Neural Networks

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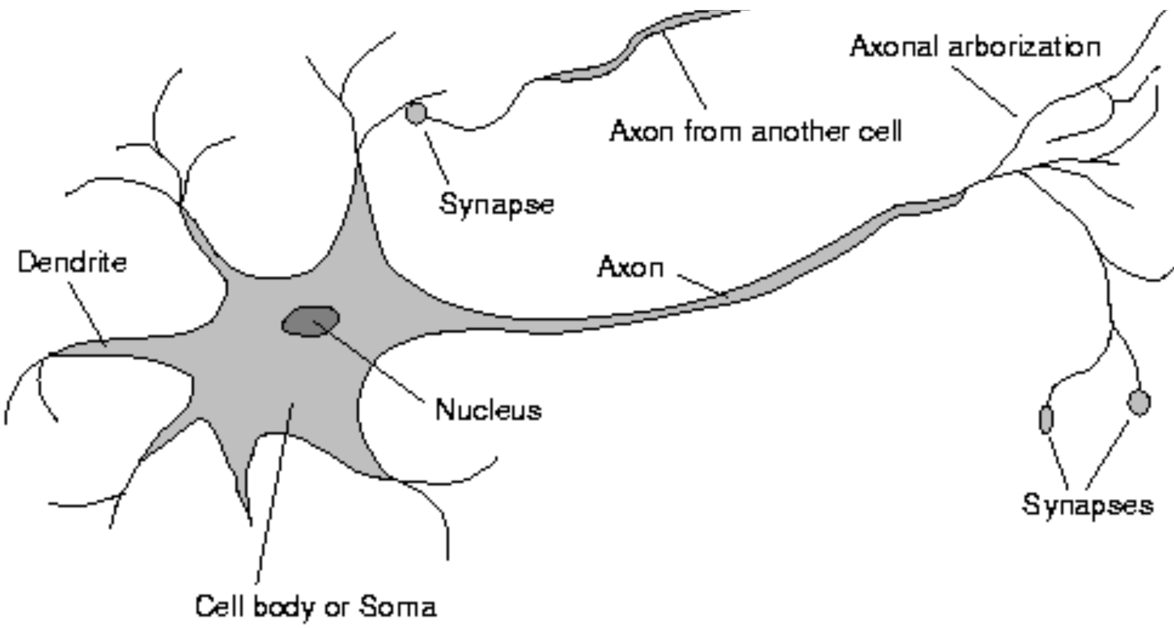
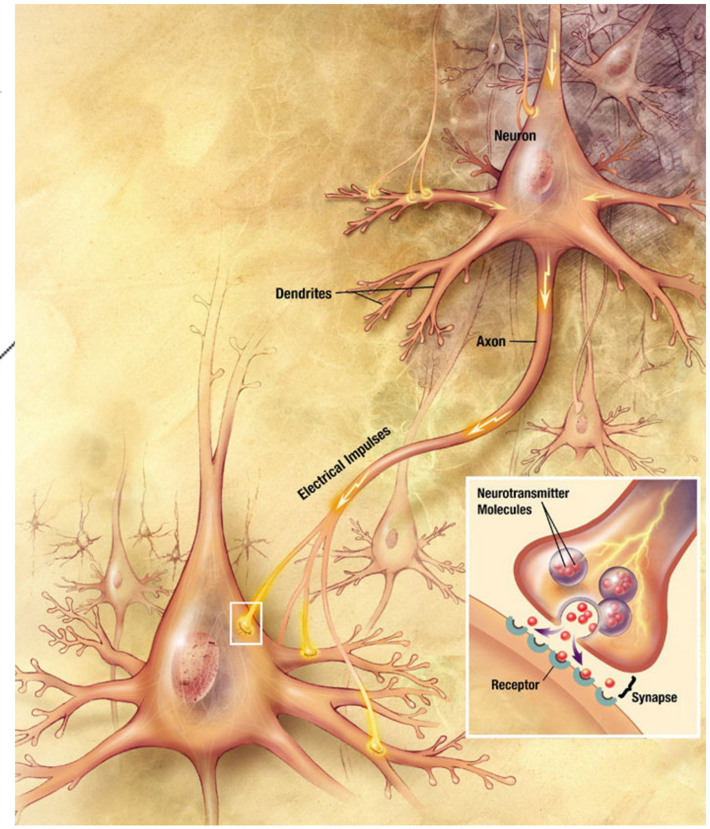
Neural Function

- Brain function (thought) occurs as the result of the firing of **neurons**
- Neurons connect to each other through **synapses**, which propagate **action potential** (electrical impulses) by releasing **neurotransmitters**
  - Synapses can be **excitatory** (potential-increasing) or **inhibitory** (potential-decreasing), and have varying **activation thresholds**
  - Learning occurs as a result of the synapses' **plasticicity**: They exhibit long-term changes in connection strength
- There are about 10^{11} neurons and about 10^{14} synapses in the human brain!

Biology of a Neuron

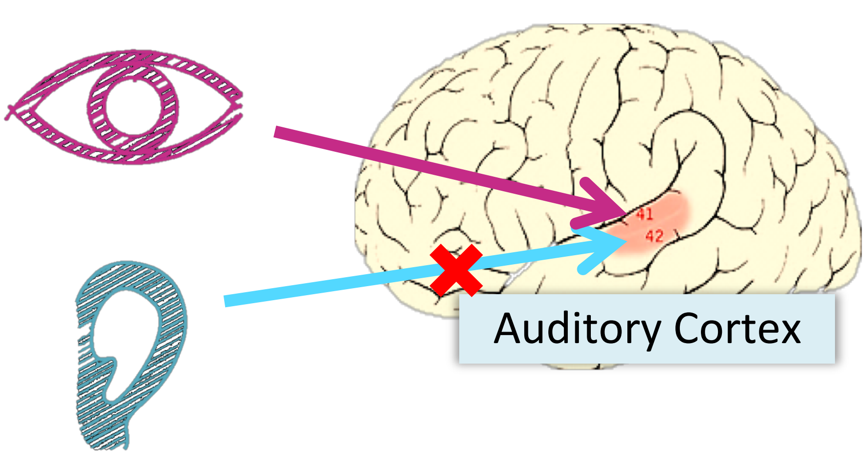




Brain Structure

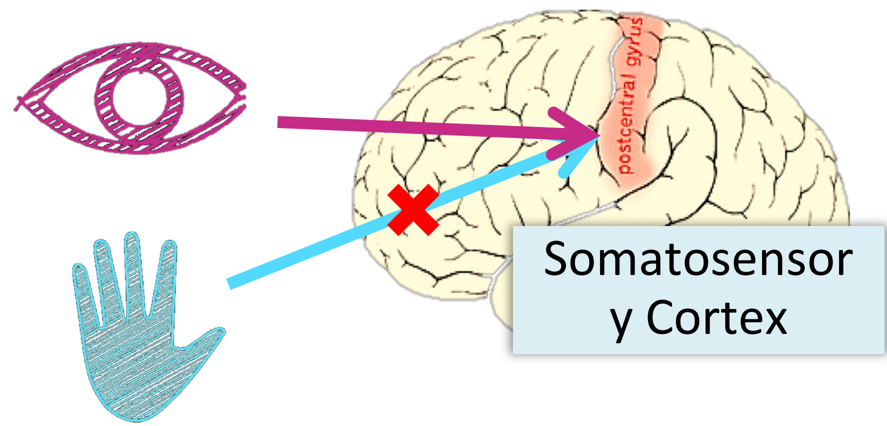
- Different areas of the brain have different functions
  - Some areas seem to have the same function in all humans (e.g., Broca's region for motor speech); the overall layout is generally consistent
  - Some areas are more plastic, and vary in their function; also, the lower-level structure and function vary greatly
- We don't know how different functions are "assigned" or acquired
  - Partly the result of the physical layout / connection to inputs (sensors) and outputs (effectors)
  - Partly the result of experience (learning)
- We *really* don't understand how this neural structure leads to what we perceive as "consciousness" or "thought"

The "One Learning Algorithm" Hypothesis



Auditory cortex learns to see

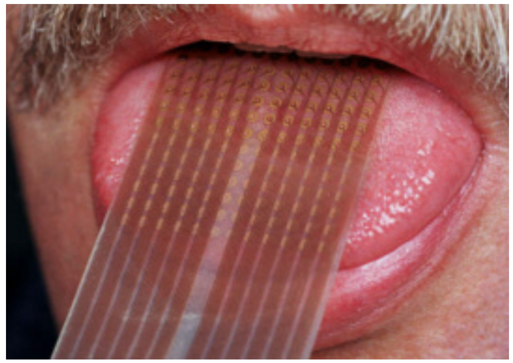
[Roe et al., 1992]



Somatosensory cortex learns to see

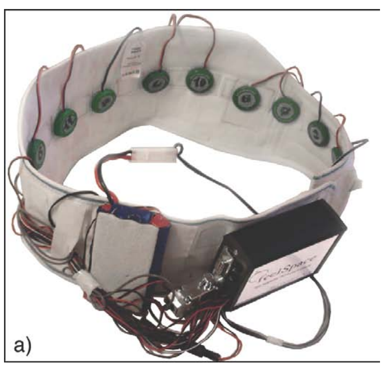
[Metin & Frost, 1989]

Sensor Representations in the Brain

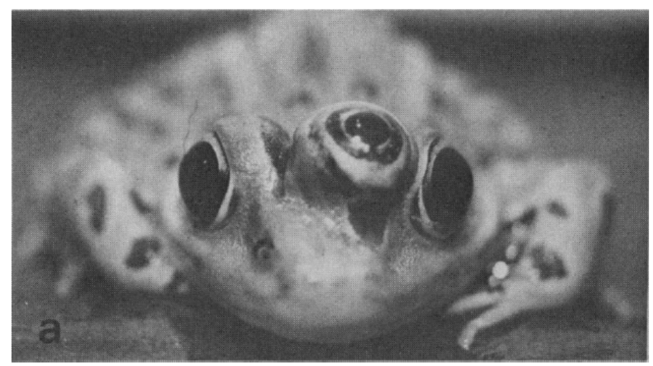



Seeing with your tongue

Human echolocation (sonar)



