Neural Networks

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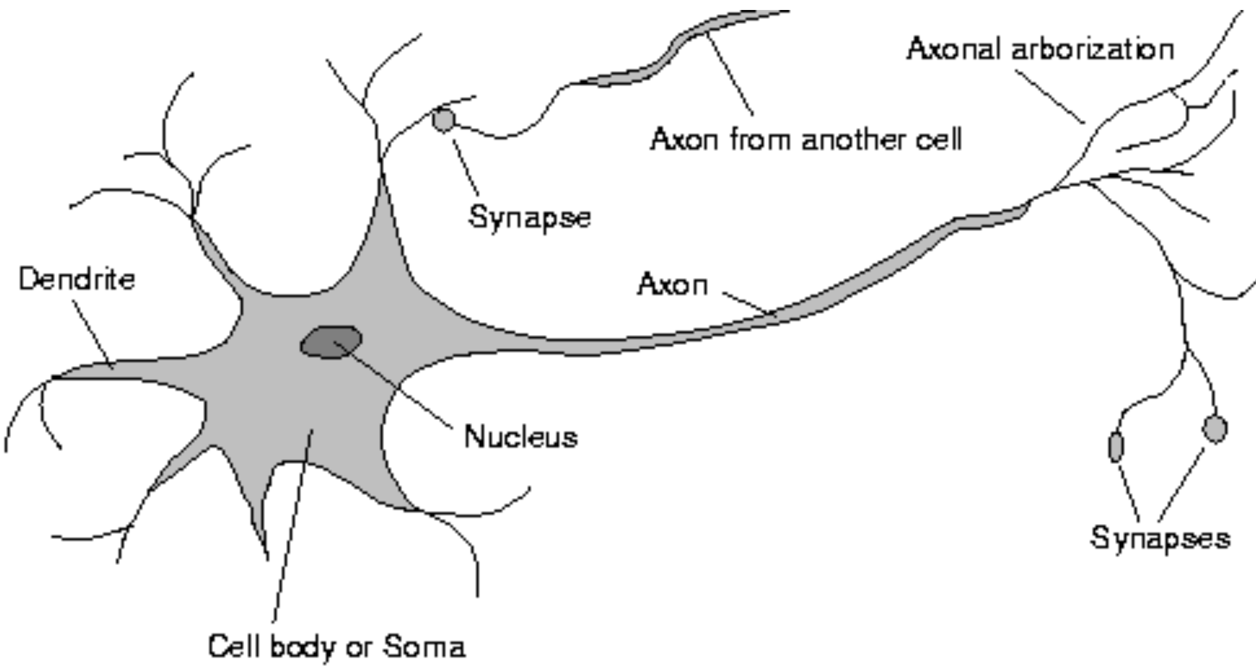
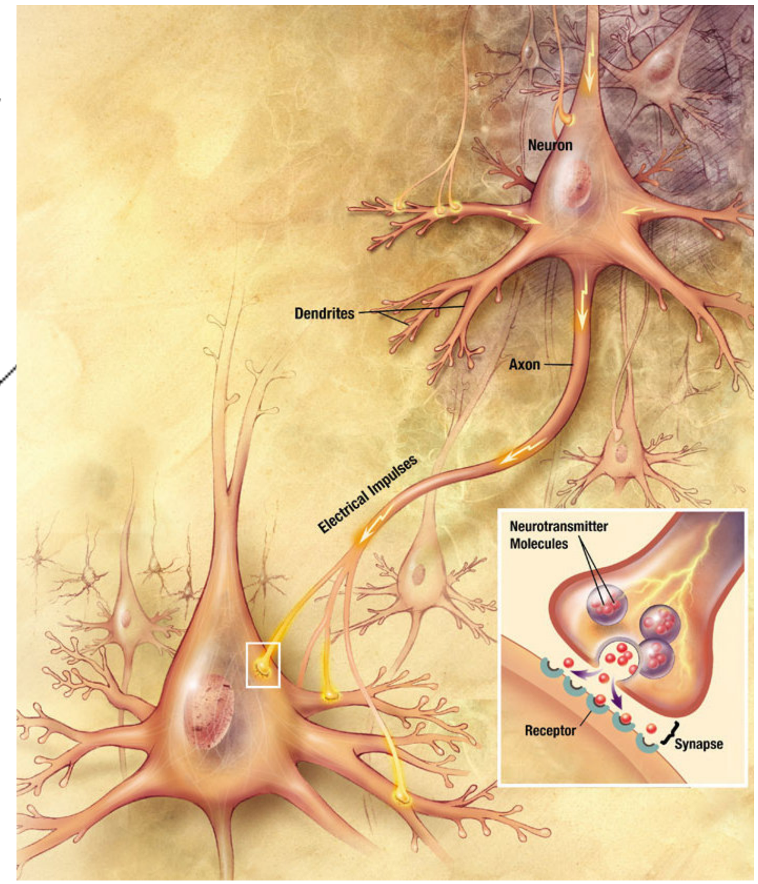
Neural Function

- 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

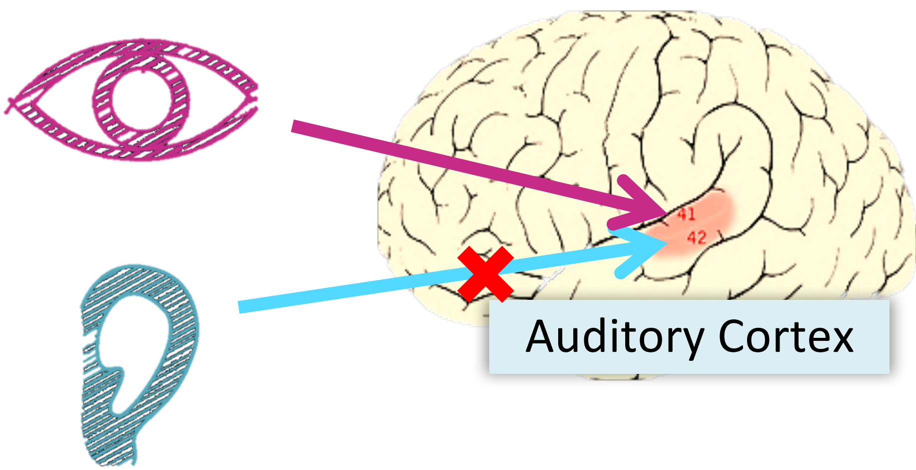




Brain Structure

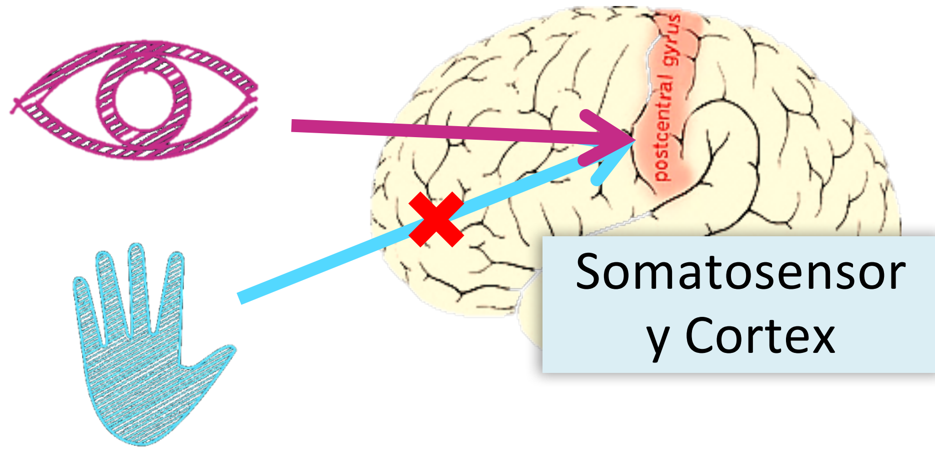
- Different areas of the brain have different functions
  - Some areas seem to have the same function in all humans (e.g., Broca's region for motor speech); the overall layout is generally consistent
  - Some areas are more plastic, and vary in their function; also, the lower-level structure and function 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]

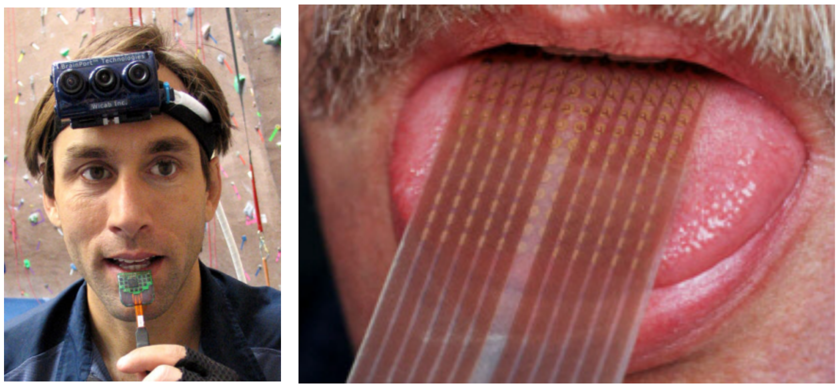


Somatosensory cortex learns to see

[Metin & Frost, 1989]

