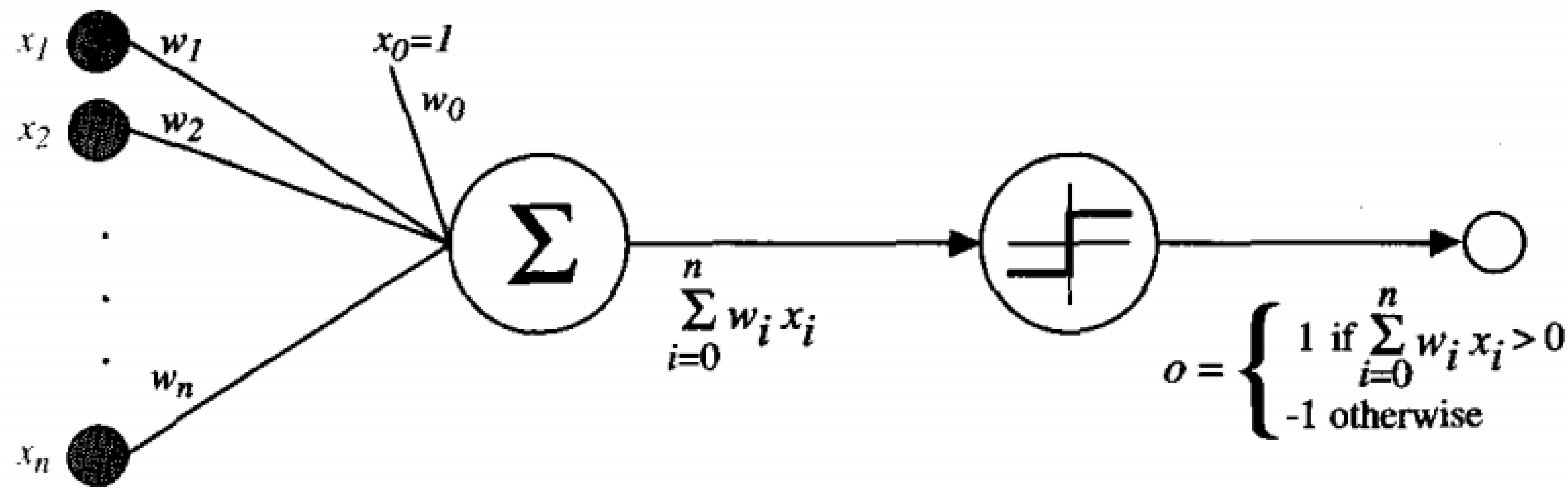
Neural Networks

- 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

When to use Neural Network

- 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

Perceptron



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

Sometimes we'll use simpler vector notation:

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

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
- η is small constant (e.g., .1) called *learning rate*

Gradient Descent

To understand, consider simpler *linear unit*, where

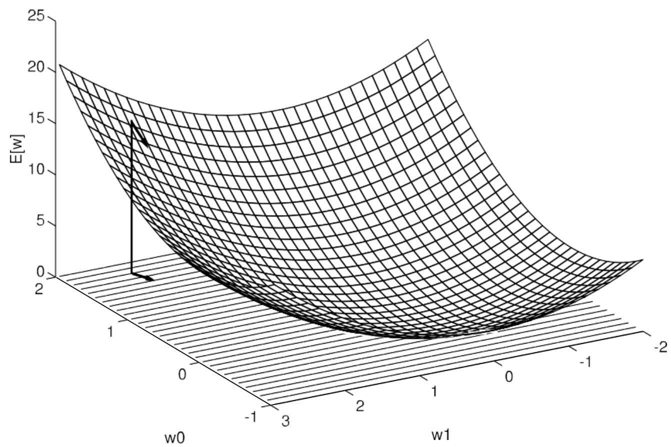
$$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$

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

GRADIENT-DESCENT(*training_examples*, η)

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. η 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 Δw_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

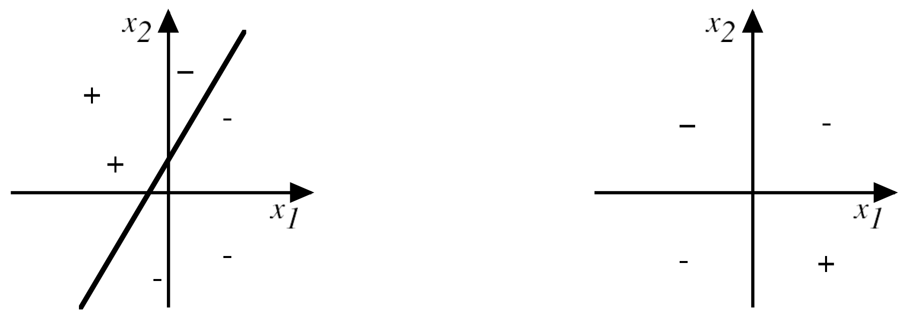
Perceptron training rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate η

Linear unit training rule uses gradient descent

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

Decision Surface of Perceptron



(a) (b)

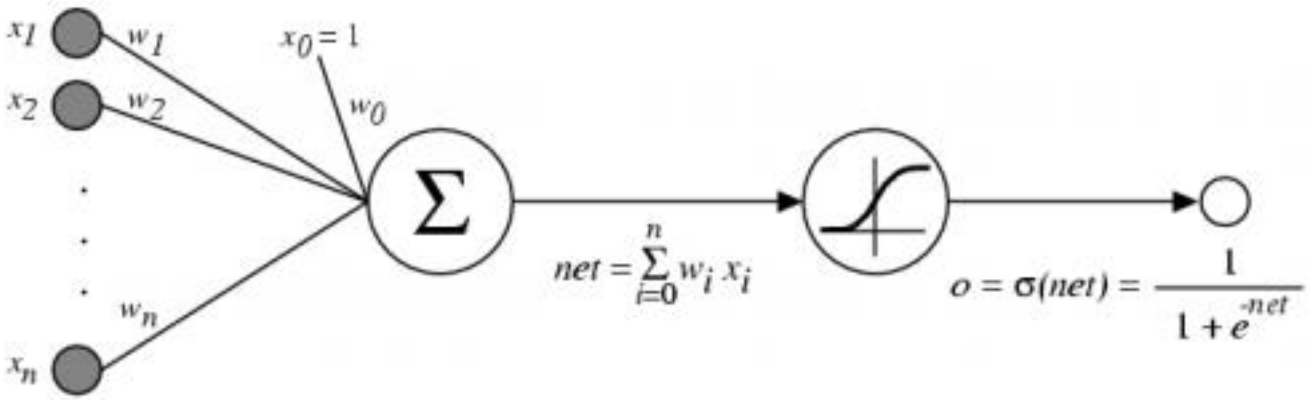
Represents some useful functions

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

But some functions not representable

- e.g., not linearly separable
- ..

Perceptron: Sigmoid Function



$$
\begin{aligned}
g'(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\
&= \frac{1}{(1+e^{-z})^2}\left(e^{-z}\right) \\
&= \frac{1}{(1+e^{-z})}\cdot\left(1-\frac{1}{(1+e^{-z})}\right) \\
&= g(z)(1-g(z)).
\end{aligned}
$$

$\sigma(x)$ is the sigmoid function

$$\frac{1}{1+e^{-x}}$$

Nice property: $\frac{d\sigma(x)}{dx} = \sigma(x)(1-\sigma(x))$

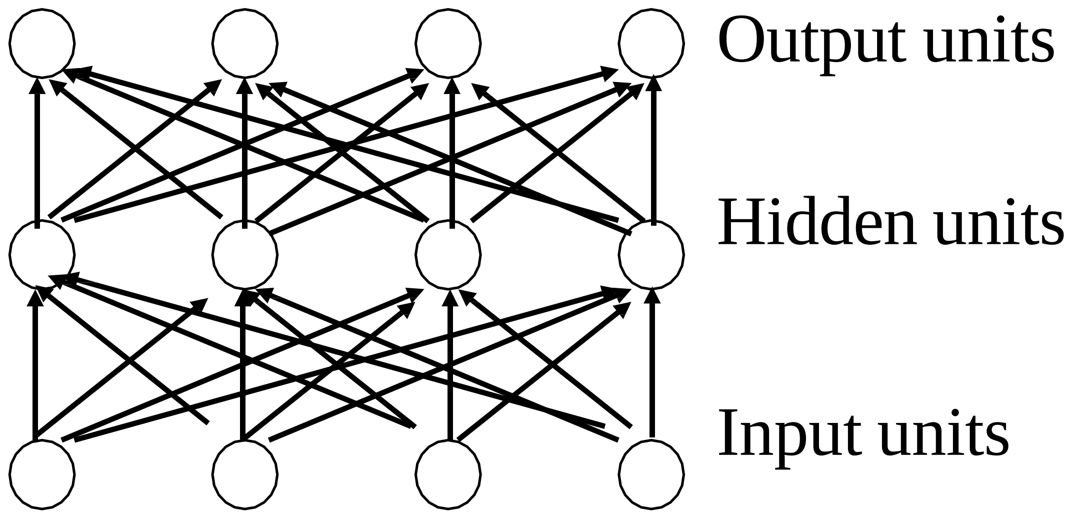
We can derive gradient decent rules to train

- One sigmoid unit
- *Multilayer networks* of sigmoid units $\rightarrow$ Backpropagation