Haptic belt: Direction sense



Implanting a 3rd eye

[BrainPort; Welsh & Blasch, 1997; Nagel et al., 2005; Constantine-Paton & Law, 2009]

Comparison of computing power

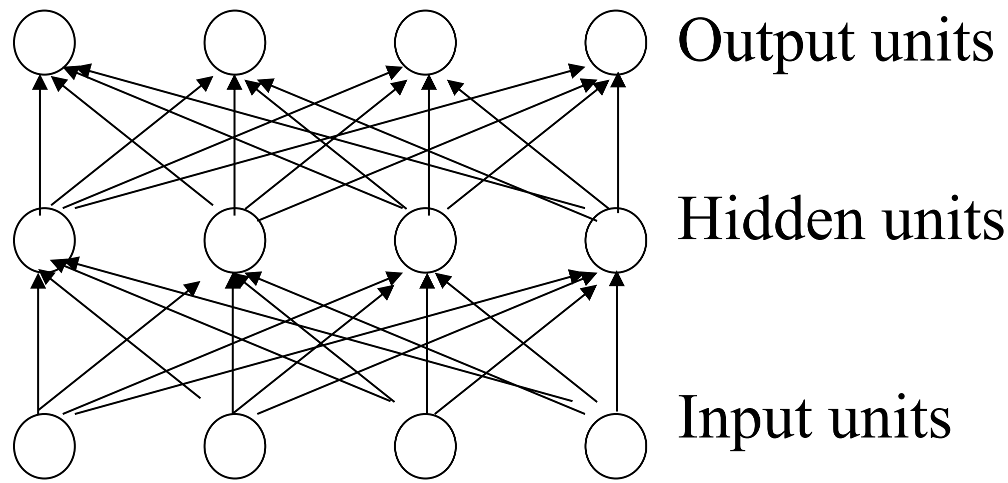
INFORMATION CIRCA 2012	Computer	Human Brain
Computation Units	10-core Xeon: 10^9 Gates	10^{11} Neurons
Storage Units	10^9 bits RAM, 10^{12} bits disk	10^{11} neurons, 10^{14} synapses
Cycle time	10^{-9} sec	10^{-3} sec
Bandwidth	10^9 bits/sec	10^{14} bits/sec

- Computers are way faster than neurons…
- But there are a lot more neurons than we can reasonably model in modern digital computers, and they all fire in parallel
- Neural networks are designed to be massively parallel
- The brain is effectively a billion times faster

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

Neural networks

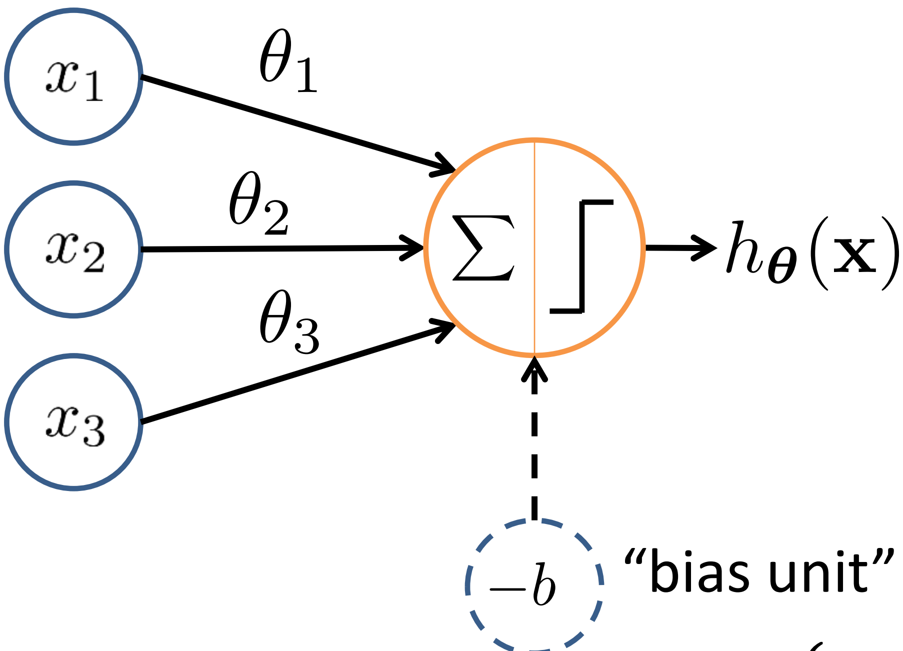


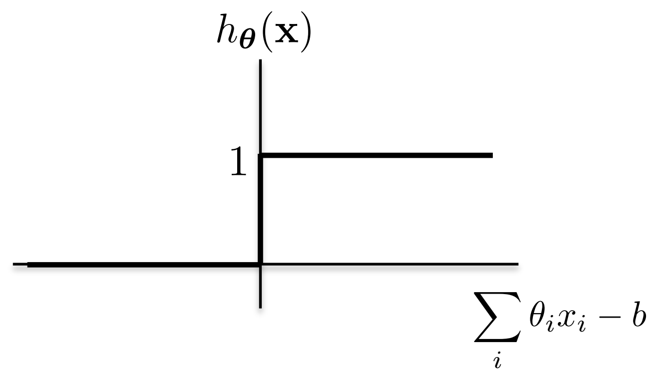
Layered feed-forward network

- 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**

Neuron Model: Threshold Unit

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$



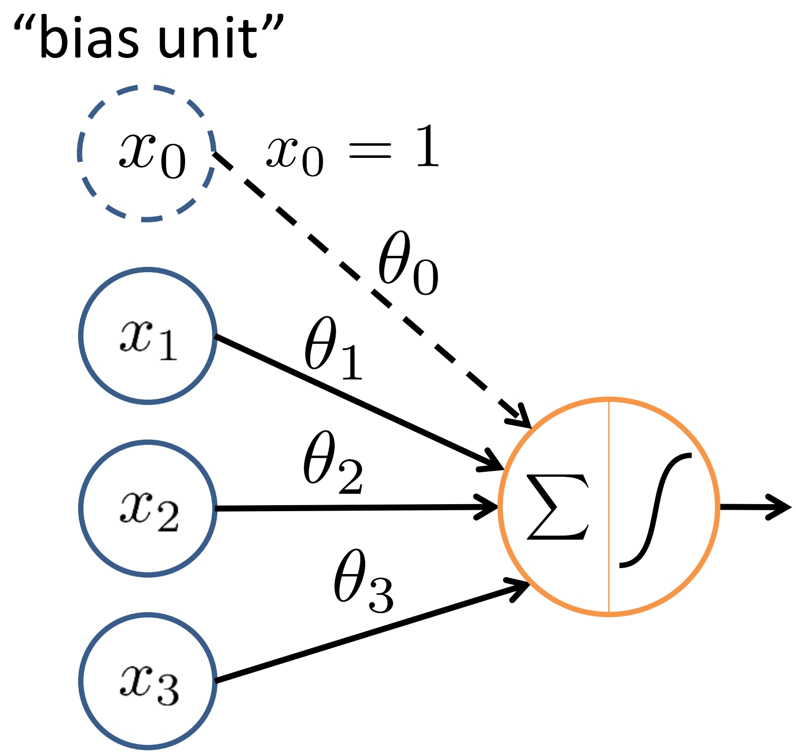


Activate if weighted sum of inputs is larger than “threshold”

Step activation function: $h_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{cases} 1 & \text{if} \quad \sum_i \theta_i x_i \geq b \\ 0 & \text{otherwise} \end{cases}$

Based on slide by Andrew Ng

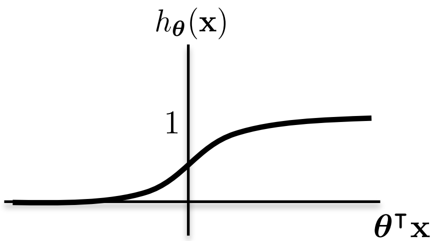
Neuron Model: Logistic Unit



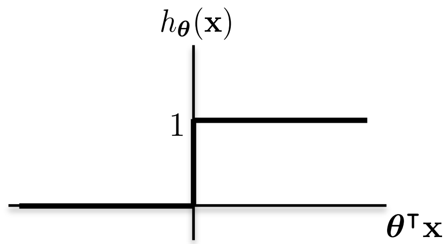
$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^\intercal \mathbf{x}\right) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\intercal \mathbf{x}}}$$