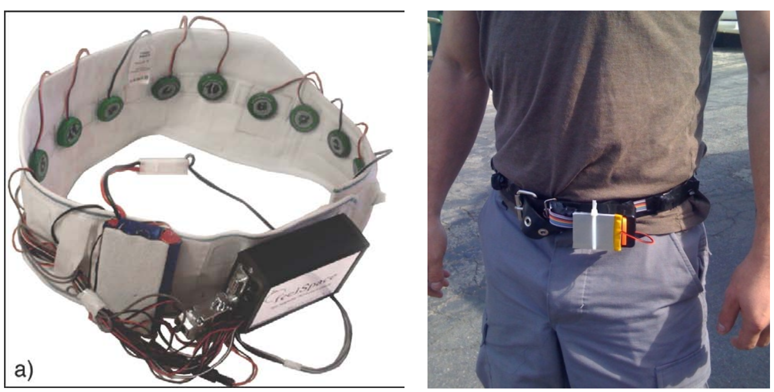
Based on slide by Andrew Ng

Sensor Representations in the Brain

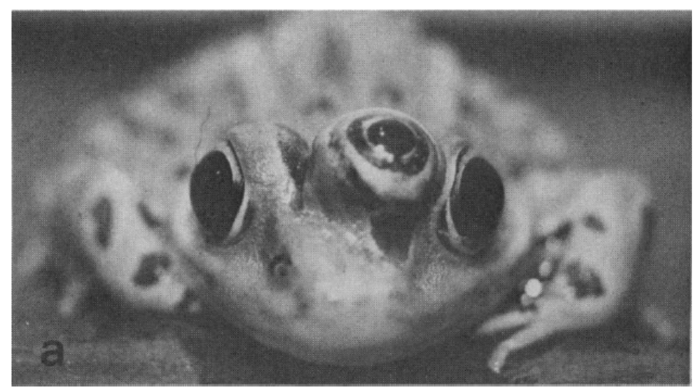


Seeing with your tongue

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

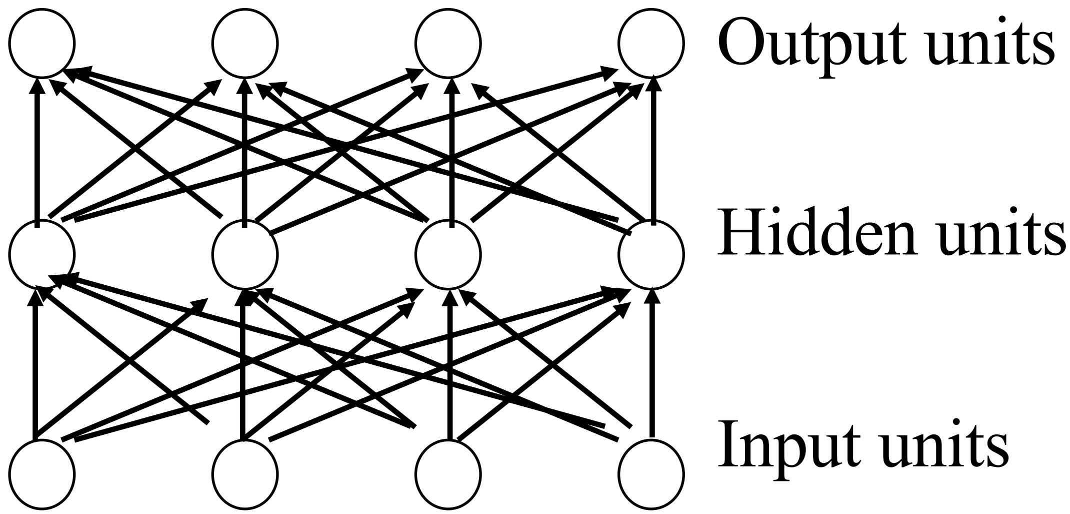
INFORMATION CIRCA 2012	**Computer**	**Human Brain**
Computation Units	10-core Xeon: 10^9 Gates	10^{11} Neurons
Storage Units	10^9 bits RAM, 10^{12} bits disk	10^{11} neurons, 10^{14} synapses
Cycle time	10^{-9} sec	10^{-3} sec
Bandwidth	10^9 bits/sec	10^{14} bits/sec