Multilayer network

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

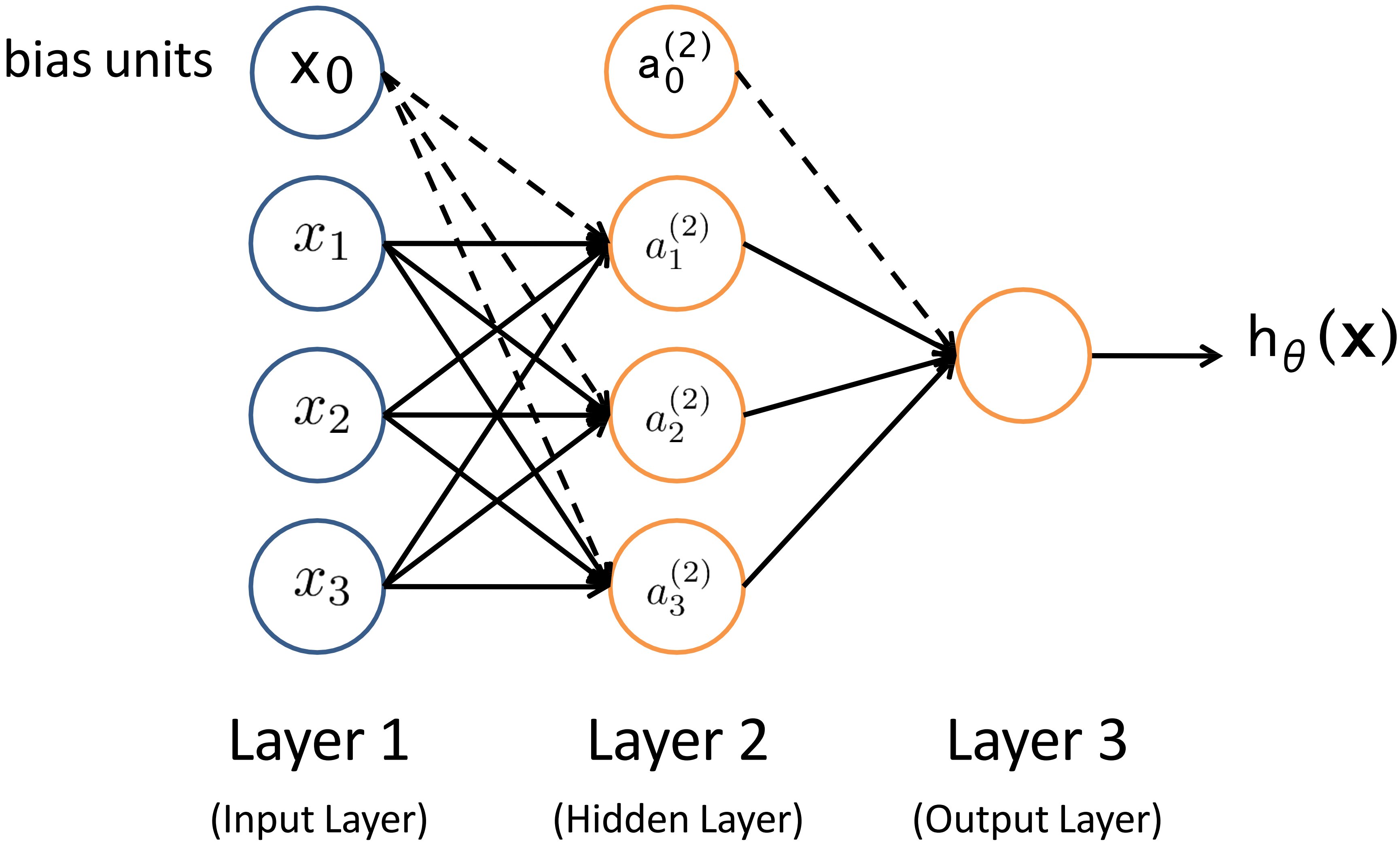
Neural networks



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

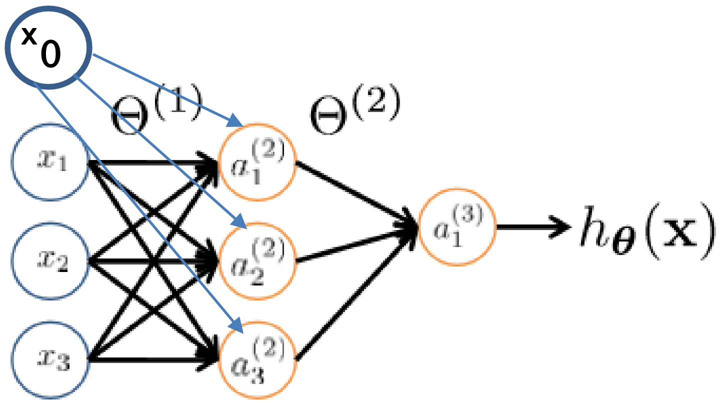
- Input layer units are set by some exterior function (think of these as **sensors**), which causes their output links to be **activated** at the specified level

- 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} × (s_j+1) .

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

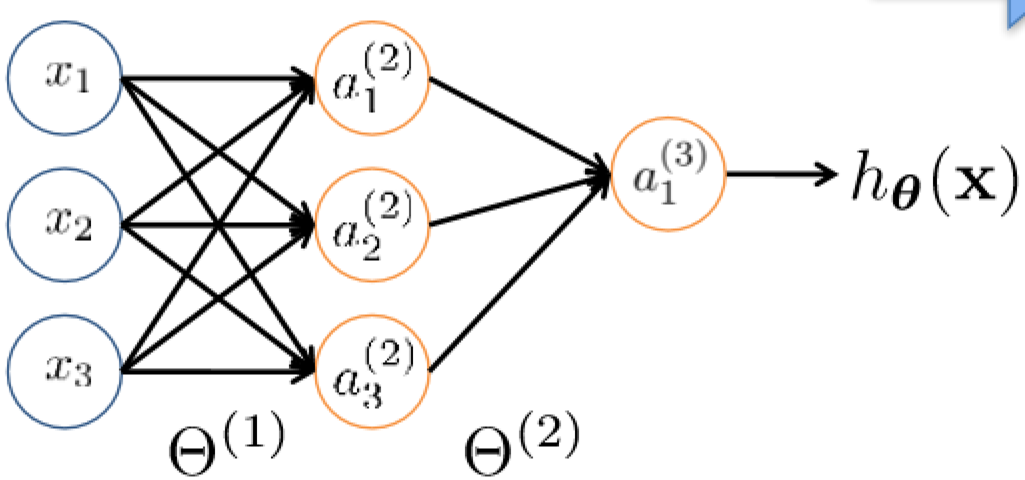
Vectorization

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

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

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

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



Feed-Forward Steps:

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

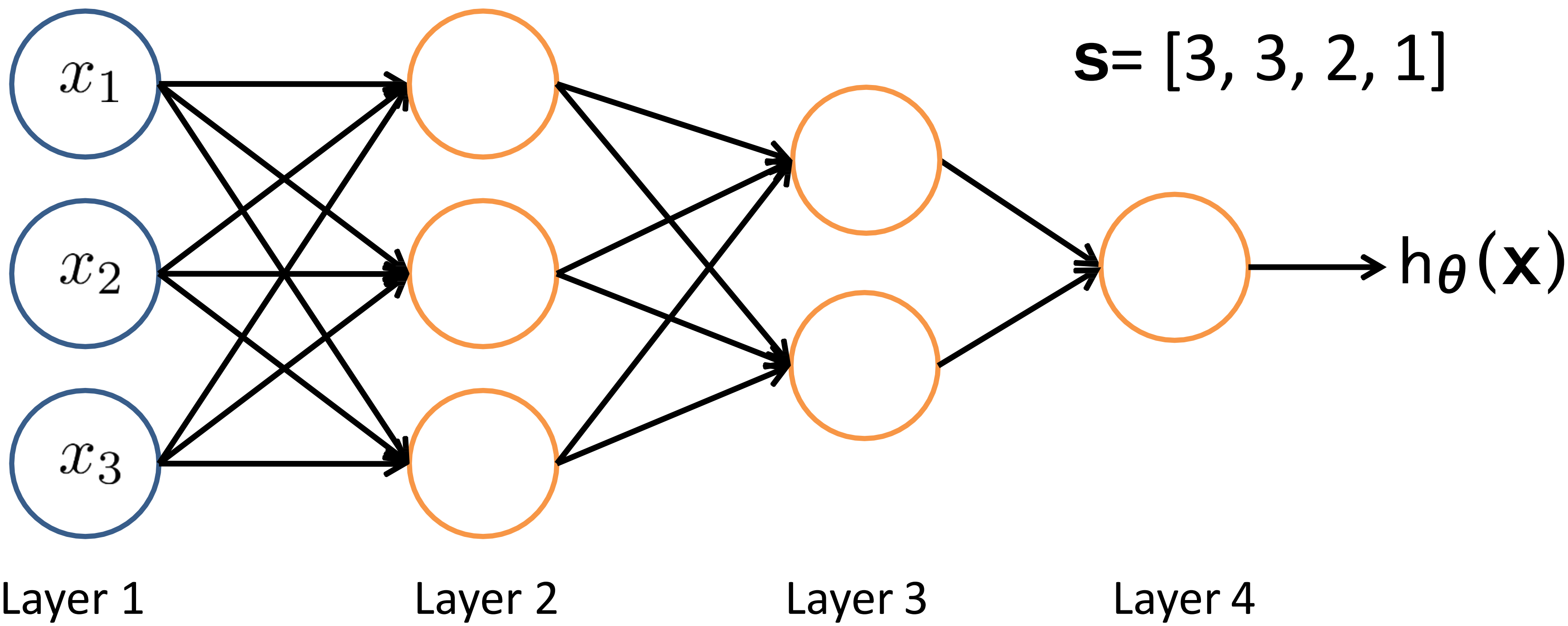
$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