Sigmoid (logistic) activation function: $g(z) = \dfrac{1}{1 + e^{-z}}$

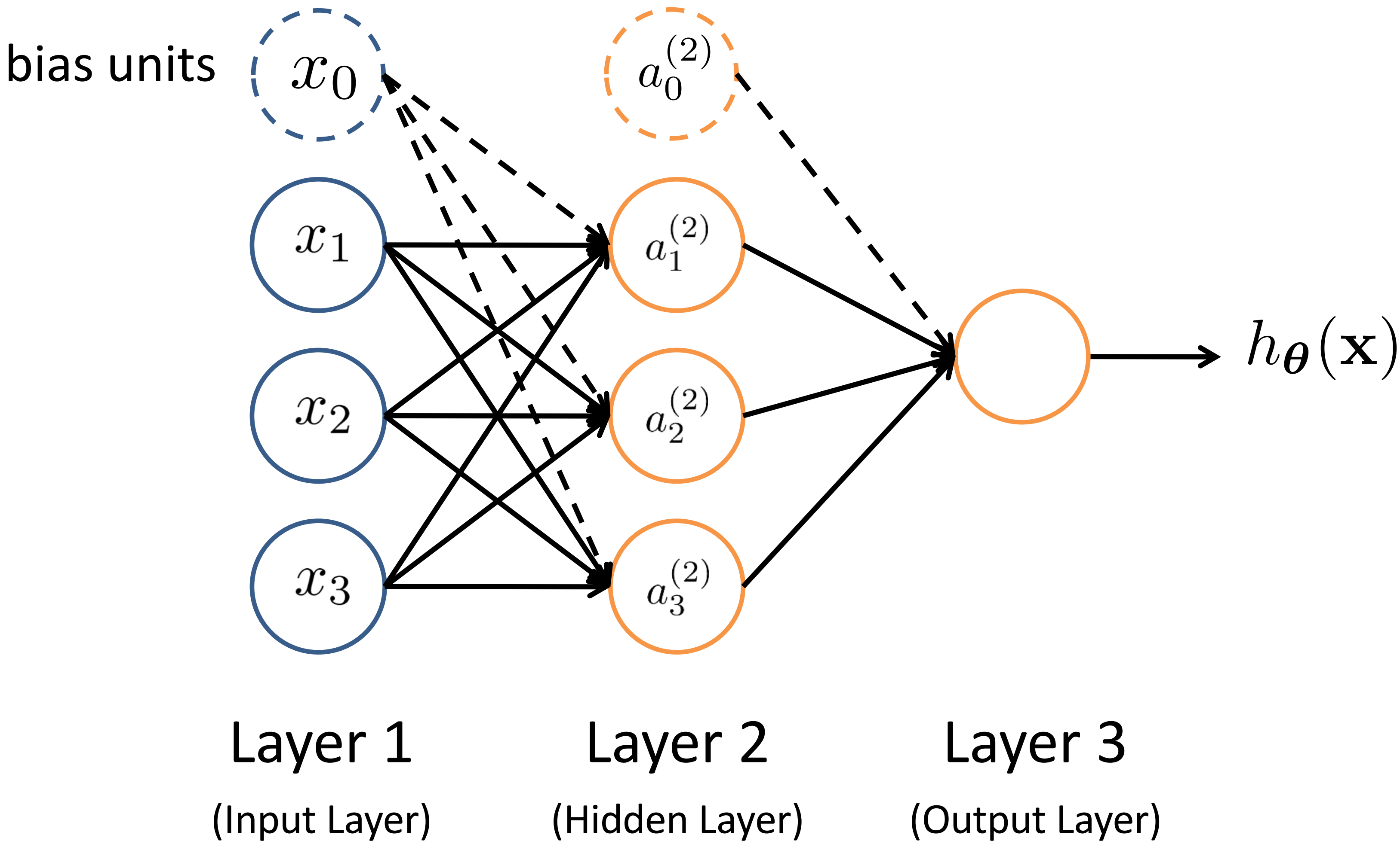


sigmoid



threshold

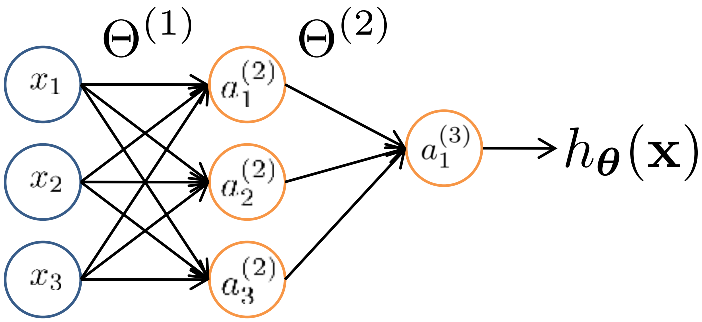
Neural Network



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

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) .

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

Slide by Andrew Ng

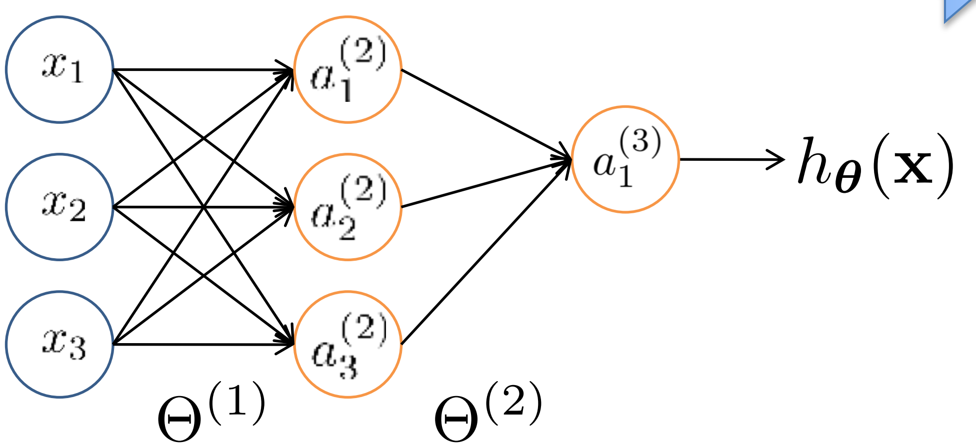
Vectorization

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

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

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

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



Feed-Forward Steps:

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

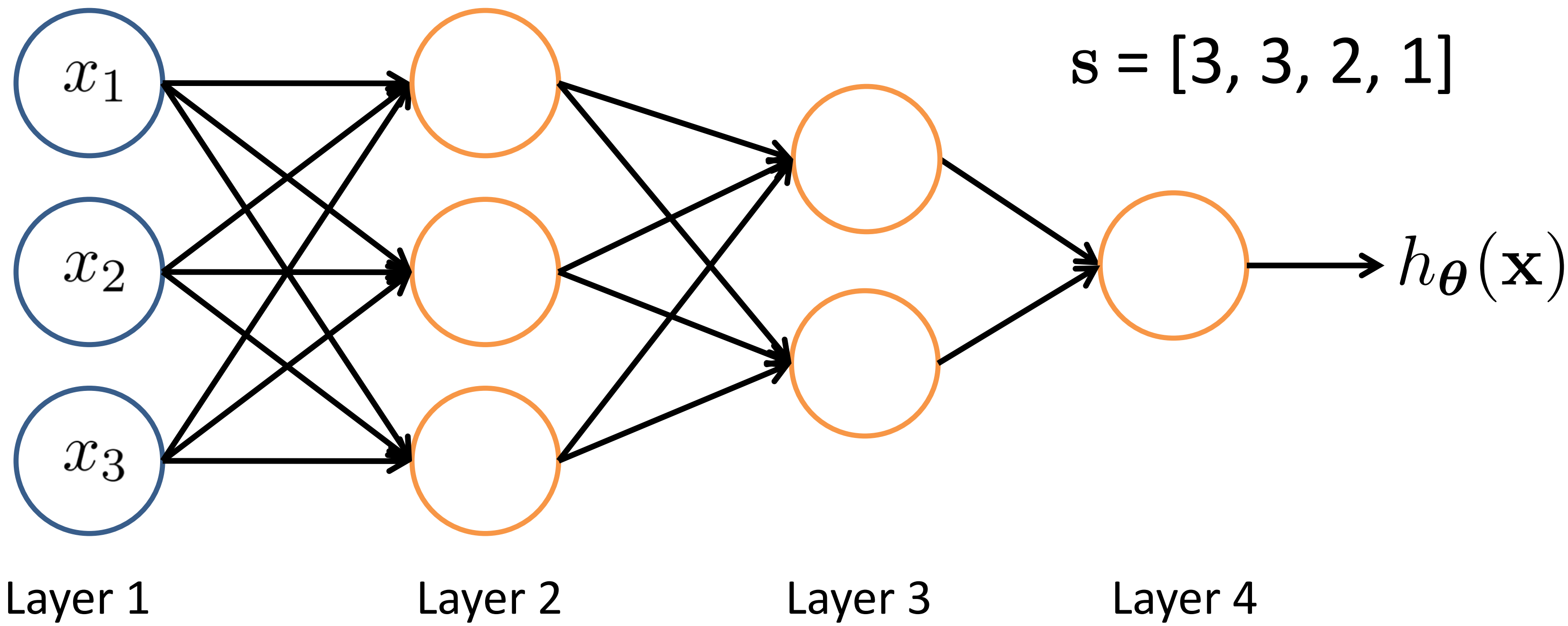
$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

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

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

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

Other Network Architectures



L denotes the number of layers

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

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

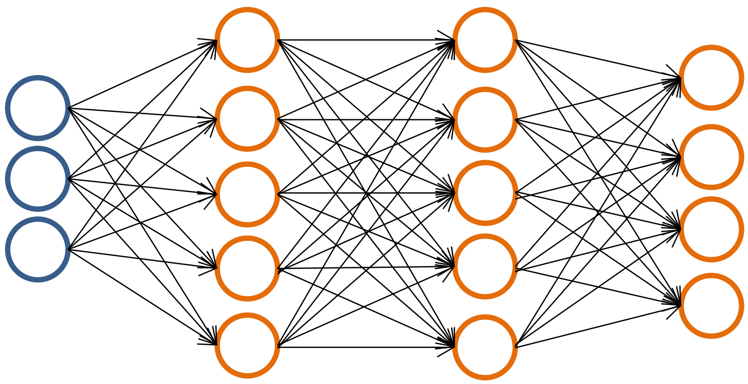
Multiple Output Units: One-vs-Rest


Pedestrian


Car


Motorcycle


Truck



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

We want:

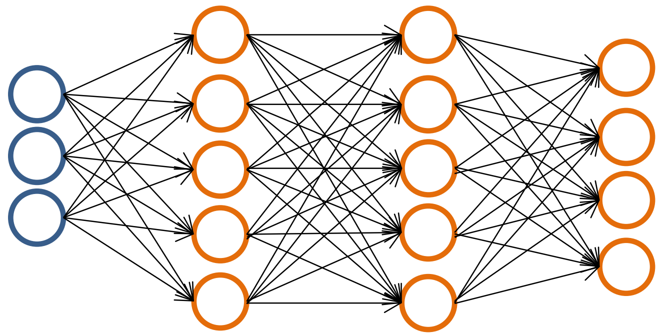
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
when pedestrian

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

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

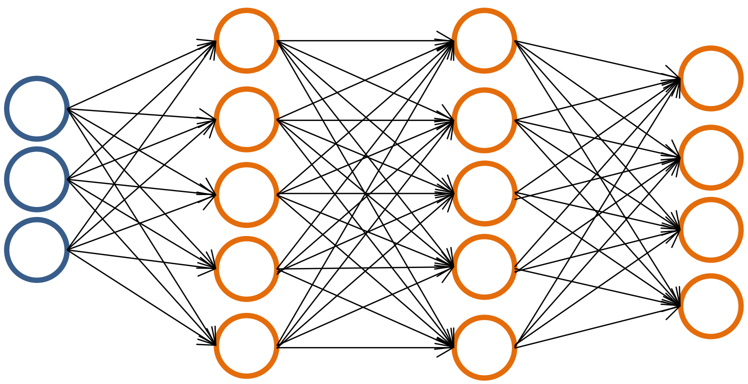
$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when motorcycle