- 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

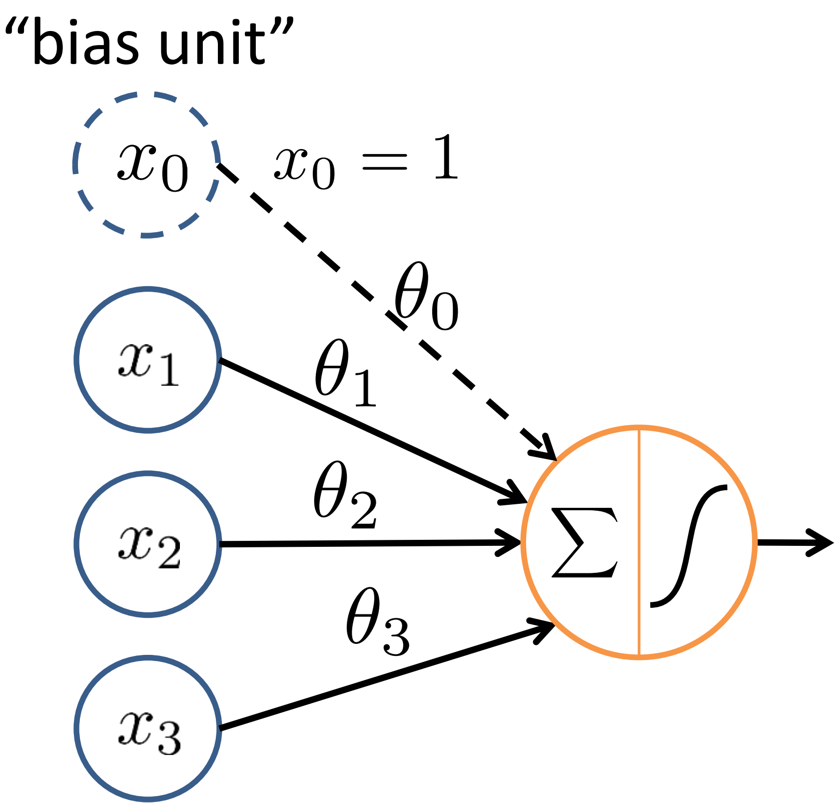
Neural networks



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: Logistic Unit

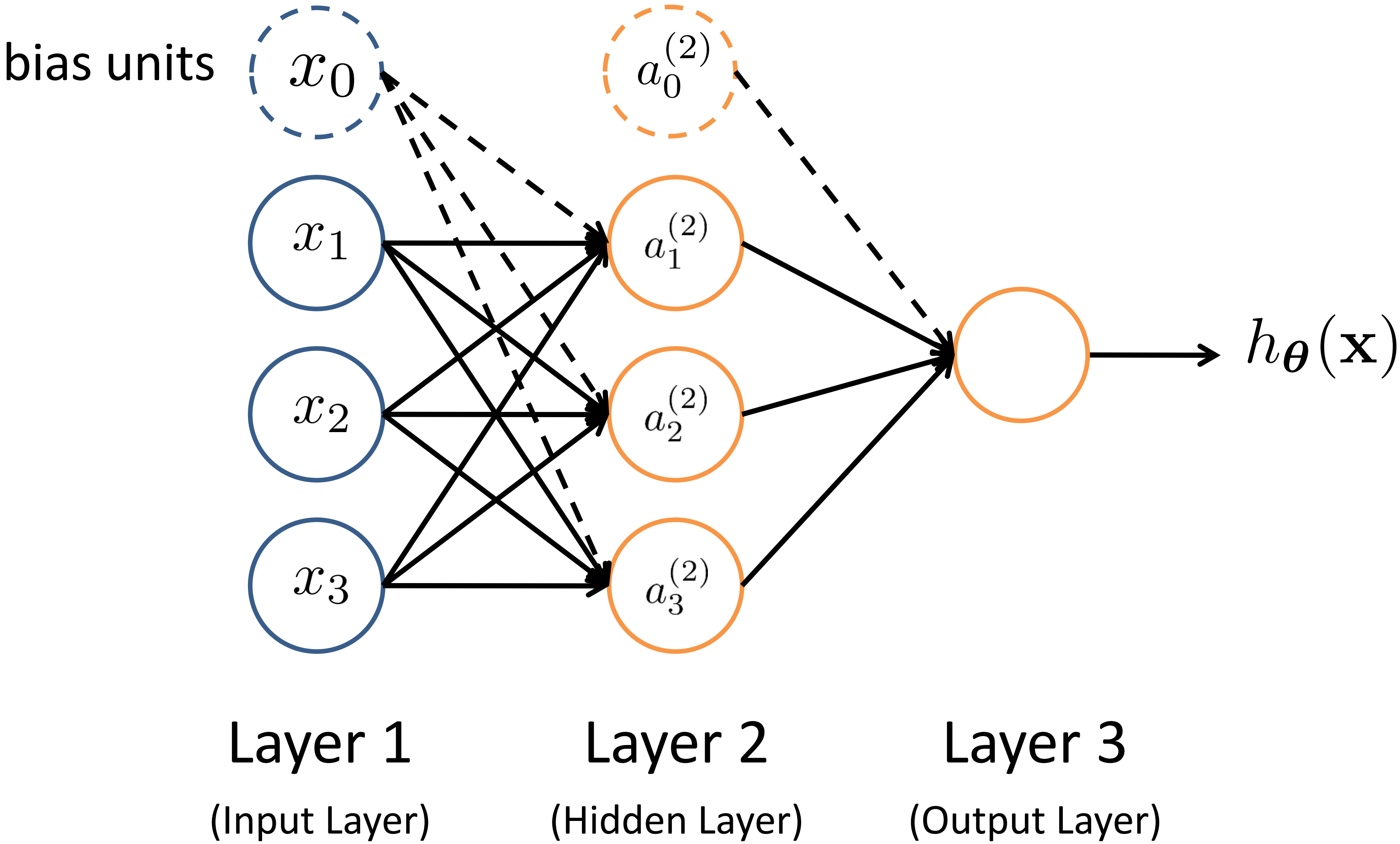


$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

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

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

Neural Network

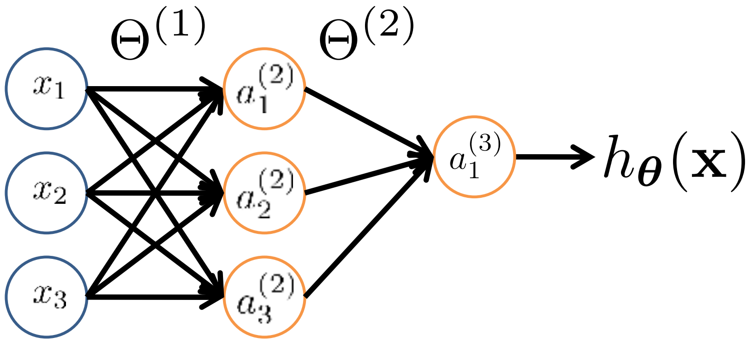


Slide by Andrew Ng

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) .

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

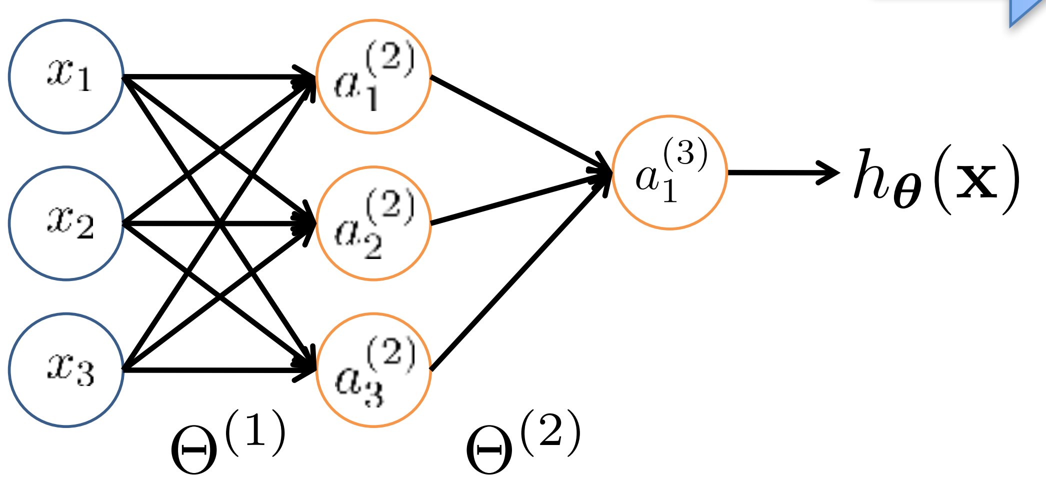
Vectorization

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

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

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

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



Feed-Forward Steps:

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

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

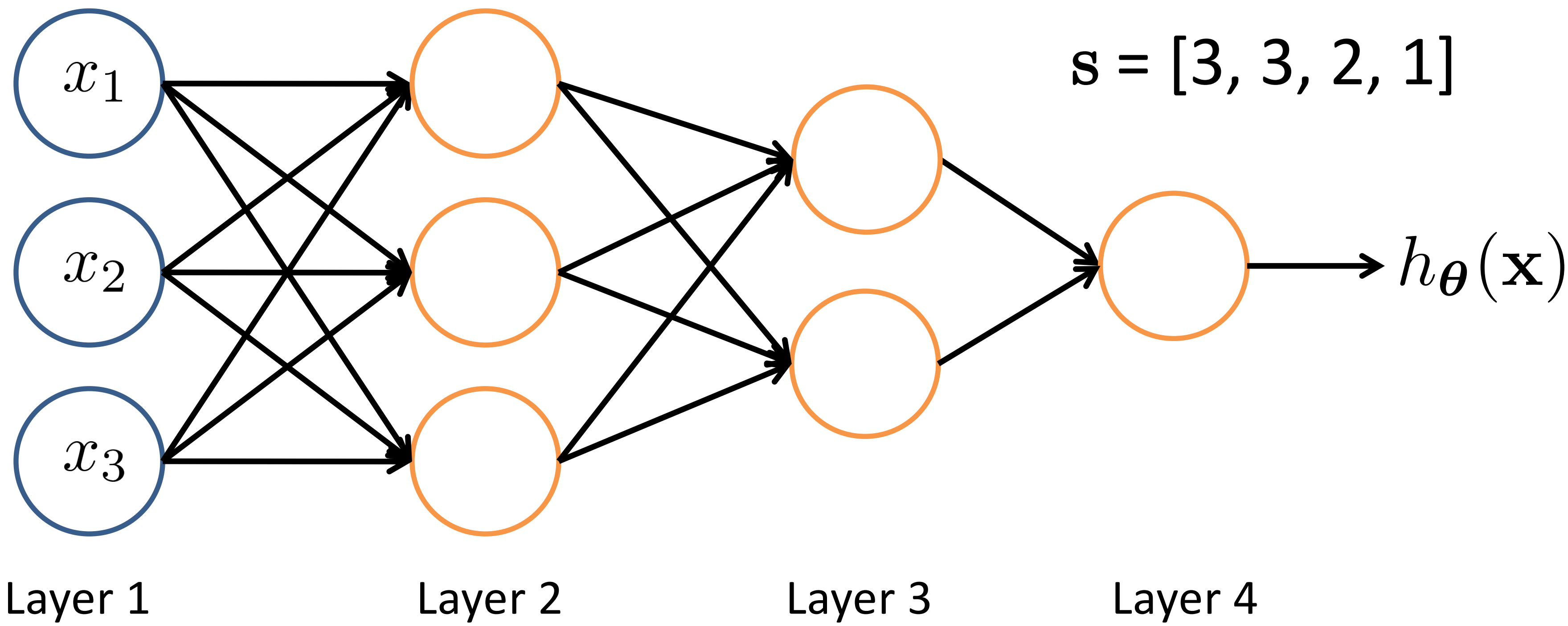
$$\text{Add } a_0^{(2)} = 1$$

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

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

Based on slide by Andrew Ng

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

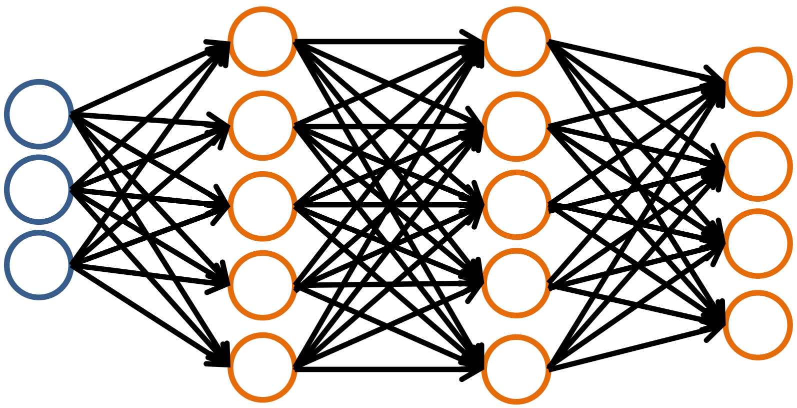
Multiple Output Units: One-vs-Rest

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

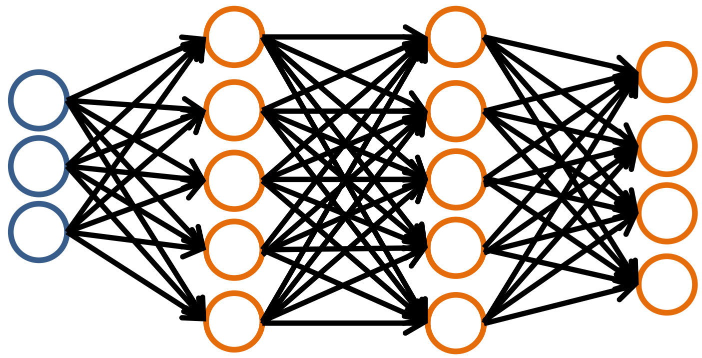
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