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

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

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

Other Network Architectures



L denotes the number of layers

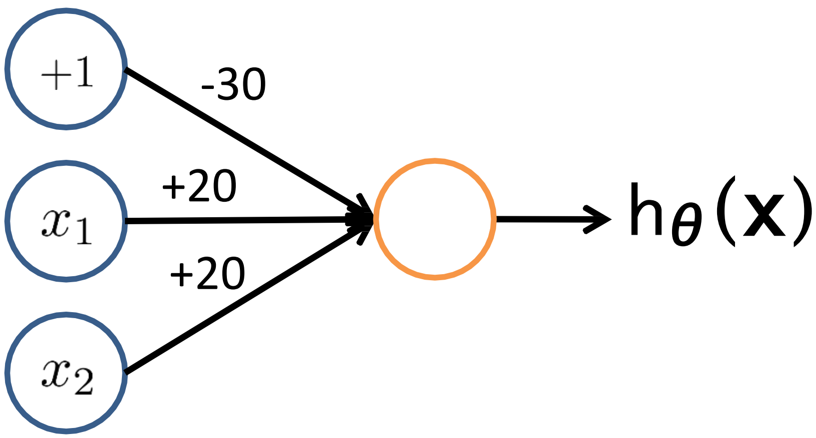
s $\in \mathbb{N}^{+L}$ contains the numbers of nodes at each layer

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

Representing Boolean Functions

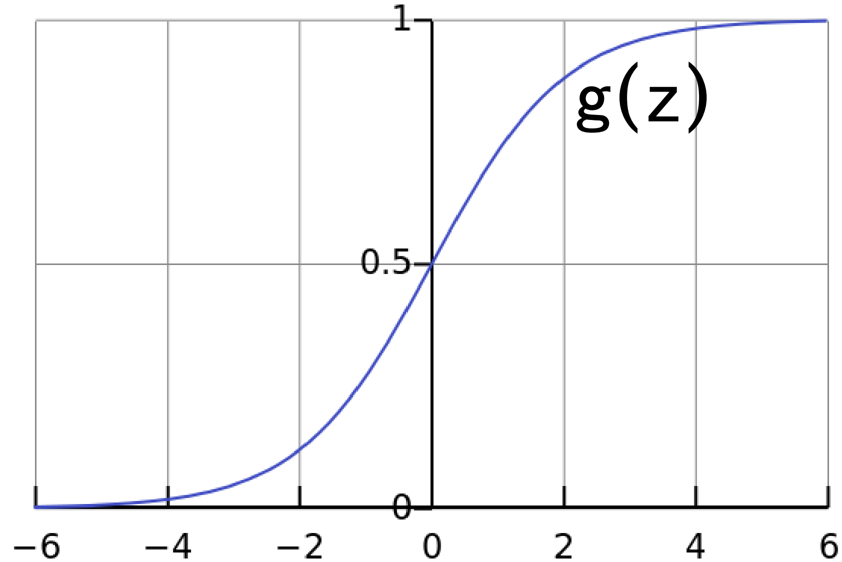
Simple example: AND

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



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

Logistic / Sigmoid Function

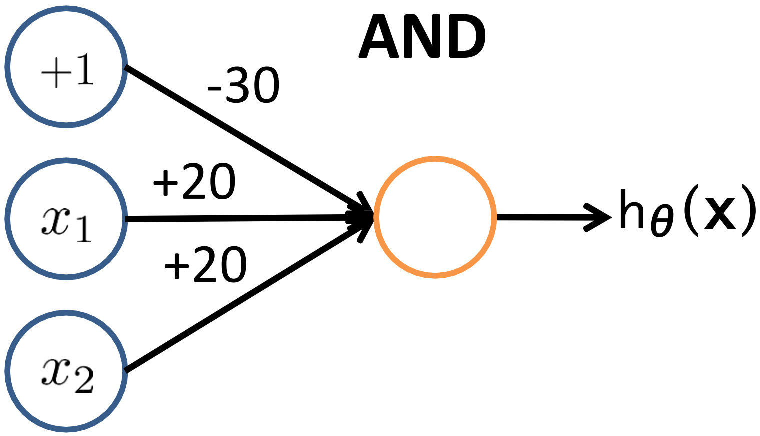


x_1	x_2	$h_\Theta(\mathbf{x})$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