$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ 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 $(s_{L\text{-}1} = 1)$

<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 $(s_{L\text{-}1} = K)$

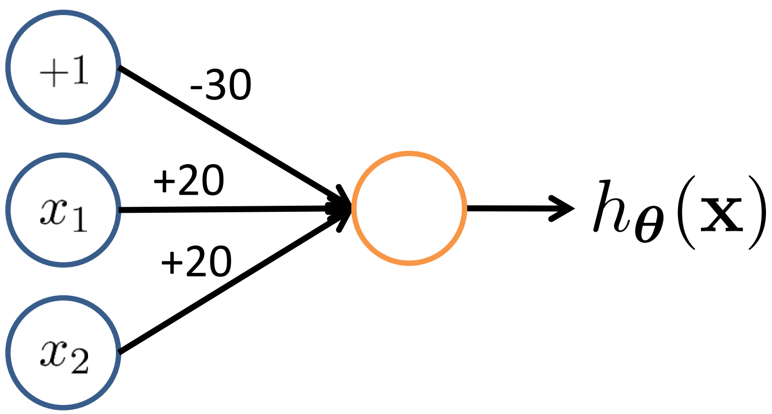
Understanding Representations

Representing Boolean Functions

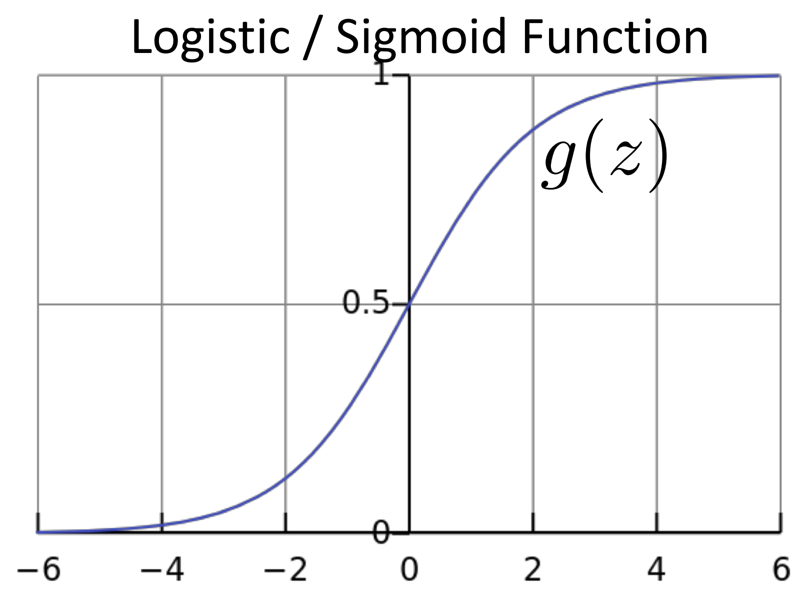
Simple example: AND

$$x_1, x_2 \in \{0, 1\}$$

$$y = x_1 \text{ AND } x_2$$



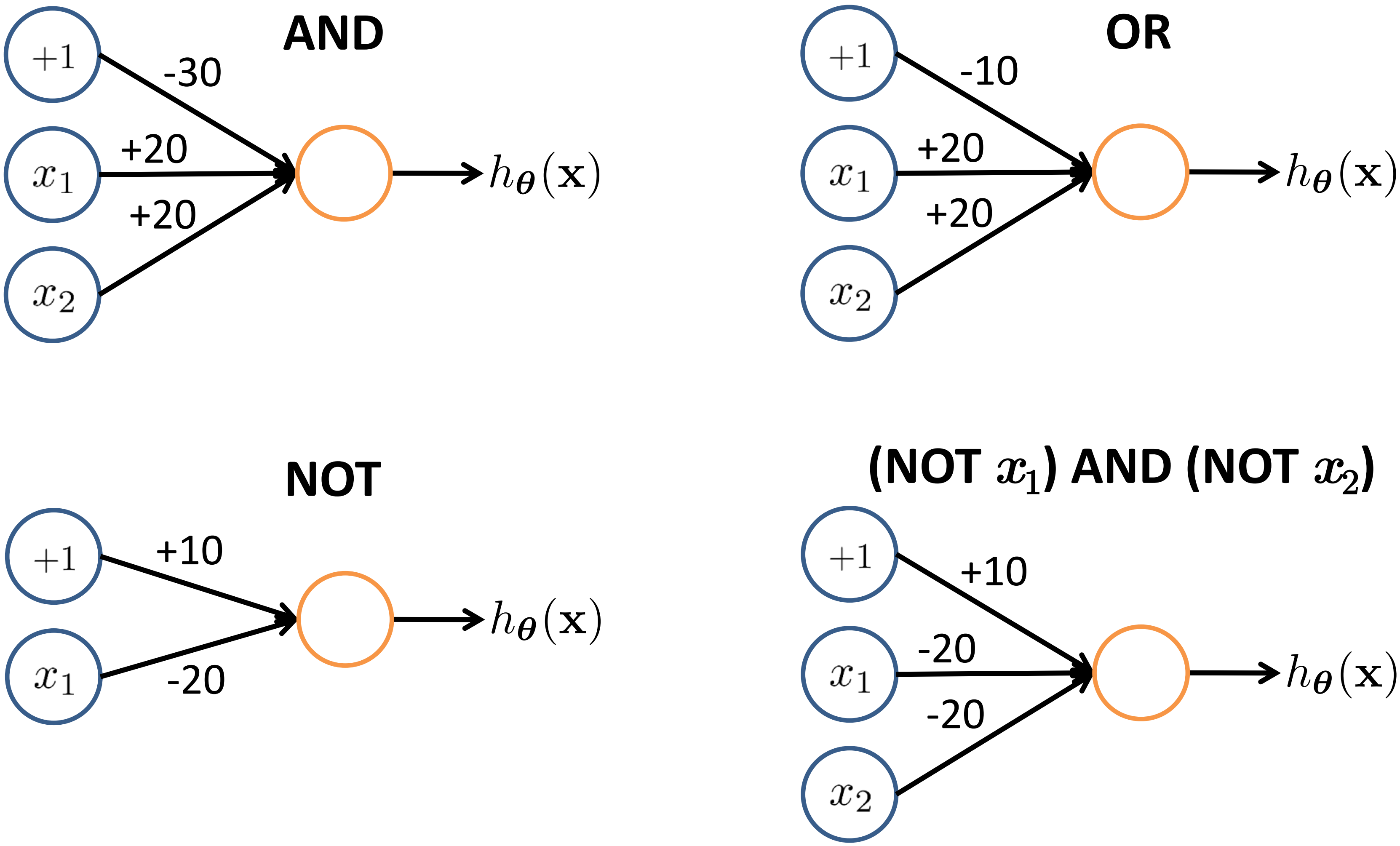
$$h_\Theta(\mathbf{x}) = g(-30 + 20x_1 + 20x_2)$$



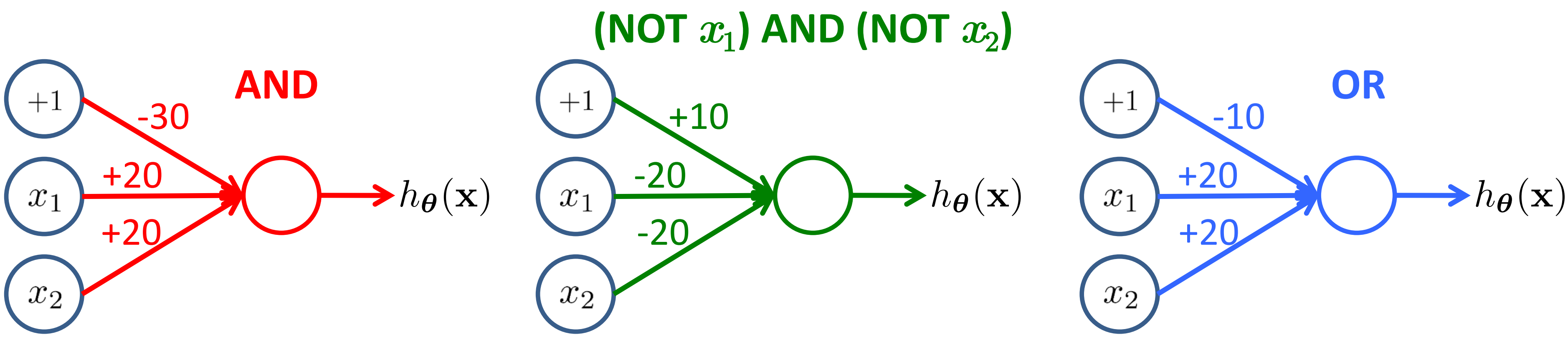
x_1	x_2	$h_\Theta(\mathbf{x})$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