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

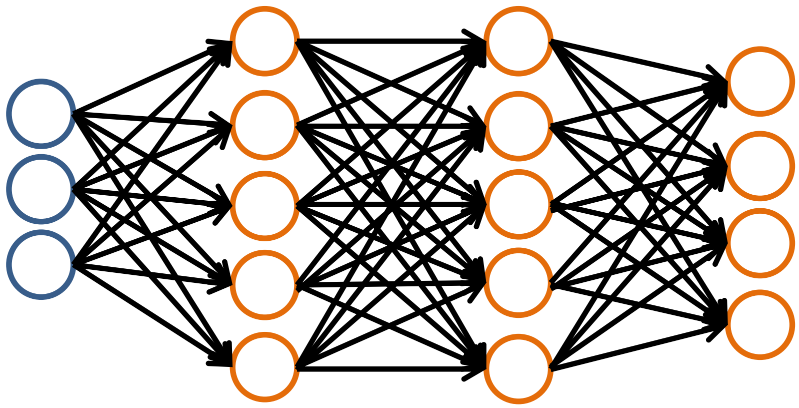
$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when motorcycle

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

Based on slide by Andrew Ng

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

Slide by Andrew Ng

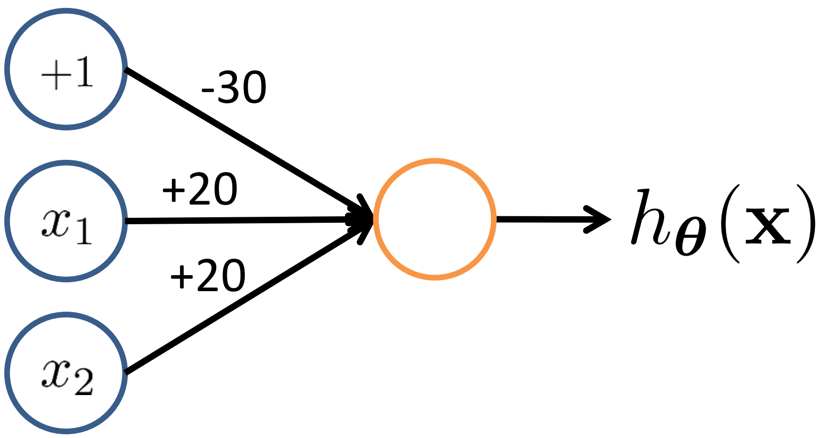
Understanding Representations

Representing Boolean Functions

Simple example: AND

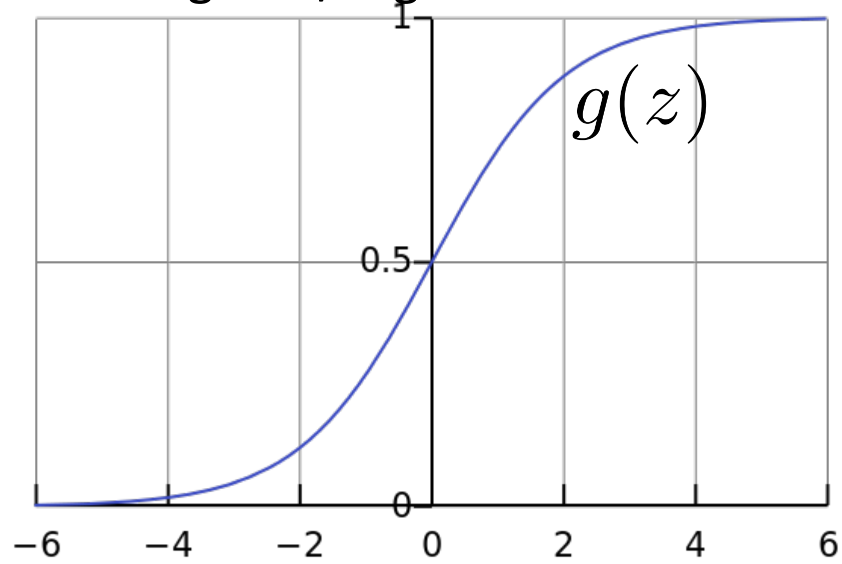
$x_1, x_2 \in \{0, 1\}$

$y = x_1 \text{ AND } x_2$



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

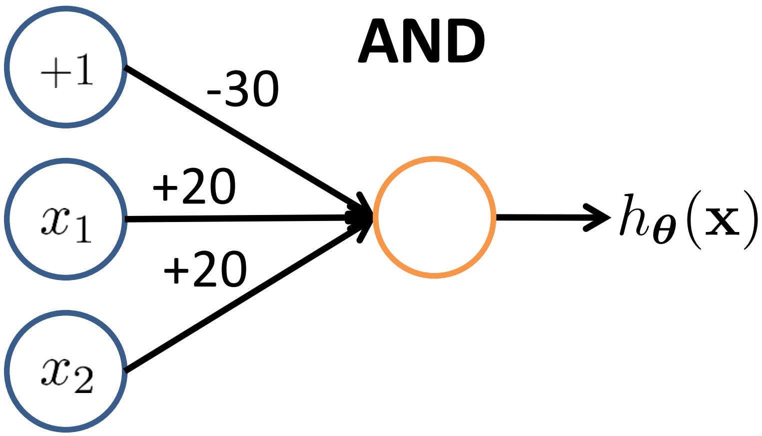
Logistic / Sigmoid Function



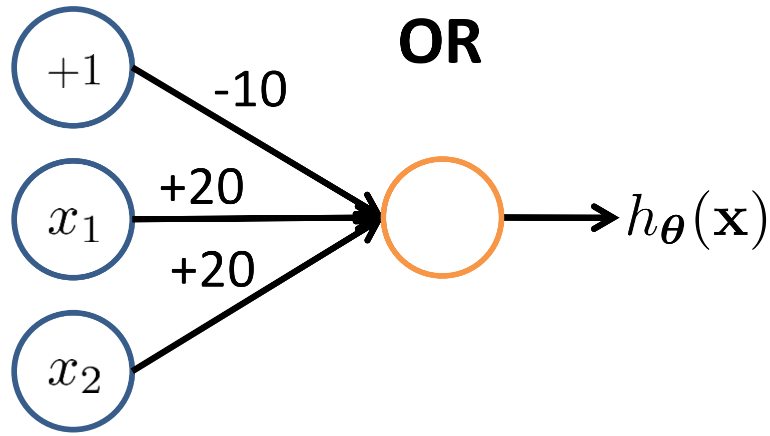
x_1	x_2	$h_\Theta(\mathbf{x})$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