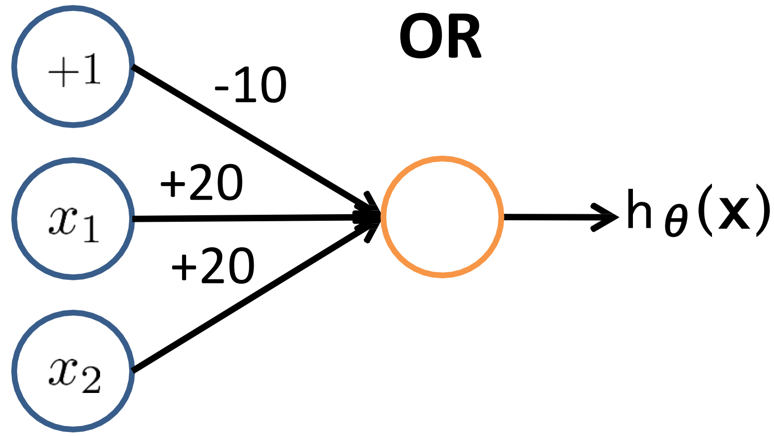
Based on slide and example by Andrew Ng

Representing Boolean Functions

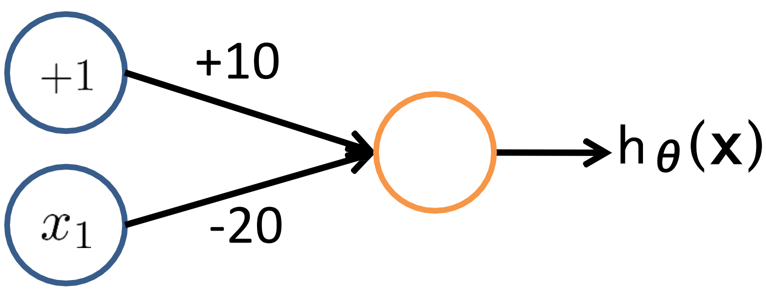
AND



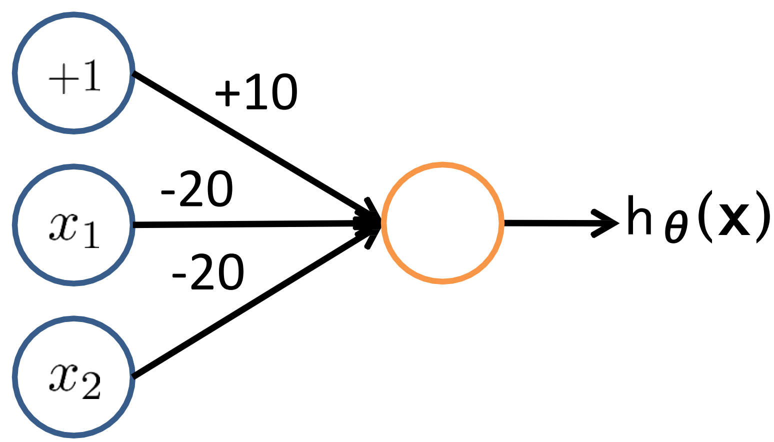
OR



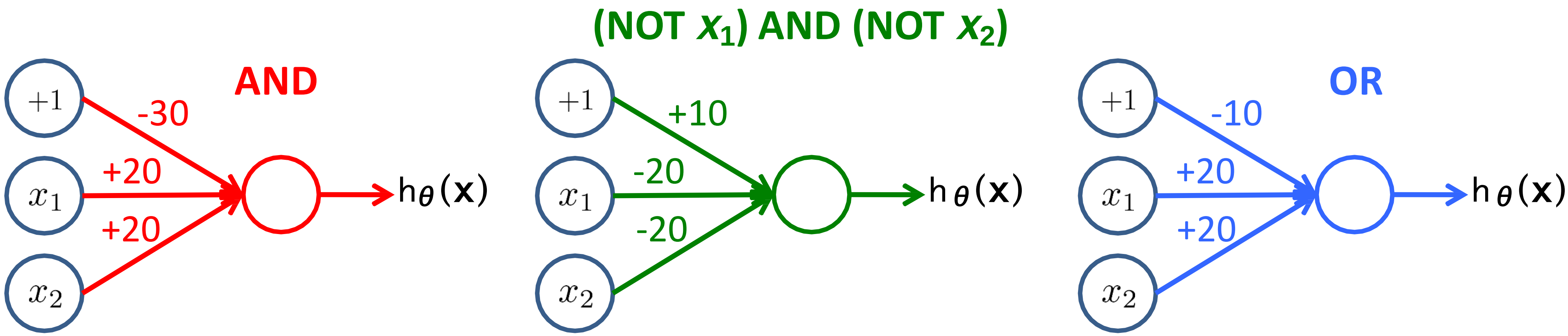
NOT

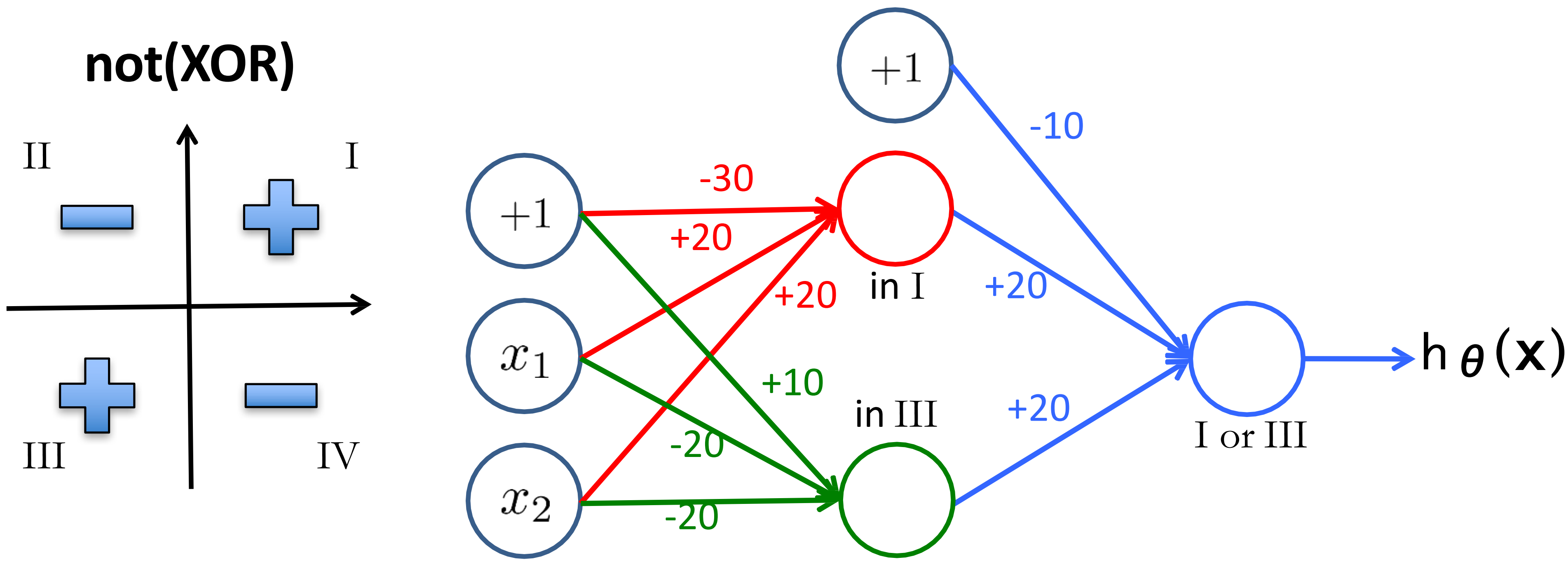


(NOT x_1) AND (NOT x_2)



Combining Representations to Create Non-Linear Functions





Based on example by Andrew Ng

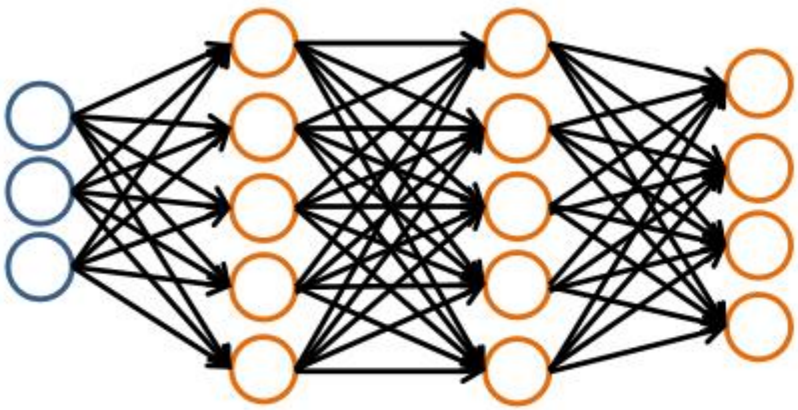
Multiple Output Units:One-vs-Rest

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

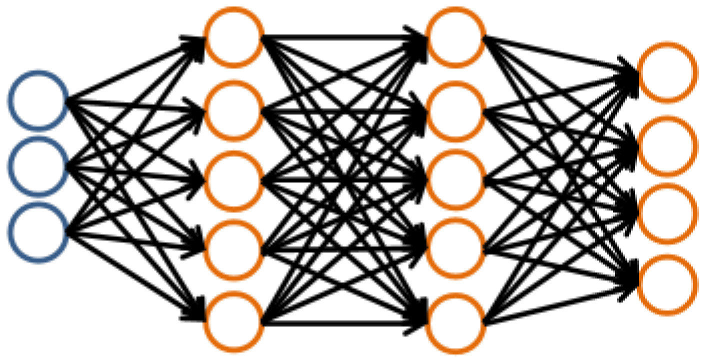
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

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

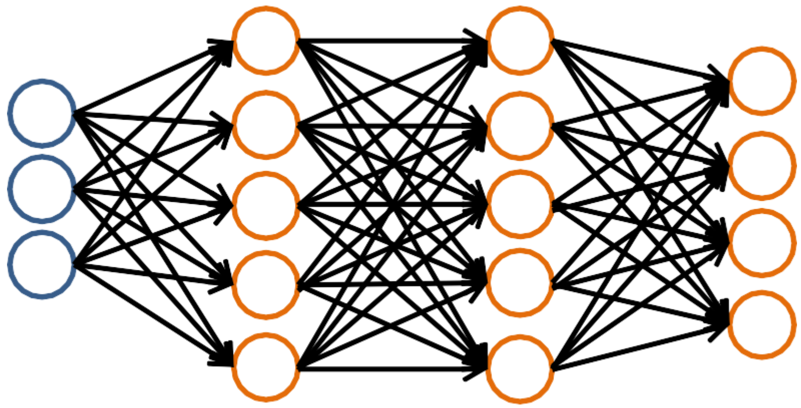
$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ when car

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

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

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

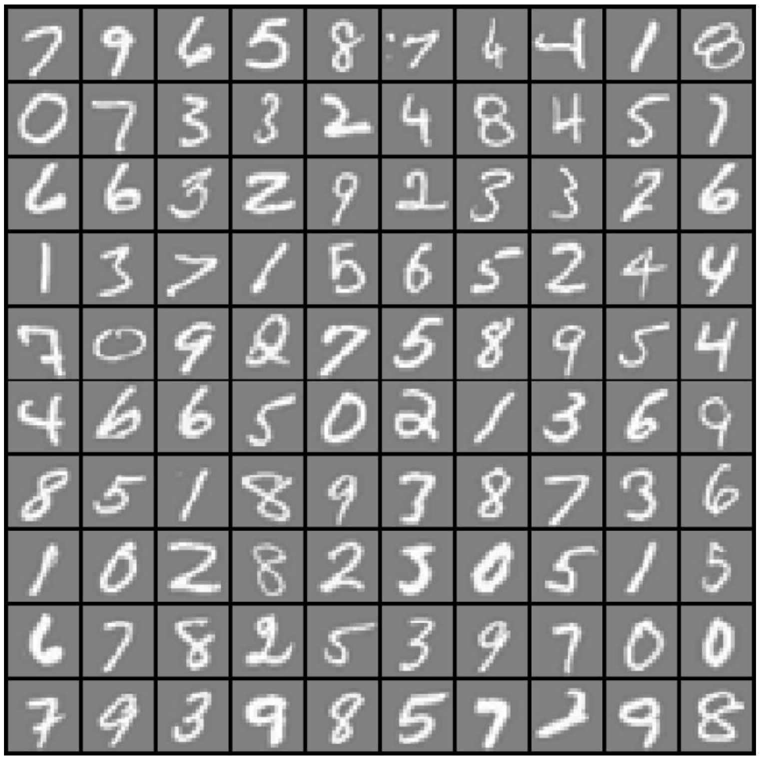
<u>Multi-class classification</u> (K classes)

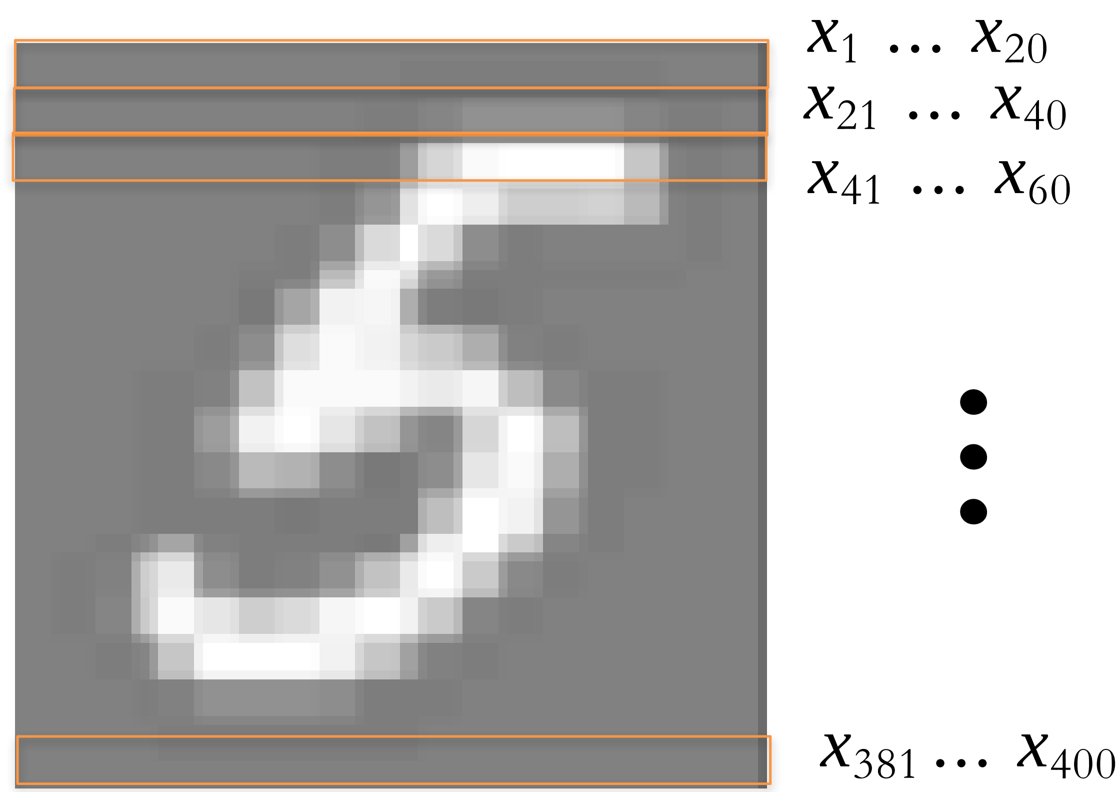
$\mathbf{y} \in \mathbb{R}^K$ e.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