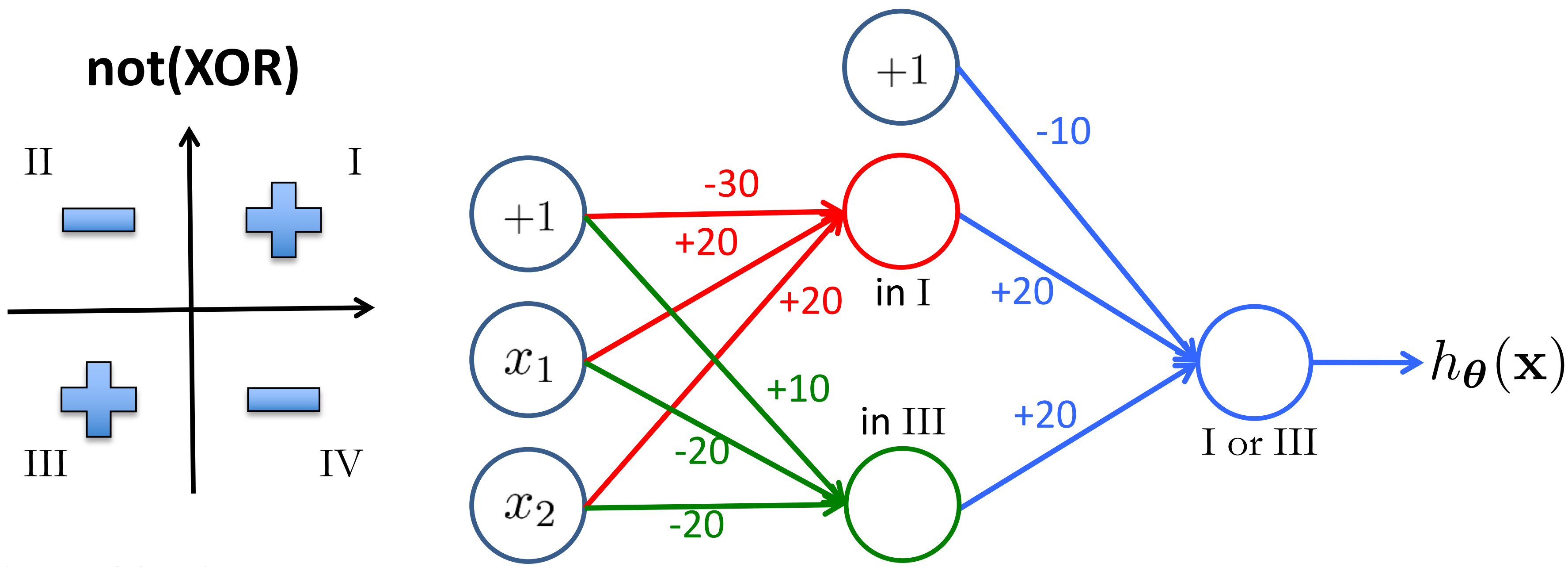
Based on slide and example by Andrew Ng

Representing Boolean Functions



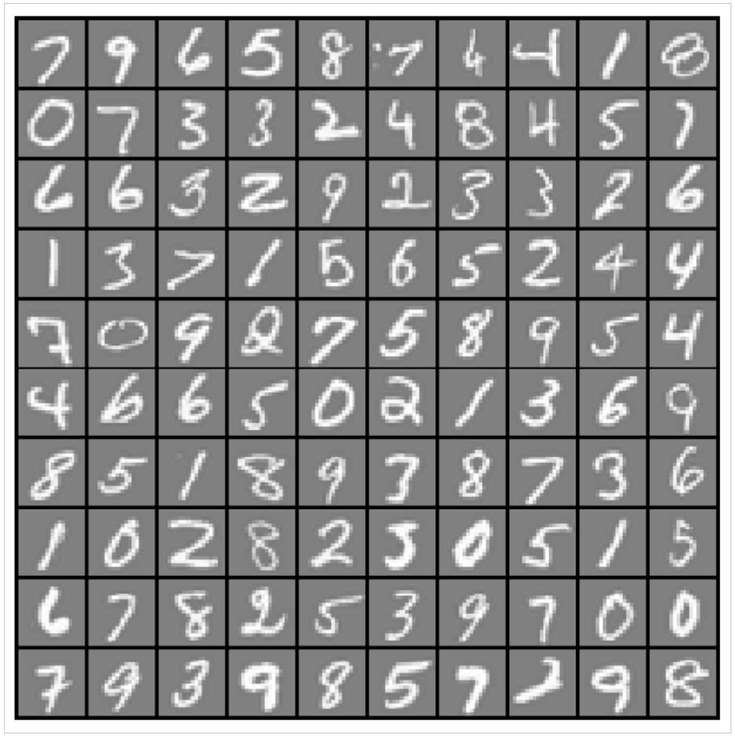
Combining Representations to Create Non-Linear Functions