Representing Boolean Functions

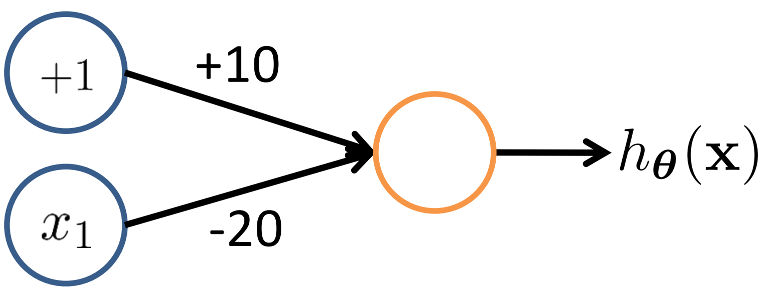
AND



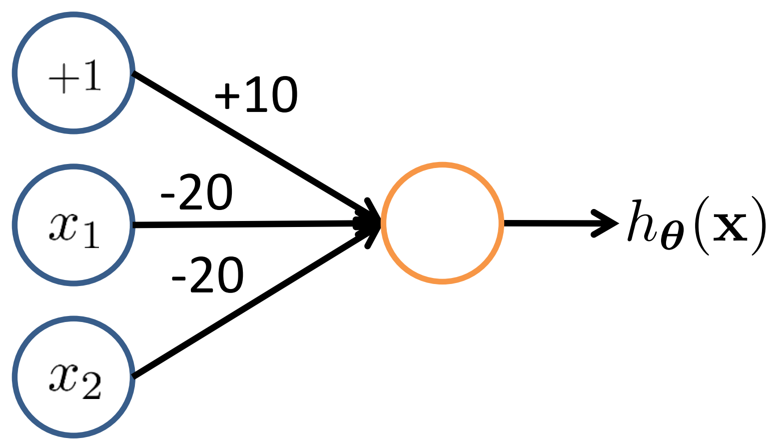
OR



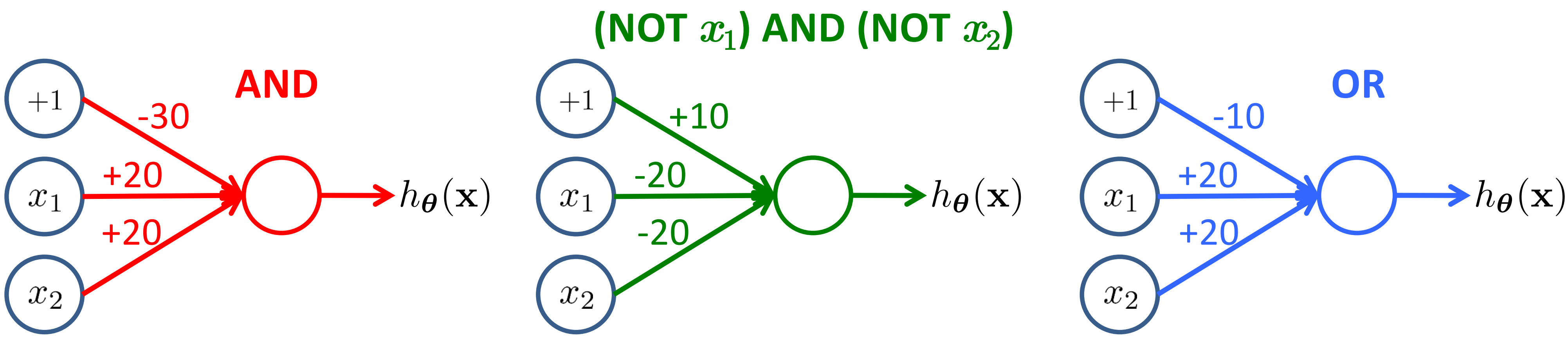
NOT

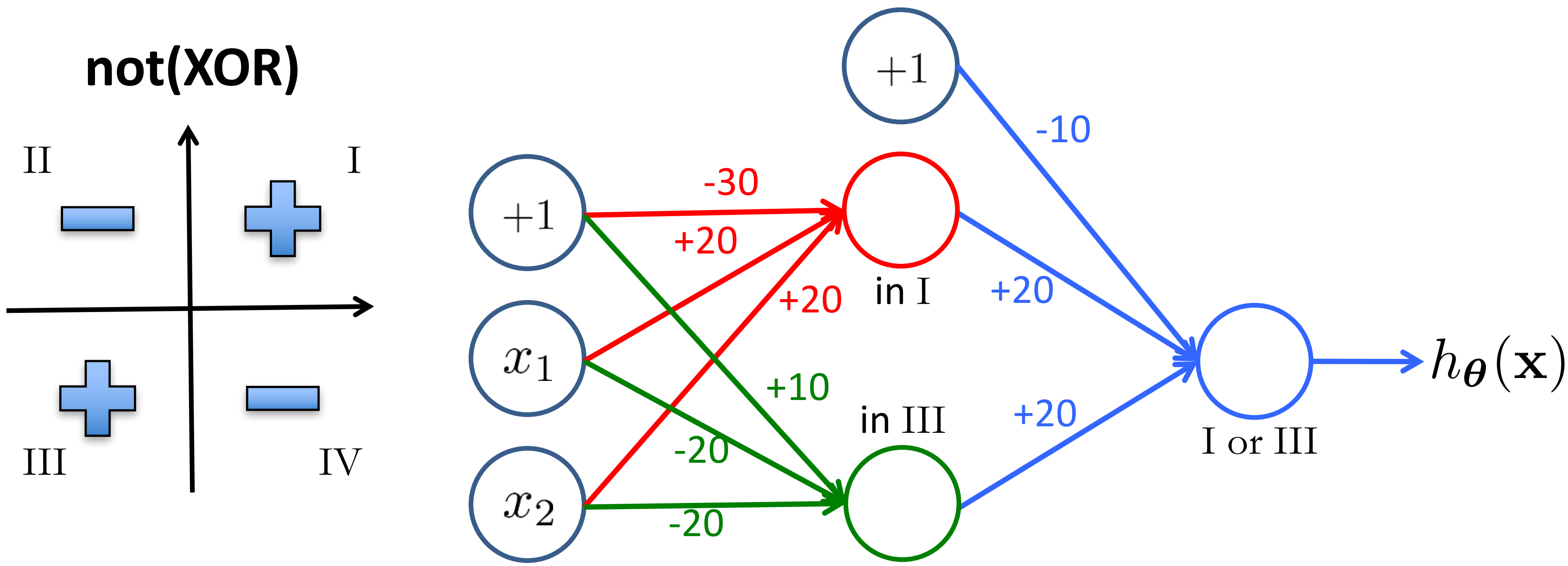


(NOT x_1) AND (NOT x_2)



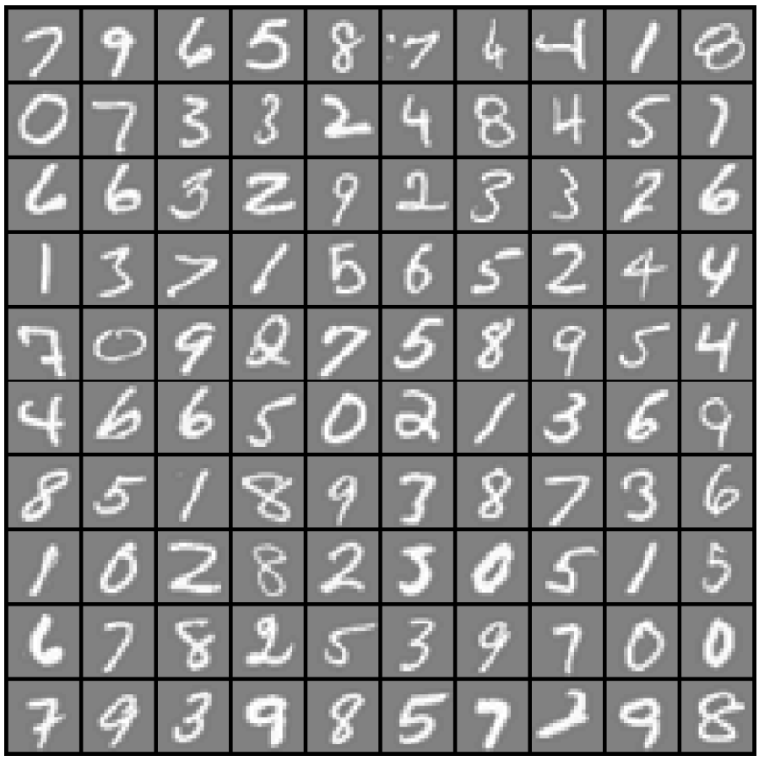
Combining Representations to Create Non-Linear Functions