pedestrian car motorcycle truck

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

Layering Representations

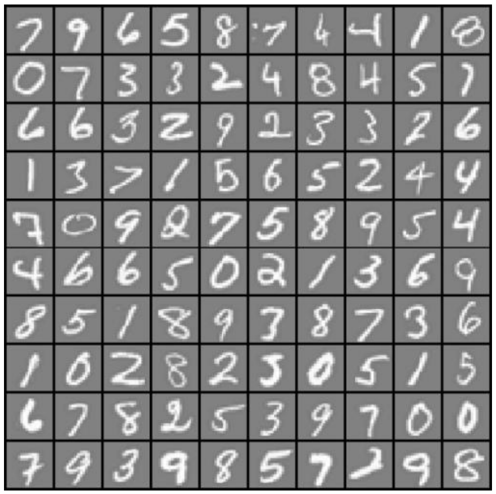


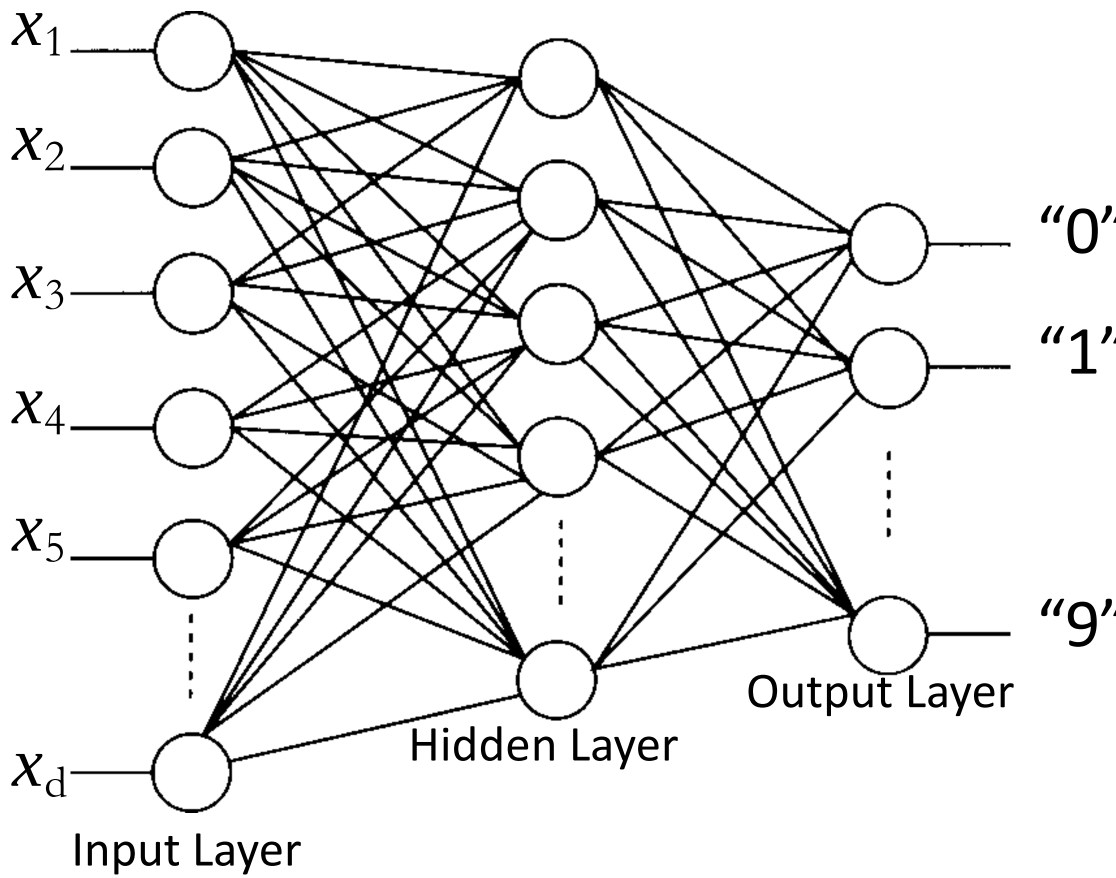


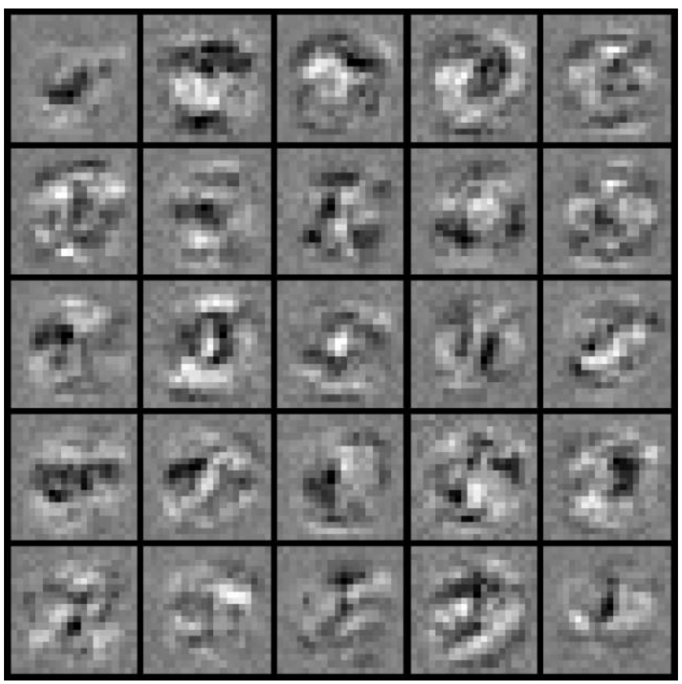
20×20 pixel images
$d = 400$ 10 classes

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

Layering Representations

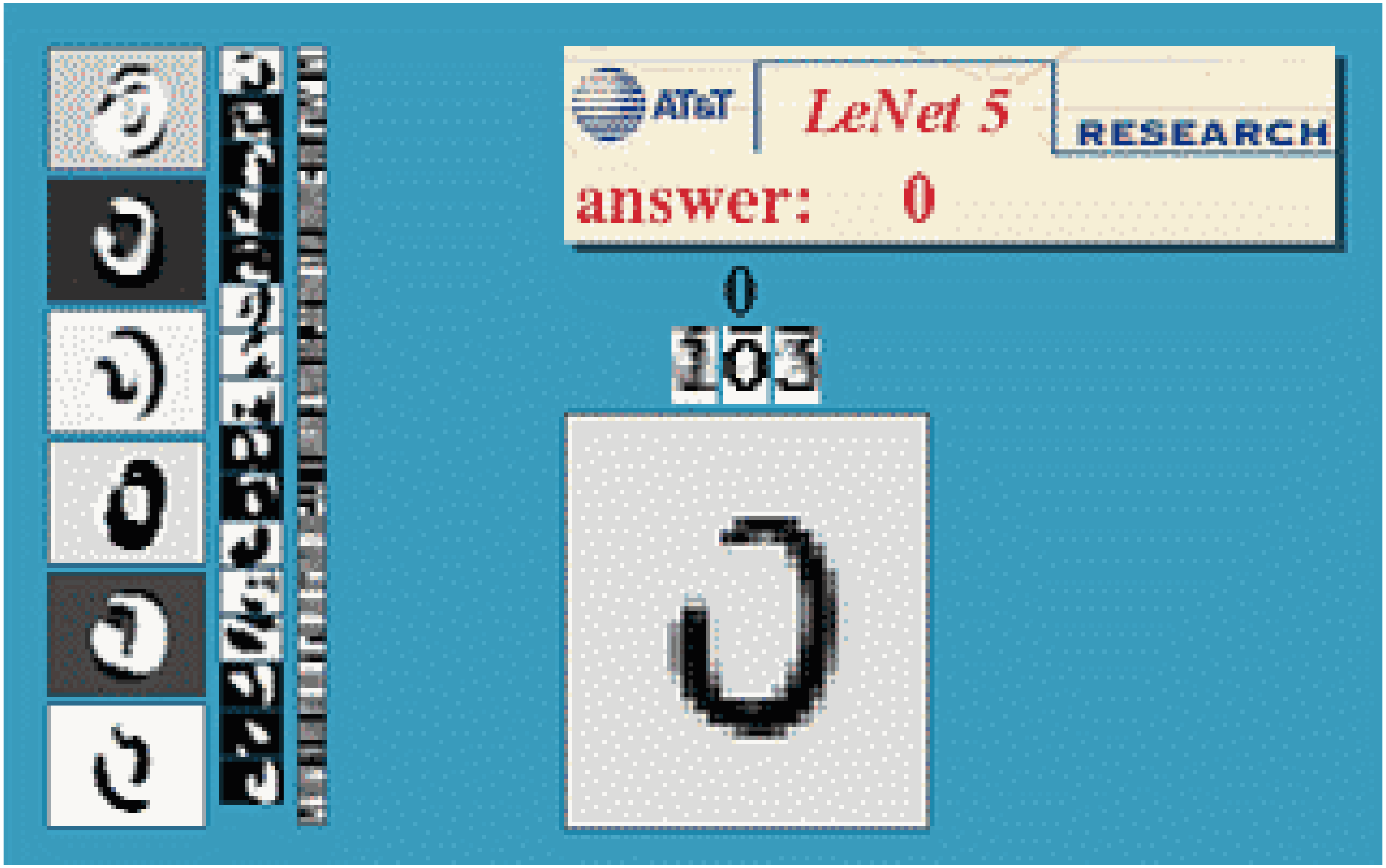






Visualization of Hidden Layer

Digit Recognition



Handwriting Recognition

LeNet 5 Demonstration:

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

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

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:

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

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

k^{th} class: true, predicted
not k^{th} class: true, predicted

Optimizing the Neural Network

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

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

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

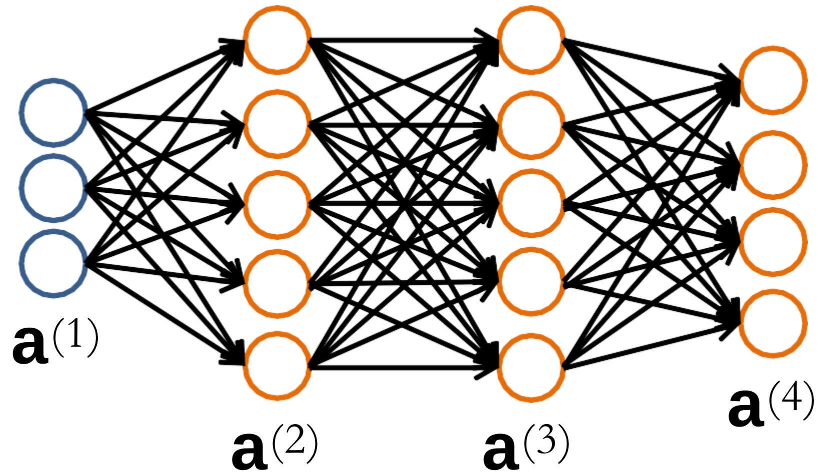
- But, tends to work well in practice

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

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

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

Chain rule

Chain Rule of Differentiation (reminder)

- The rate of change of a function of a function is the multiple of the derivatives of those functions.

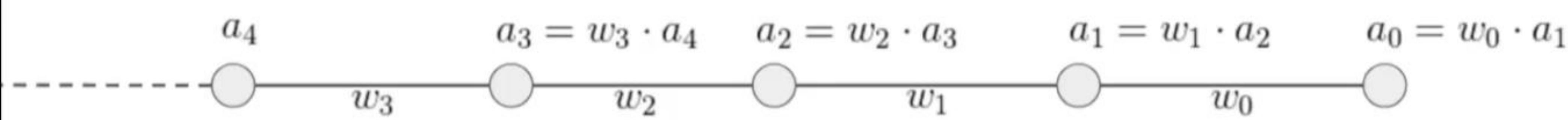
- You have probably learned this in school (nothing new here)

$$\frac{\partial}{\partial x} f(g(x)) = g'(x) \cdot f'(g)$$

$$\frac{\partial}{\partial x} f(g(h(i(j(k(x)))))) = \frac{\partial k}{\partial x}\frac{\partial j}{\partial k}\frac{\partial i}{\partial j}\frac{\partial h}{\partial i}\frac{\partial g}{\partial h}\frac{\partial f}{\partial g}$$

Backpropogation

Backpropagation Generalized to several layers



$$-r \frac{\partial a_0}{\partial w_0} \frac{\partial C}{\partial a_0}$$

$$-r \frac{\partial a_1}{\partial w_1} \frac{\partial a_0}{\partial a_1} \frac{\partial C}{\partial a_0}$$

$$C = (a_0 - y)^2$$

$$-r \frac{\partial a_2}{\partial w_2} \frac{\partial a_1}{\partial a_2} \frac{\partial a_0}{\partial a_1} \frac{\partial C}{\partial a_0}$$

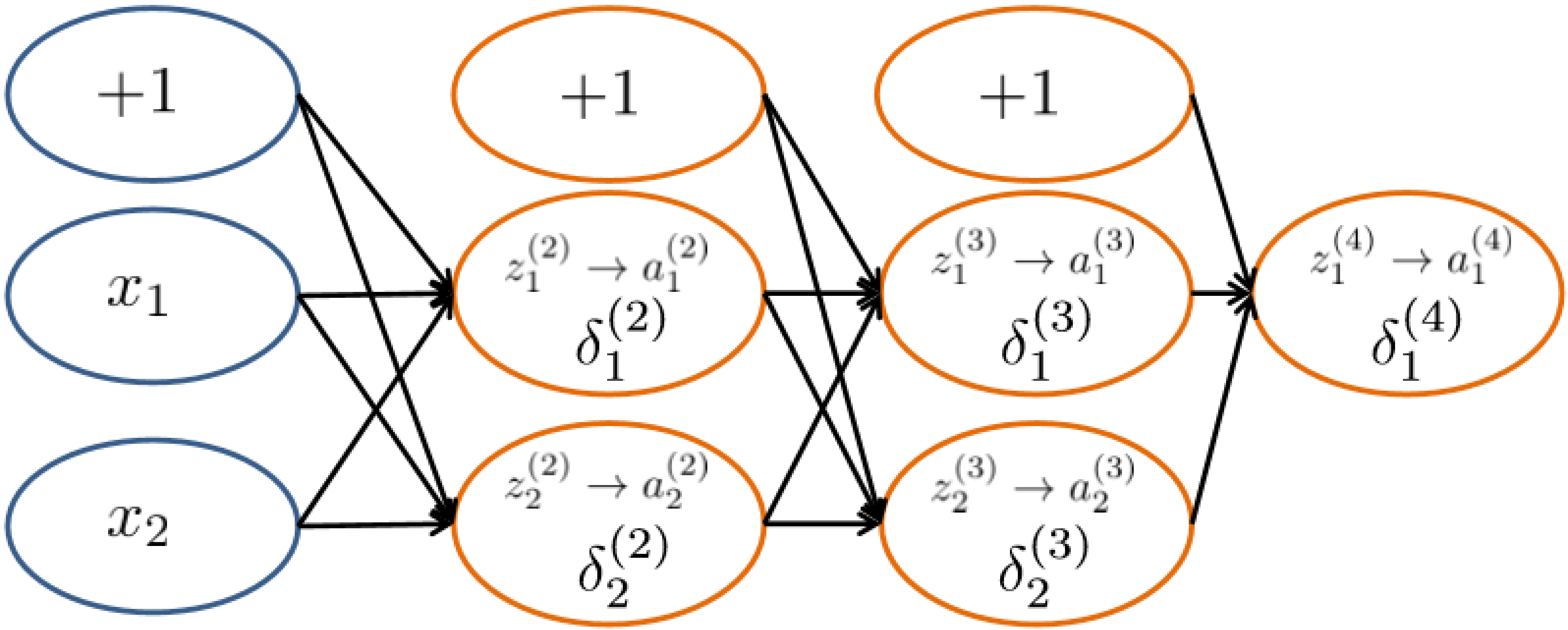
$$-r \frac{\partial a_3}{\partial w_3} \frac{\partial a_2}{\partial a_3} \frac{\partial a_1}{\partial a_2} \frac{\partial a_0}{\partial a_1} \frac{\partial C}{\partial a_0}$$

For example, we adjust w3 as follows:

$$w_3' = w_3 - r \cdot a_4 \cdot w_2 \cdot w_1 \cdot w_0 \cdot 2(a_0 - y)$$

$$-r \frac{\partial a_3}{\partial w_3} \frac{\partial a_2}{\partial a_3} \frac{\partial a_1}{\partial a_2} \frac{\partial a_0}{\partial a_1} \frac{\partial C}{\partial a_0}$$