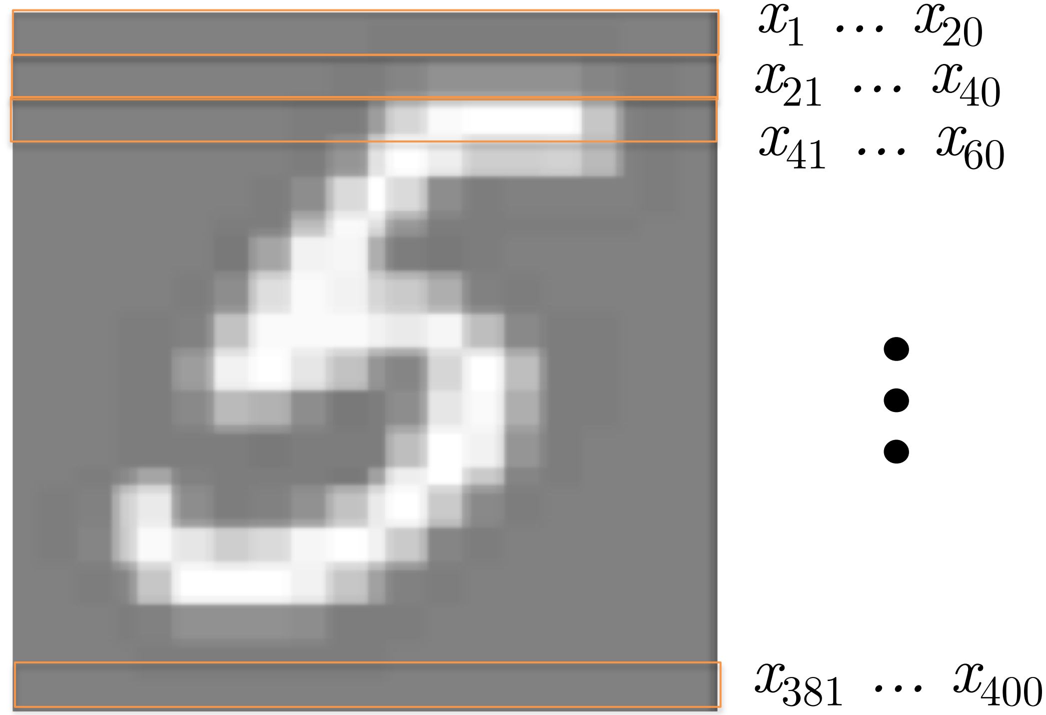


Based on example by Andrew Ng

Layering Representations

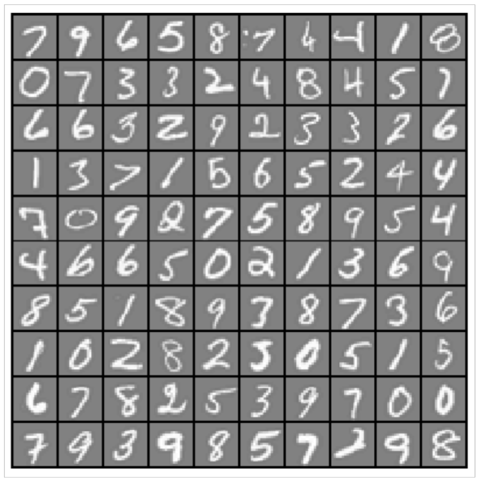


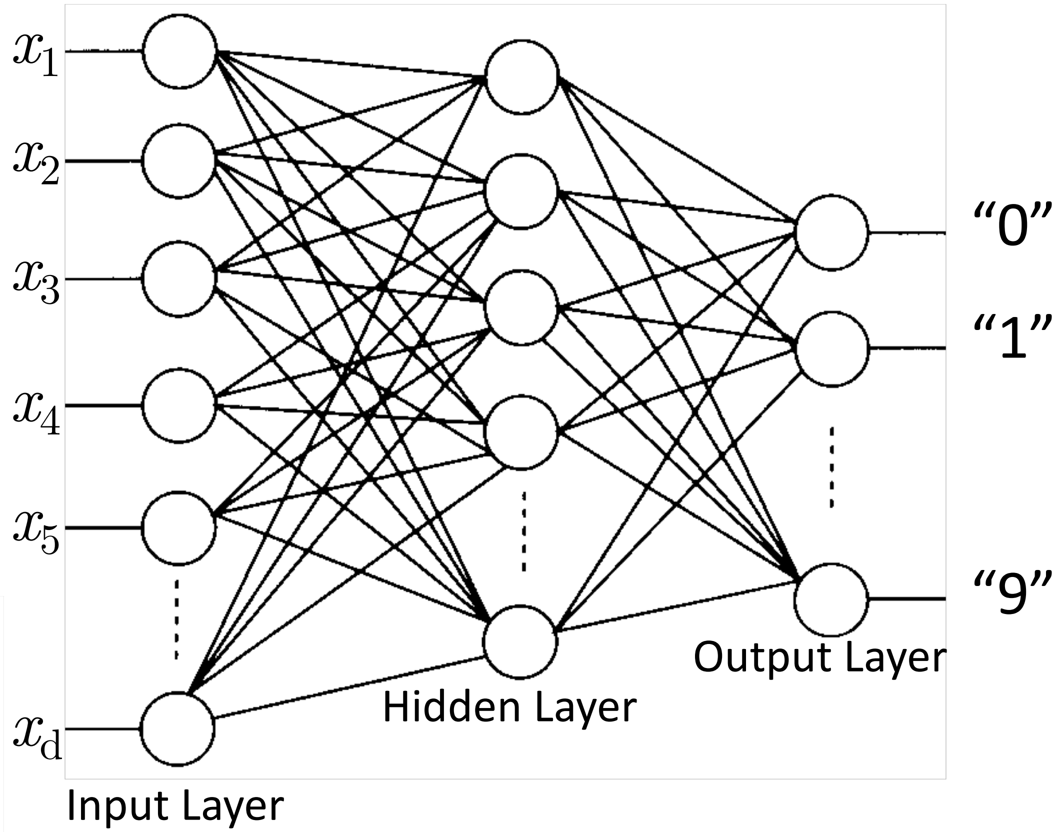
20 × 20 pixel images
d = 400 10 classes

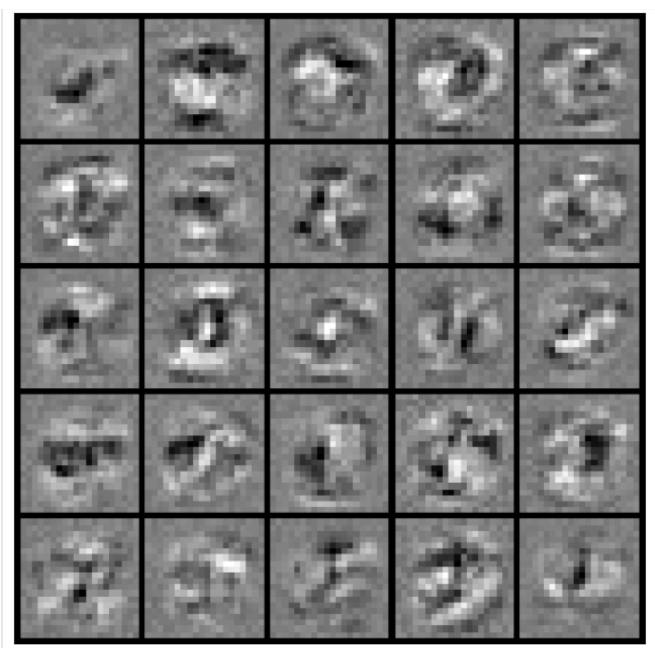


Each image is "unrolled" into a vector $\mathbf{x}$ of pixel intensities

Layering Representations







Visualization of Hidden Layer

LeNet 5 Demonstration: http://yann.lecun.com/exdb/lenet/

Neural Network Learning

Learning in NN: Backpropagation

- 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

Cost Function

Logistic Regression:

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

Neural Network:

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

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

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

k^{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

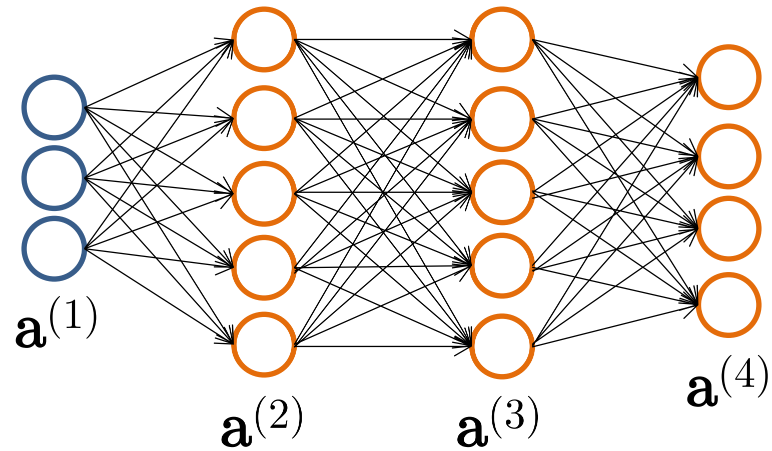
- But, tends to work well in practice

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

Backpropagation Intuition

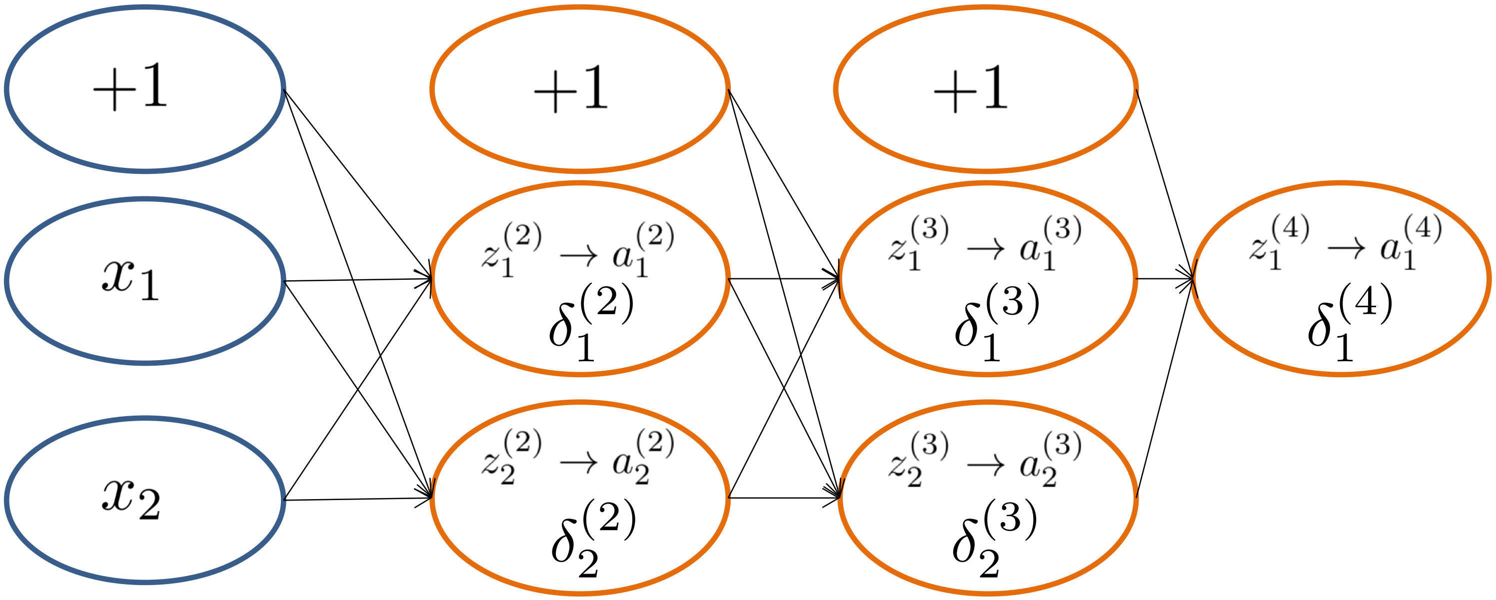
- Each hidden node j is "responsible" for some fraction of the error $\delta_j^{(l)}$ in each of the output nodes to which it connects