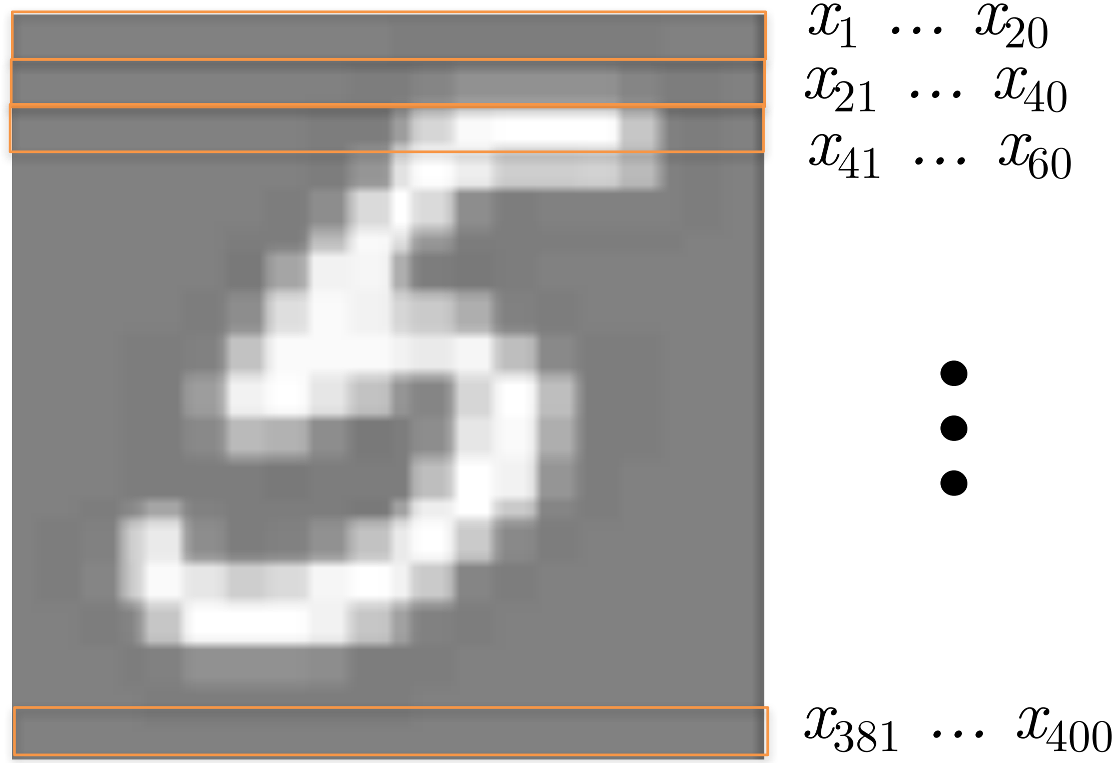
Based on example by Andrew Ng

Layering Representations



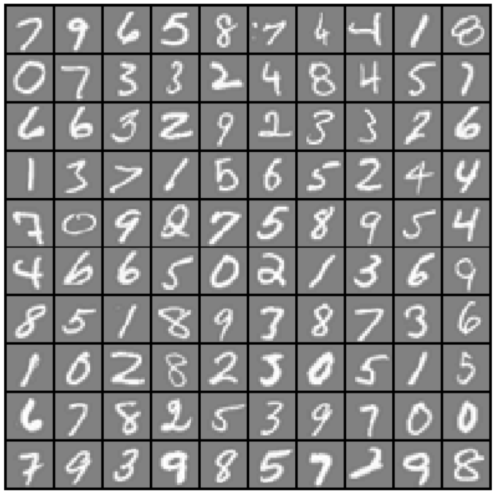
20 × 20 pixel images

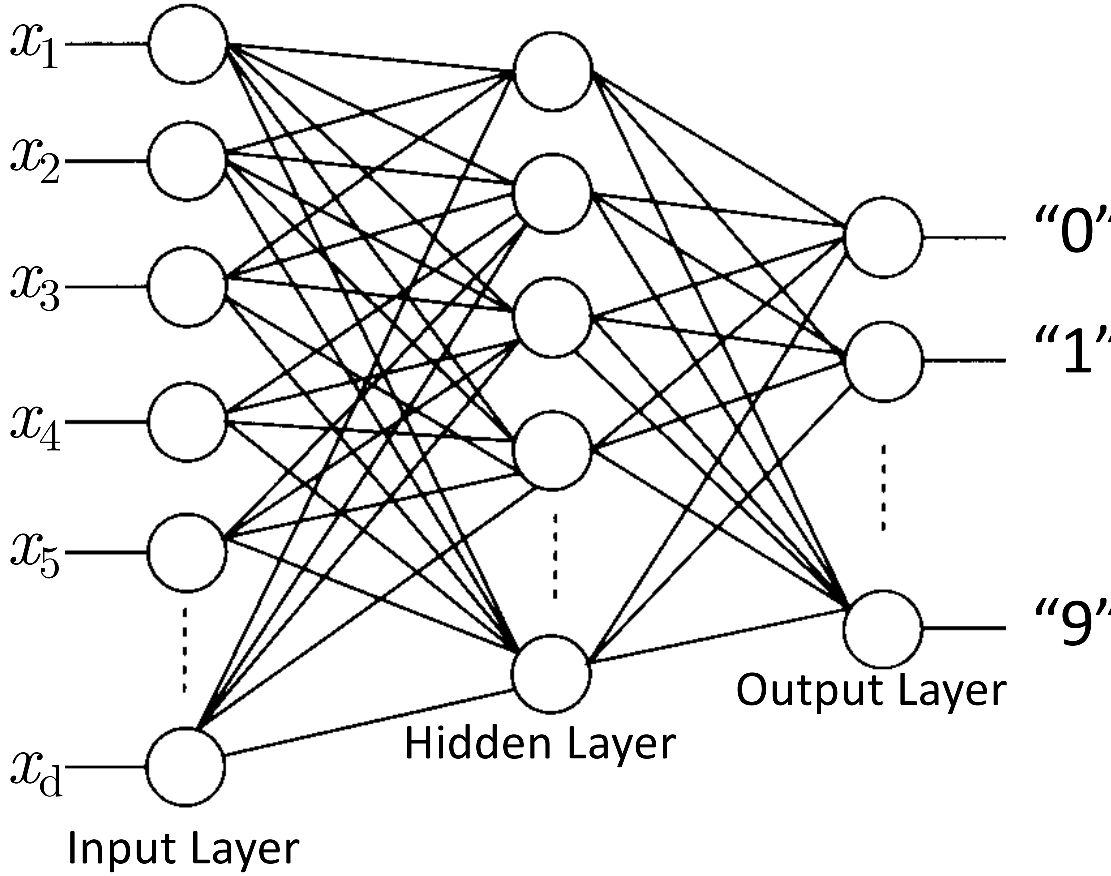
d = 400   10 classes

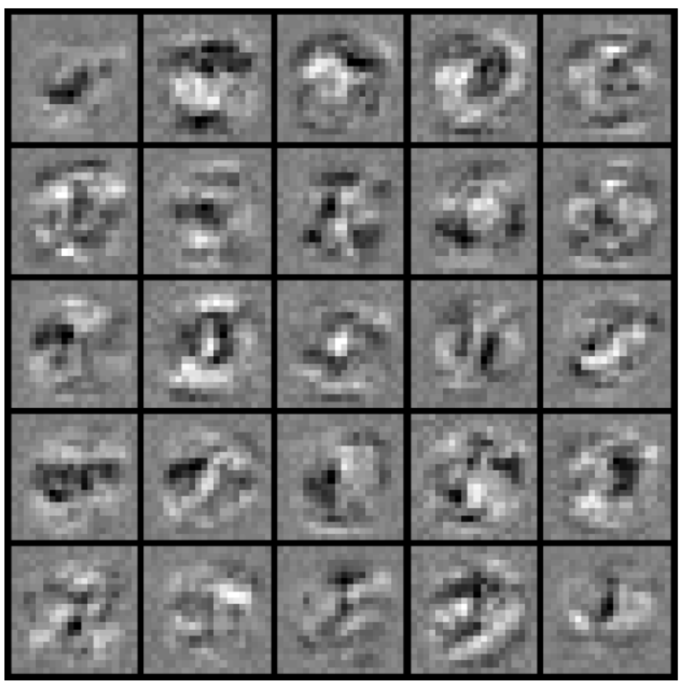


Each image is “unrolled” into a vector $\mathbf{x}$ of pixel intensities

Layering Representations







Visualization of Hidden Layer

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

Neural Network Learning

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]

Batch Perceptron

Given training data $\{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{n}$
Let $\boldsymbol{\theta} \leftarrow [0, 0, \ldots, 0]$
Repeat:
  Let $\boldsymbol{\Delta} \leftarrow [0, 0, \ldots, 0]$
  for $i = 1 \ldots n$, do
    if $y^{(i)}\boldsymbol{x}^{(i)}\boldsymbol{\theta} \leq 0$ // prediction for i^{th} instance is incorrect
      $\boldsymbol{\Delta} \leftarrow \boldsymbol{\Delta} + y^{(i)}\boldsymbol{x}^{(i)}$
  $\boldsymbol{\Delta} \leftarrow \boldsymbol{\Delta}/n$ // compute average update
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\boldsymbol{\Delta}$
Until $\|\boldsymbol{\Delta}\|_2 < \epsilon$

- Simplest case: α = 1 and don't normalize, yields the fixed increment perceptron
- Each increment of outer loop is called an **epoch**

Based on slide by Alan Fern

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

Cost Function

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^{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:

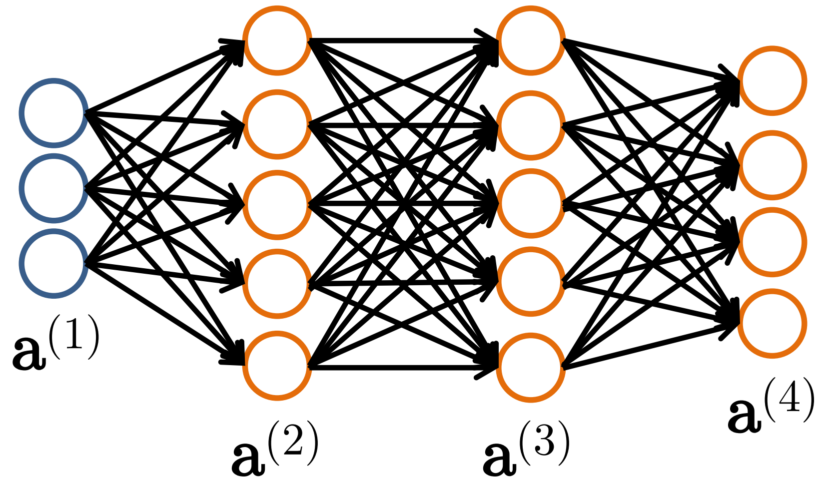
- $J(\Theta)$
- $\frac{\partial}{\partial\Theta_{ij}^{(l)}}J(\Theta)$