Backpropagation Intuition

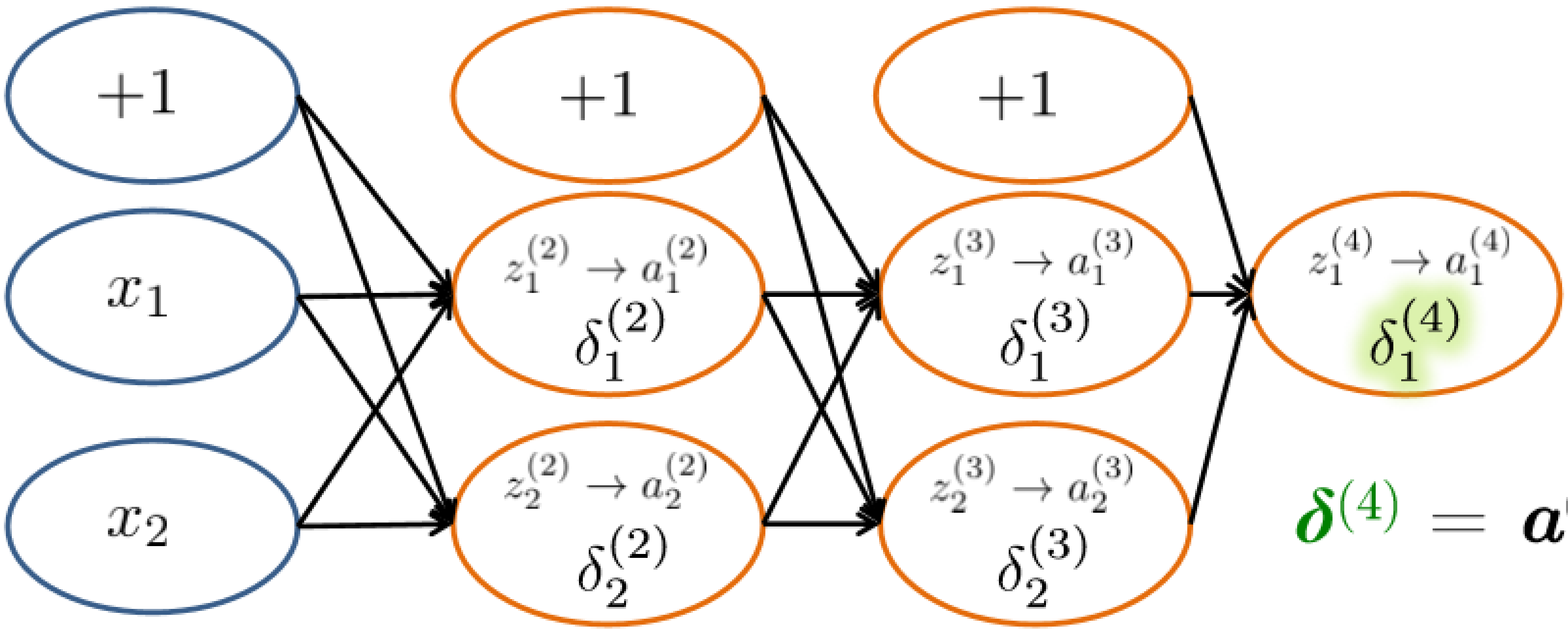


$\delta_j^{(l)} =$ "error" of node j in layer l

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 Intuition

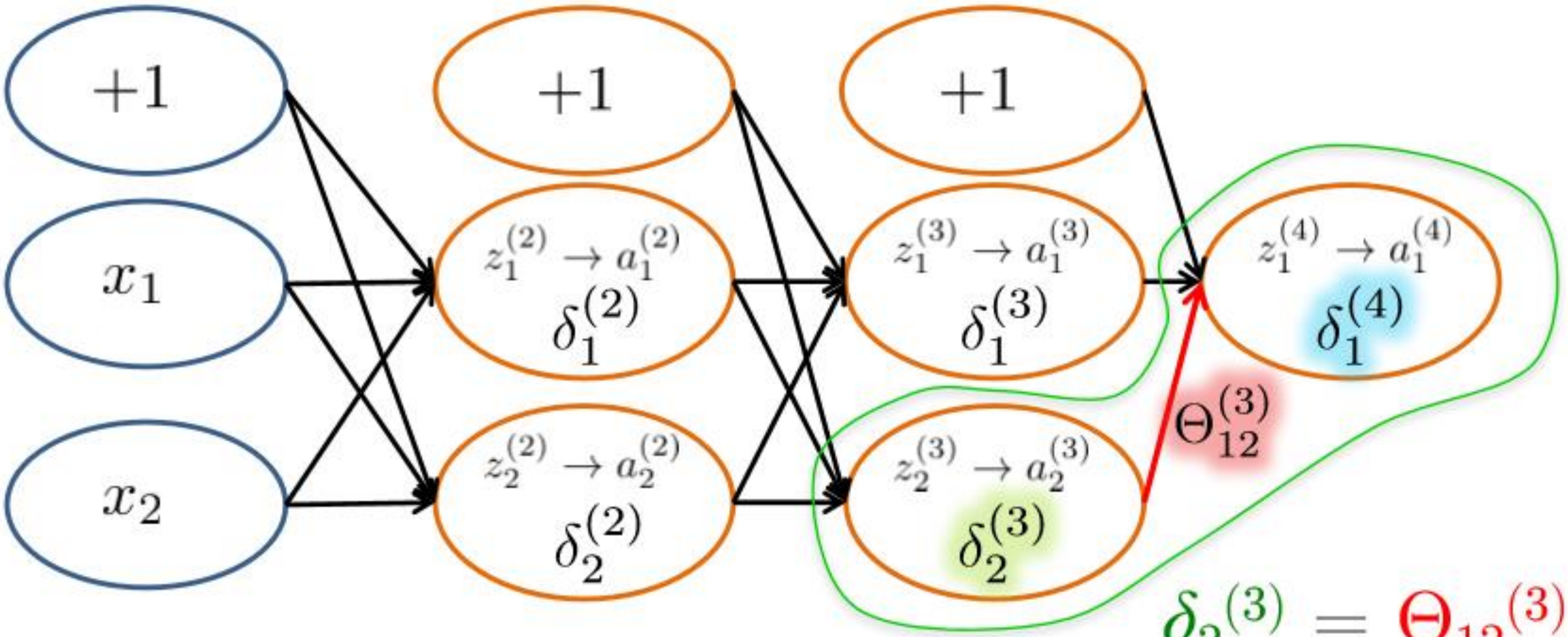


$$\boldsymbol{\delta}^{(4)} = \boldsymbol{a}^{(4)} - \mathbf{y}$$

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

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

Backpropagation Intuition



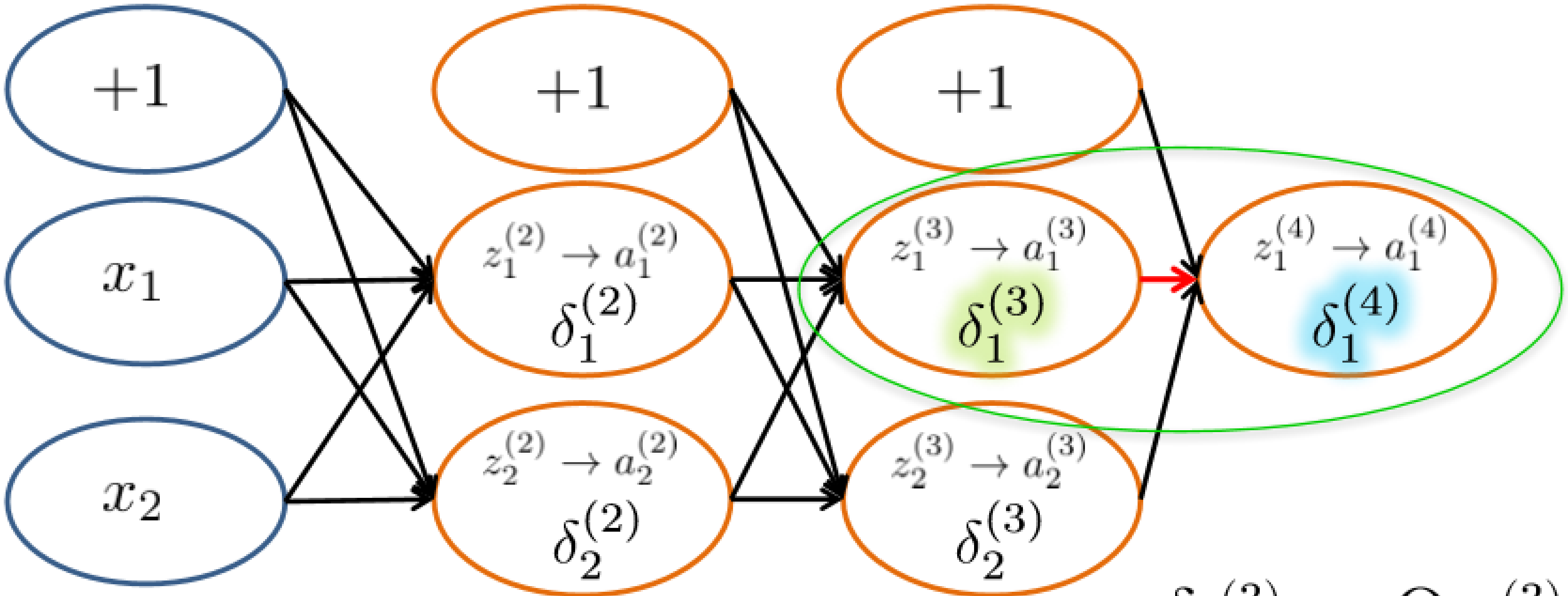
$$\delta_2{}^{(3)} = \Theta_{12}{}^{(3)} \times \delta_1{}^{(4)}$$

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

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

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



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

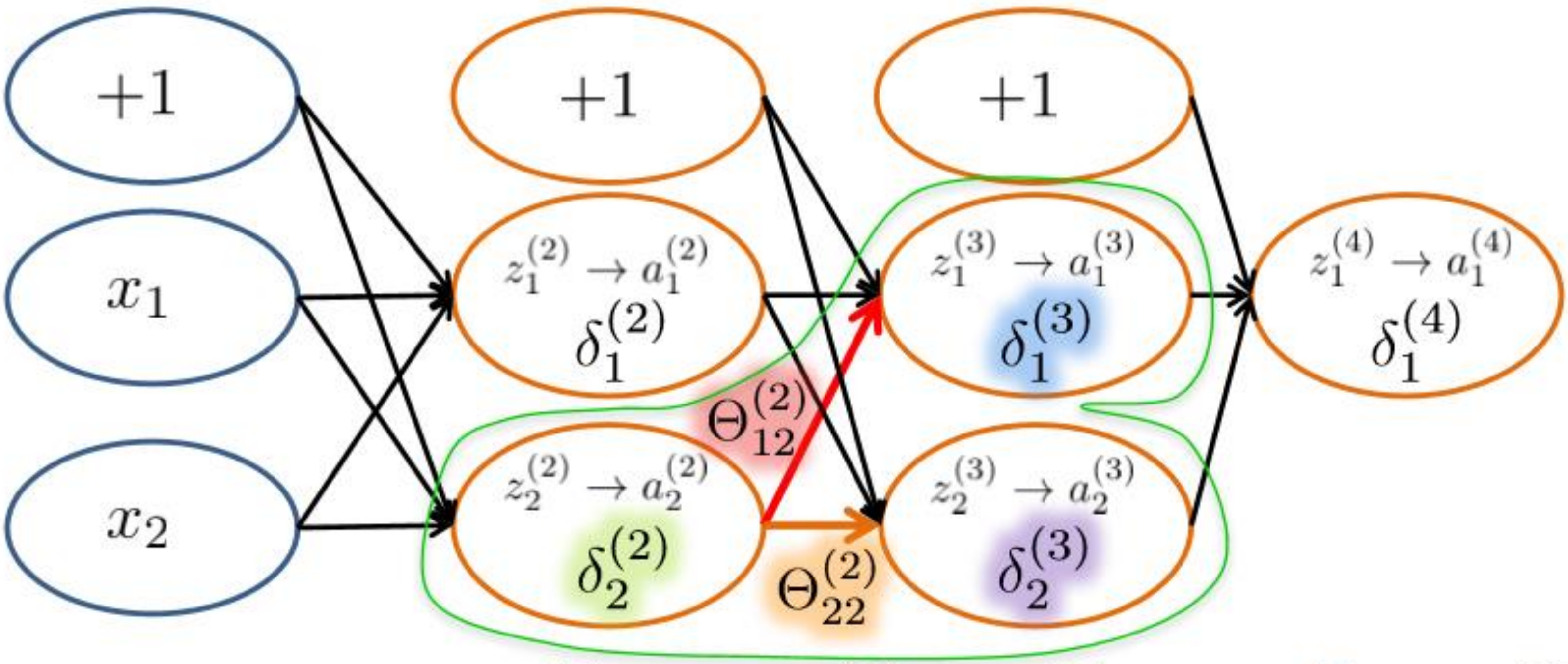
$$\delta_1{}^{(3)} = \Theta_{11}{}^{(3)} \times \delta_1{}^{(4)}$$