- $\delta_j^{(l)}$ 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

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

Backpropagation Intuition

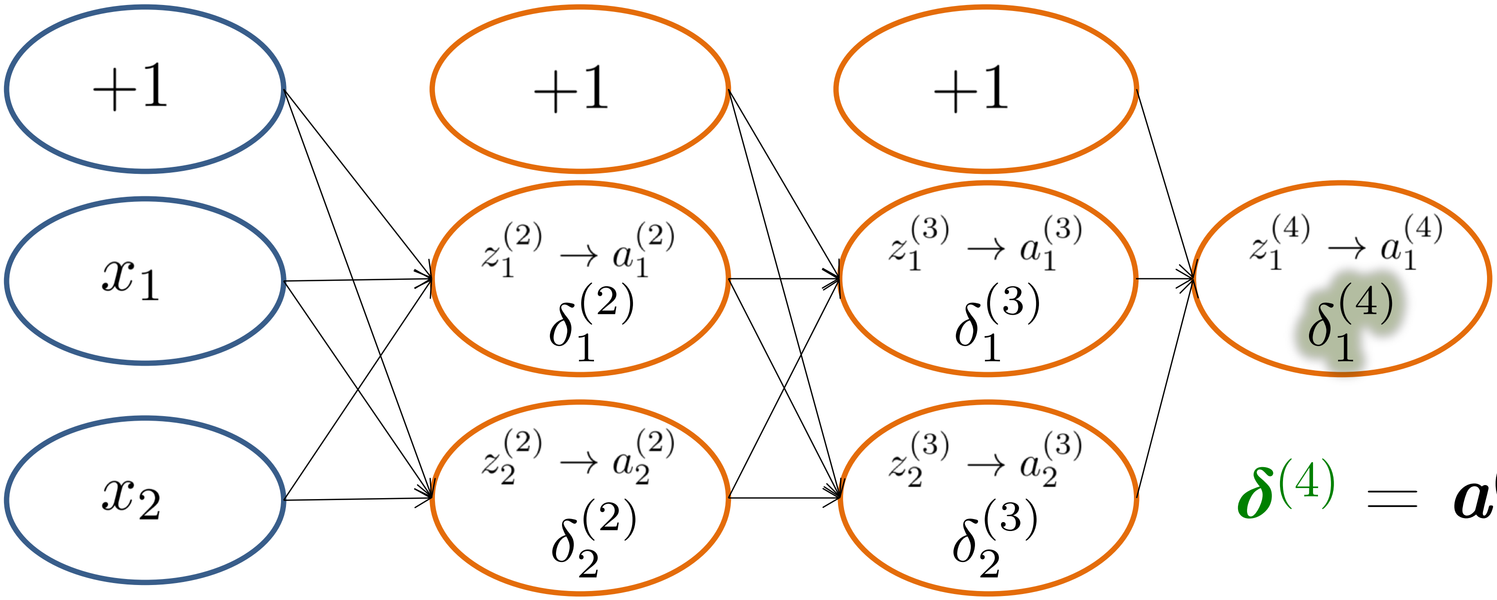


$\delta_j^{(l)} =$ "error" of node j in layer l

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



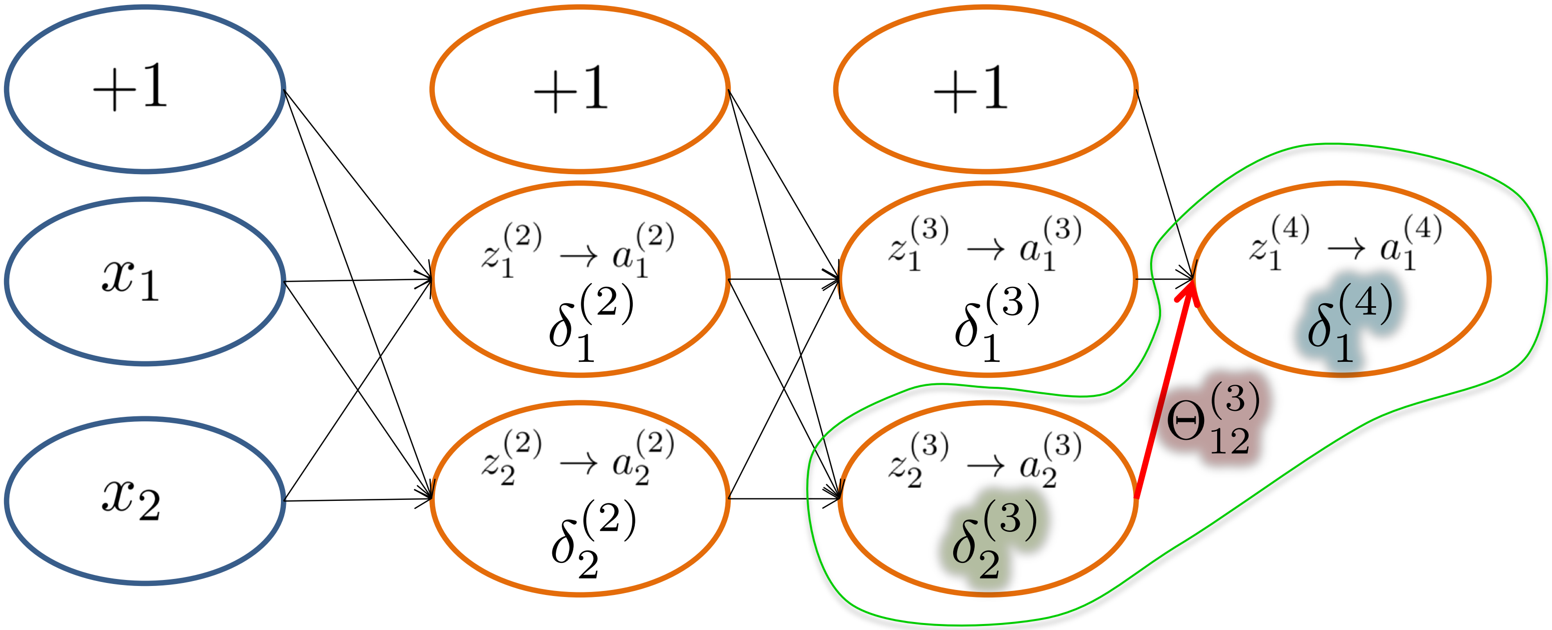
$$\boldsymbol{\delta}^{(4)} = \boldsymbol{a}^{(4)} - \mathbf{y}$$

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

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

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

Backpropagation Intuition



$$\delta_2{}^{(3)} = \Theta_{12}{}^{(3)} \times \delta_1{}^{(4)} \times g_2{}'^{(3)}$$

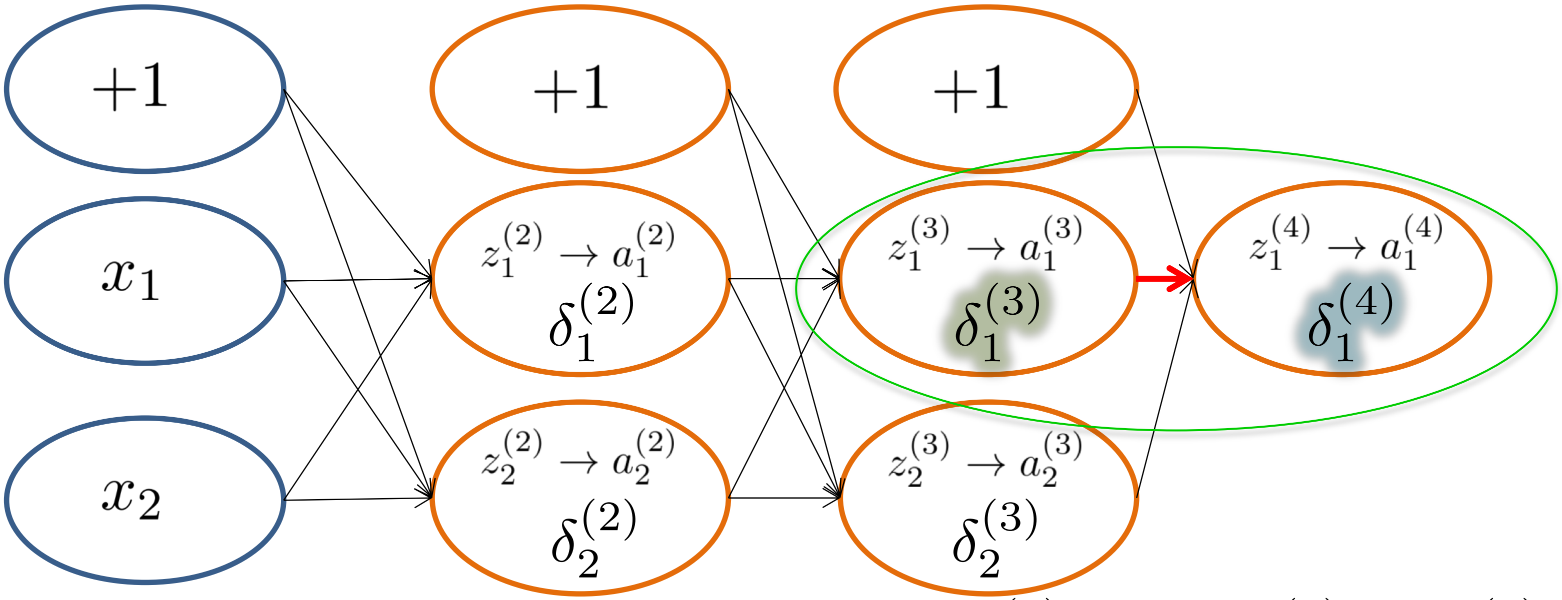
$\delta_j^{(l)} =$ "error" of node j in layer l

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

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

Based on slide by Andrew Ng

Backpropagation Intuition



$$\delta_2{}^{(3)} = \Theta_{12}{}^{(3)} \times \delta_1{}^{(4)} \times g_2{}'^{(3)}$$

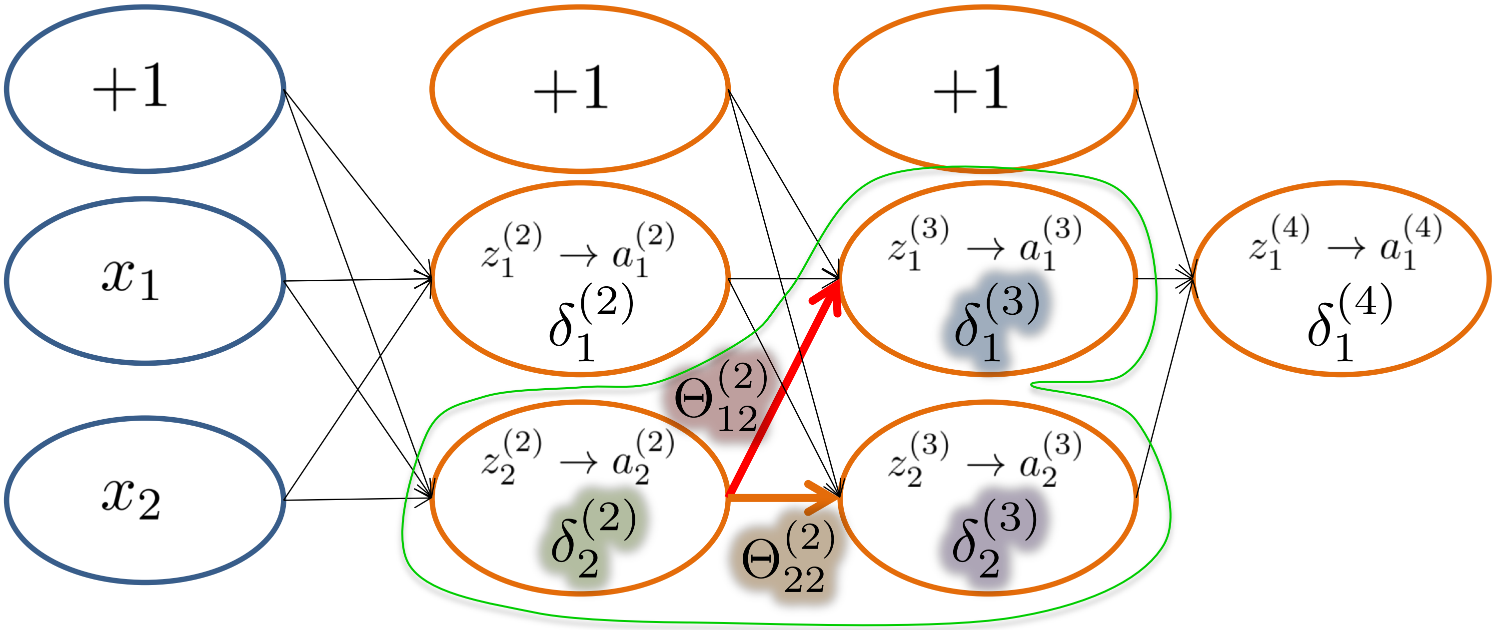
$$\delta_1{}^{(3)} = \Theta_{11}{}^{(3)} \times \delta_1{}^{(4)} \times g_1{}'^{(3)}$$

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

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

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

Backpropagation Intuition



$$\delta_2^{(2)} = [\Theta_{12}^{(2)} \times \delta_1^{(3)} + \Theta_{22}^{(2)} \times \delta_2^{(3)}] \times g_2'^{(2)}$$

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

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

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

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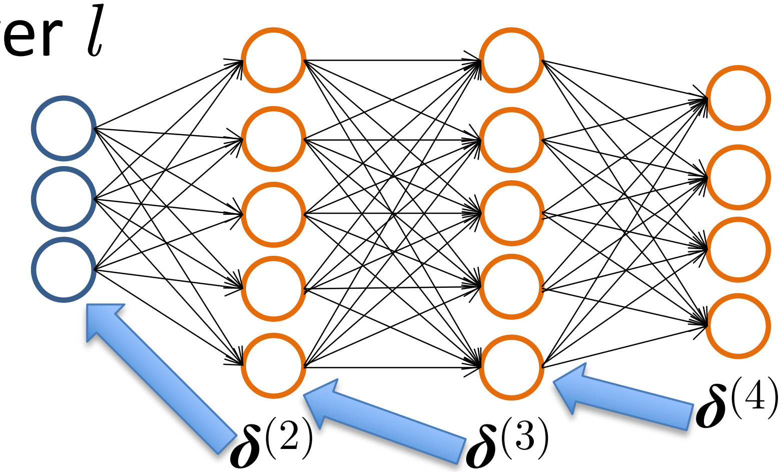
Backpropagation: Gradient Computation