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



Based on slide by Andrew Ng

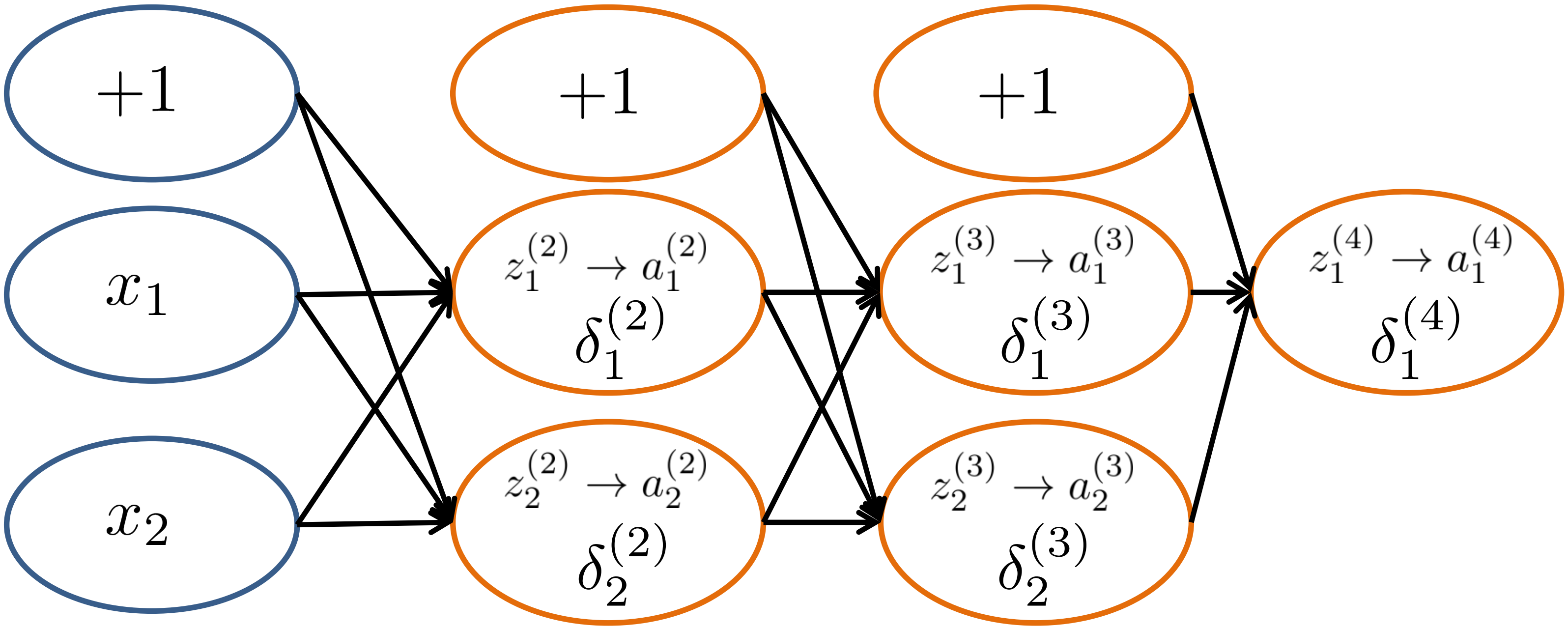
Backpropagation Intuition

- 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

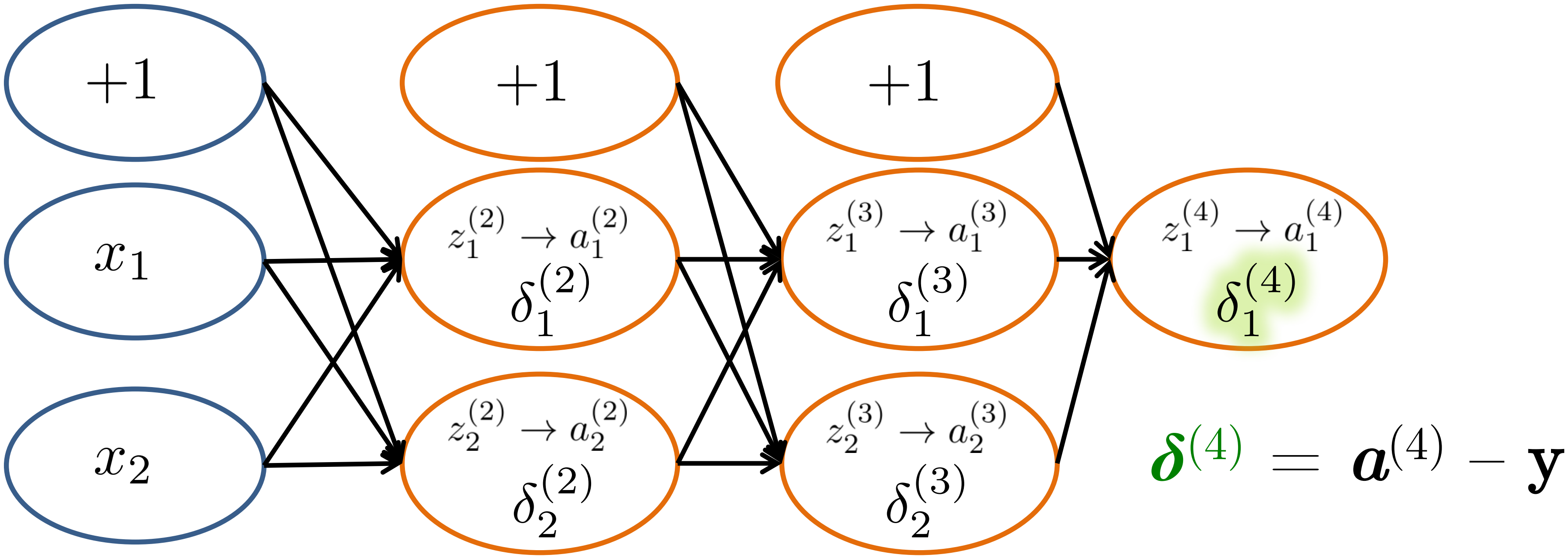


$\delta_j^{(l)}$ = "error" of node j in layer l

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

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

Backpropagation Intuition



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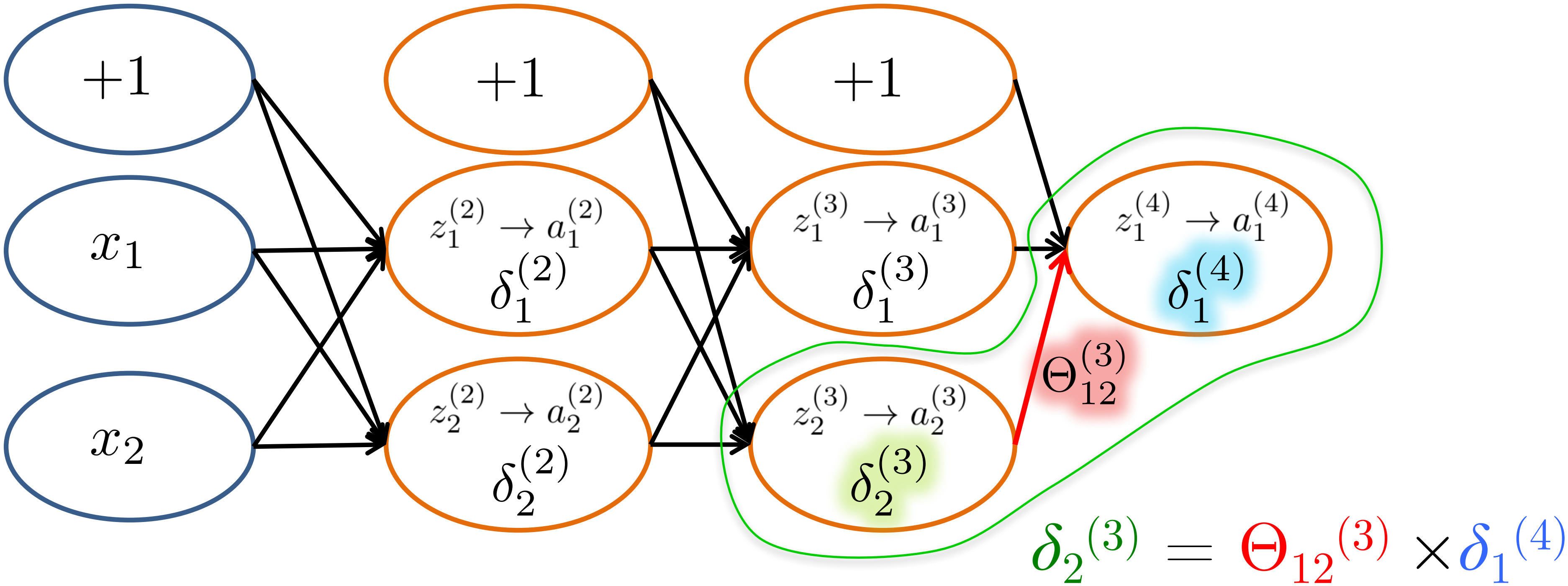
Backpropagation Intuition