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

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

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

Backpropagation Intuition



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

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

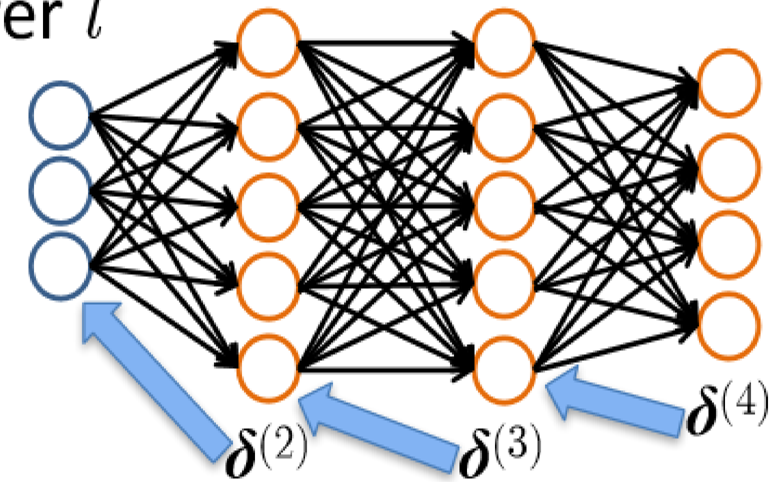
Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \mathrm{cost}(\mathbf{x}_i)$

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

Backpropagation: Gradient Computation

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

(#layers L = 4)



<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 $\boldsymbol{\delta}^{(1)}$)

Element-wise product .*

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

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

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$$ (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 $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

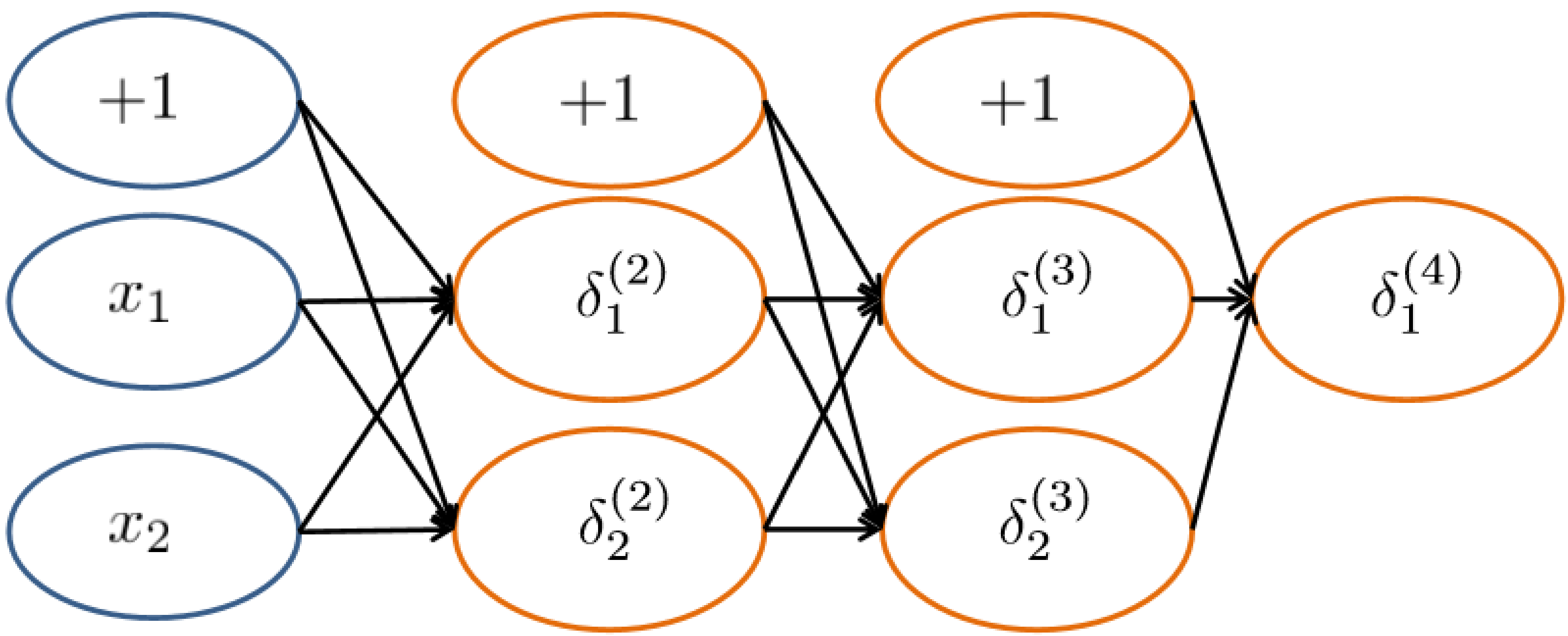
Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

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

Backpropagation

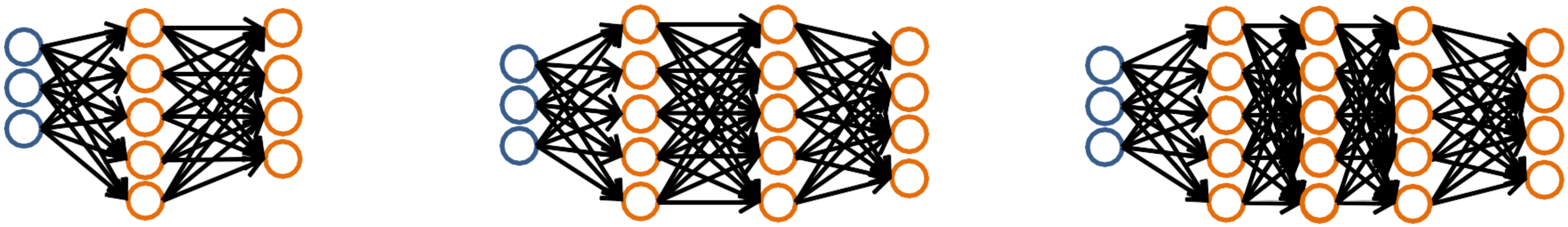
Random Initialization

- 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



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)

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

Based on slide by Andrew Ng

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

Gradient Descent

Initialise w, b

Iterate over data:

$compute\ \hat{y}$

$compute\ \mathscr{L}(w, b)$

$$w_{t+1} = w_t - \eta \Delta w_t$$

$$b_{t+1} = b_t - \eta \Delta b_t$$

till satisfied

Please note that w and θ are the two notations used to represent weights of the model. Some books refer as w and some books refer as θ .

Derivative of cross entropy

$$\mathcal{L}(\theta) = -[(1-y)\log(1-\hat{y}) + y\log\hat{y})]$$

Using Chain Rule: $$\Delta w = \frac{\partial \mathcal{L}(\theta)}{\partial w} = \frac{\partial \mathcal{L}(\theta)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w}$$

$$\frac{\partial \mathcal{L}(\theta)}{\partial \hat{y}} = \frac{\partial}{\partial \hat{y}}\{-(1-y)\log(1-\hat{y}) - y\log\hat{y})\}$$

$$= (-)(-1)\frac{(1-y)}{(1-\hat{y})} - \frac{y}{\hat{y}}$$

$$= \frac{\hat{y}(1-y) - y(1-\hat{y})}{(1-\hat{y})\hat{y}}$$

$$= \frac{\hat{y}-y}{(1-\hat{y})\hat{y}}$$

Derivative of cross entropy

$$\frac{\partial \hat{y}}{\partial w} = \frac{\partial}{\partial w}\left(\frac{1}{1+e^{-(wx+b)}}\right)$$

$$= \frac{-1}{(1+e^{-(wx+b)})^2}\frac{\partial}{\partial w}(e^{-(wx+b)}))$$

$$= \frac{-1}{(1+e^{-(wx+b)})^2} * (e^{-(wx+b)})\frac{\partial}{\partial w}(-(wx+b)))$$

$$= \frac{-1}{(1+e^{-(wx+b)})} * \frac{e^{-(wx+b)}}{(1+e^{-(wx+b)})} * (-x)$$

$$= \frac{1}{(1+e^{-(wx+b)})} * \frac{e^{-(wx+b)}}{(1+e^{-(wx+b)})} * (x)$$

$$= \hat{y} * (1 - \hat{y}) * x$$

$$\Delta w = (\hat{y} - y) * x$$