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



(#layers L = 4)

Element-wise product .*

Backpropagation

- $\boldsymbol{\delta}^{(4)} = \boldsymbol{a}^{(4)} - \mathbf{y}$
- $\boldsymbol{\delta}^{(3)} = (\Theta^{(3)})^{\mathsf{T}}\boldsymbol{\delta}^{(4)} \;.\!*\; g'(\mathbf{z}^{(3)})$
- $\boldsymbol{\delta}^{(2)} = (\Theta^{(2)})^{\mathsf{T}}\boldsymbol{\delta}^{(3)} \;.\!*\; g'(\mathbf{z}^{(2)})$
- (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 $\Delta_{i,j}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)

For each training instance $(\mathbf{x}_k, y_k)$:

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

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

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

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 $\boldsymbol{\Delta}^{(l)} = \boldsymbol{\Delta}^{(l)} + \boldsymbol{\delta}^{(l+1)} \mathbf{a}^{(l)\mathsf{T}}$

Training a Neural Network via Gradient Descent with Backprop

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 $\Delta_{i,j}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)
For each training instance $(\mathbf{x}_k, y_k)$:
Set $\mathbf{a}^{(1)} = \mathbf{x}_k$
Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation
Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_k$
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 $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

Backpropagation

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

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Training a Neural Network via Stochastic Gradient Descent with Backprop

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
    Loop
        Sample training instance $(\mathbf{x}_k, y_k)$ without replacement
        Set $\mathbf{a}^{(1)} = \mathbf{x}_k$
        Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation
        Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_k$
        Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \ldots, \boldsymbol{\delta}^{(2)}\}$
        Compute gradients $\Delta_{ij}^{(l)} = a_j^{(l)} \delta_i^{(l+1)}$
        Compute stochastic regularized gradient $D_{ij}^{(l)} = \begin{cases} \Delta_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$
        Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$
    Until all training instances are seen
Until weights converge or max #epochs is reached

Backpropagation

Training a Neural Network via Mini-batch Gradient Descent with Backprop

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
  Loop // each iteration is a mini-batch
    Set $\Delta_{i,j}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)
    Sample m training instances $\mathcal{X} = \{(\mathbf{x}'_1, y'_1), \ldots, (\mathbf{x}'_m, y'_m)\}$ without replacement
    For each instance in $\mathcal{X}$, $(\mathbf{x}_k, y_k)$:
      Set $\mathbf{a}^{(1)} = \mathbf{x}_k$
      Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation
      Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_k$
      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 mini-batch regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{m}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{m}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$
    Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$
  Until all training instances are seen
Until weights converge or max #epochs is reached

Backpropagation

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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

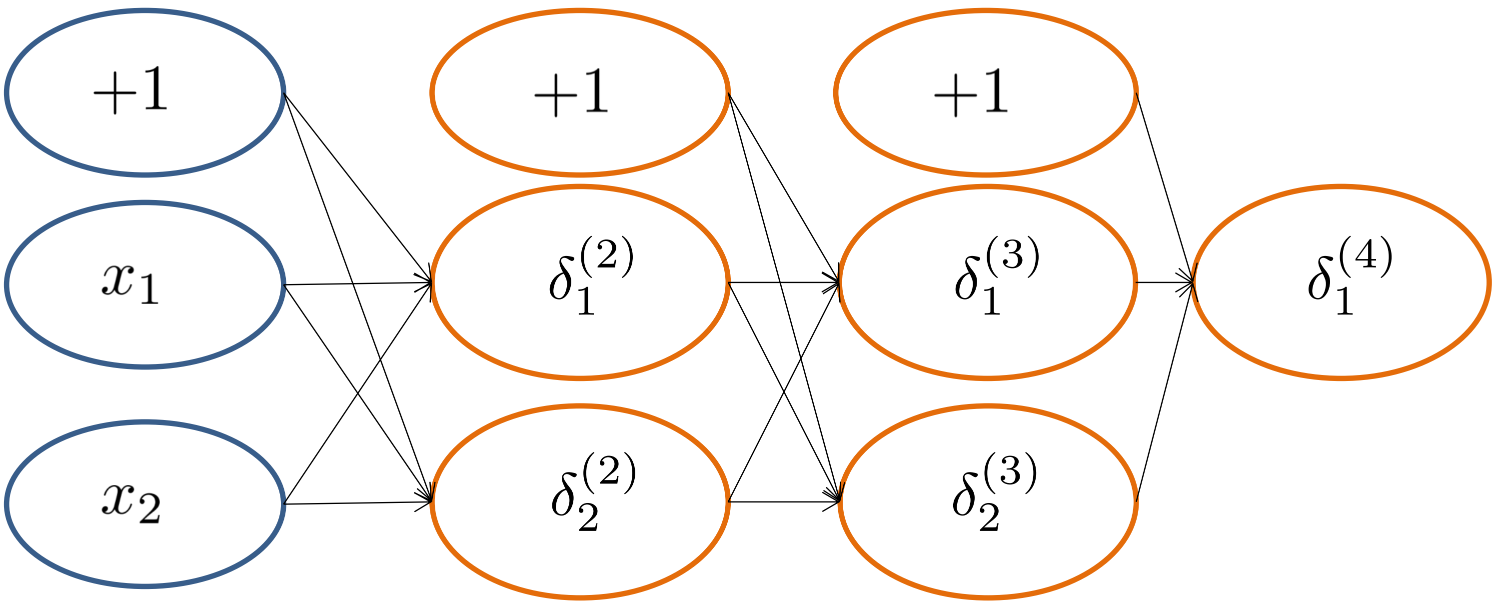
Problems:

- black box
- local minima

Implementation Details

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

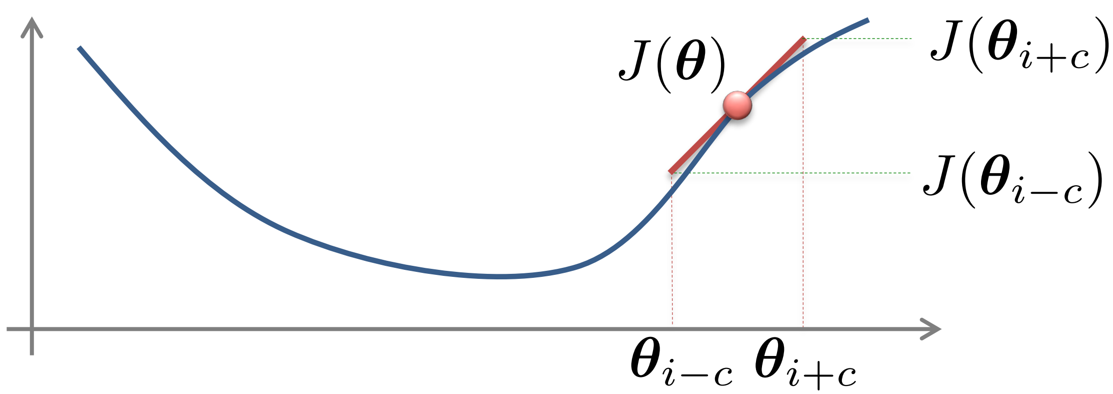
```
theta1 = reshape(theta[0:100], (10, 10))
```

- 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



$$\frac{\partial}{\partial \theta_i} J(\boldsymbol{\theta}) \approx \frac{J(\boldsymbol{\theta}_{i+c}) - J(\boldsymbol{\theta}_{i-c})}{2c}$$

$$c \approx 1\text{E-}4$$

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

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

Gradient Checking

$\boldsymbol{\theta} \in \mathbb{R}^m \qquad \boldsymbol{\theta}$ 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`

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

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

$$\vdots$$

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

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

Implementation Steps

- Implement backprop to compute `DVec`
  - `DVec` is the unrolled $\{D^{(1)}, D^{(2)}, \ldots\}$ matrices
- Implement numerical gradient checking to compute `gradApprox`
- Make sure `DVec` has similar values to `gradApprox`
- Turn off gradient checking. Use backprop code for learning.

Important: Be sure to disable your gradient checking code before training your classifier.

- If you run the numerical gradient computation on every iteration of gradient descent, your code will be very slow

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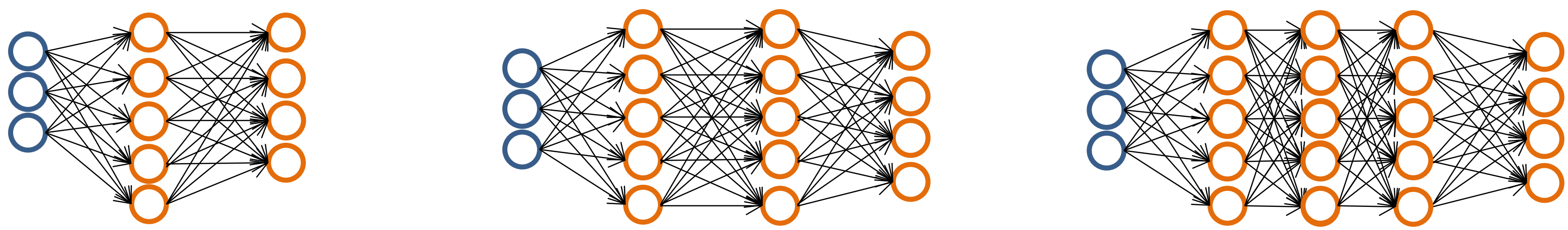
Putting It All Together

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 $\frac{\partial}{\partial \Theta^{(l)}_{jk}} J(\Theta)$
5. Use gradient checking to compare $\frac{\partial}{\partial \Theta^{(l)}_{jk}} J(\Theta)$ computed using backpropagation vs. the numerical gradient estimate.
   - Then, disable gradient checking code
6. Use gradient descent with backprop to fit the network

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