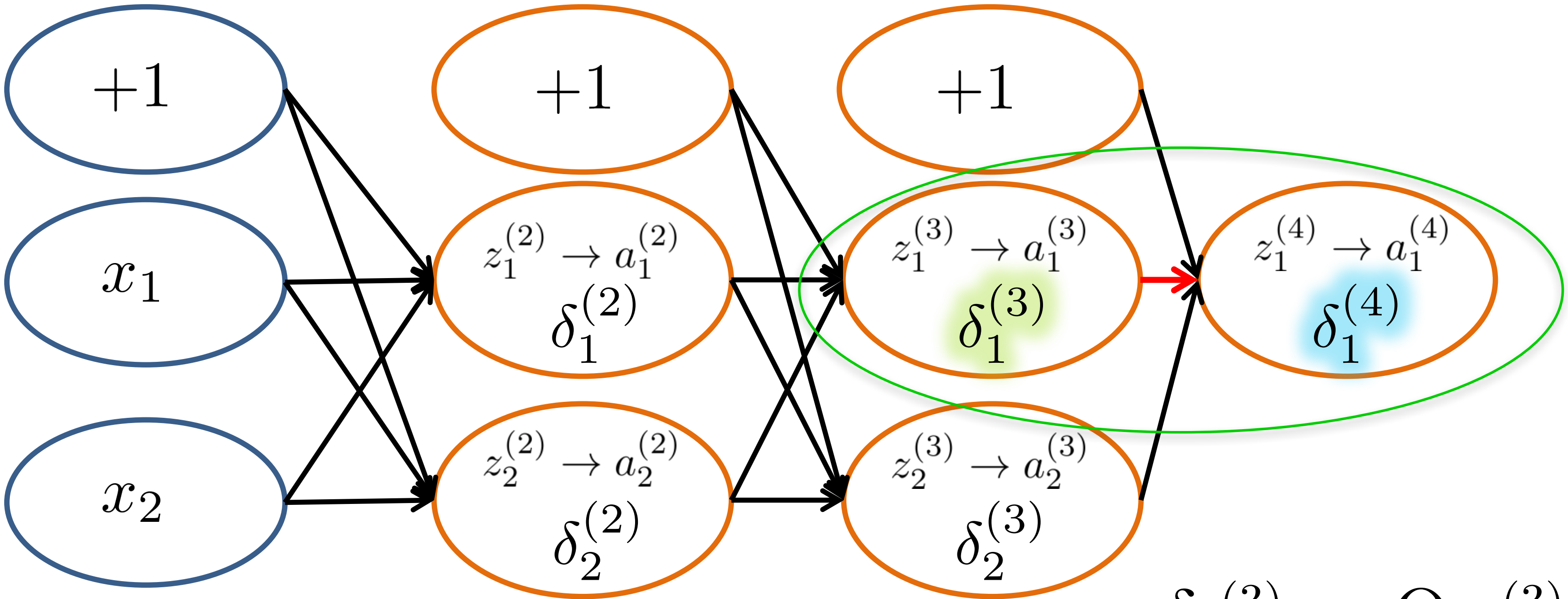
$\delta_j^{(l)} =$ "error" of node j in layer l

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

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

Based on slide by Andrew Ng

Backpropagation Intuition



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

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

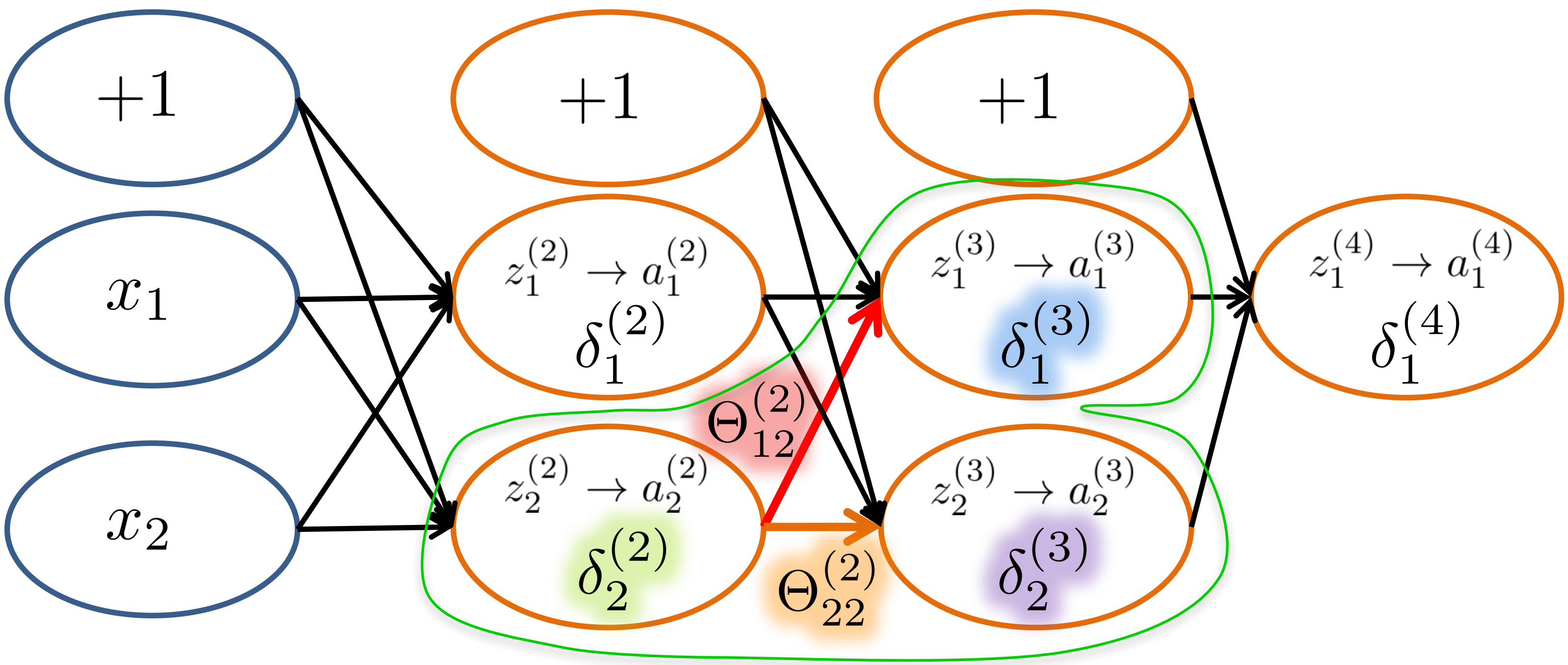
$\delta_j{}^{(l)}$ = "error" of node j in layer l

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

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

Based on slide by Andrew Ng

Backpropagation Intuition



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

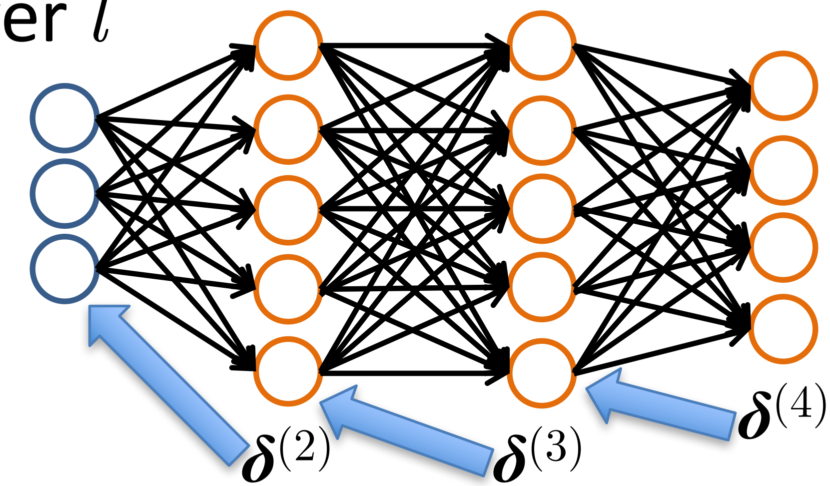
$\delta_j^{(l)} =$ "error" of node j in layer l

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

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

Backpropagation: Gradient Computation

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



(#layers L = 4)

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

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

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 $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (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

Based on slide by Andrew Ng

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

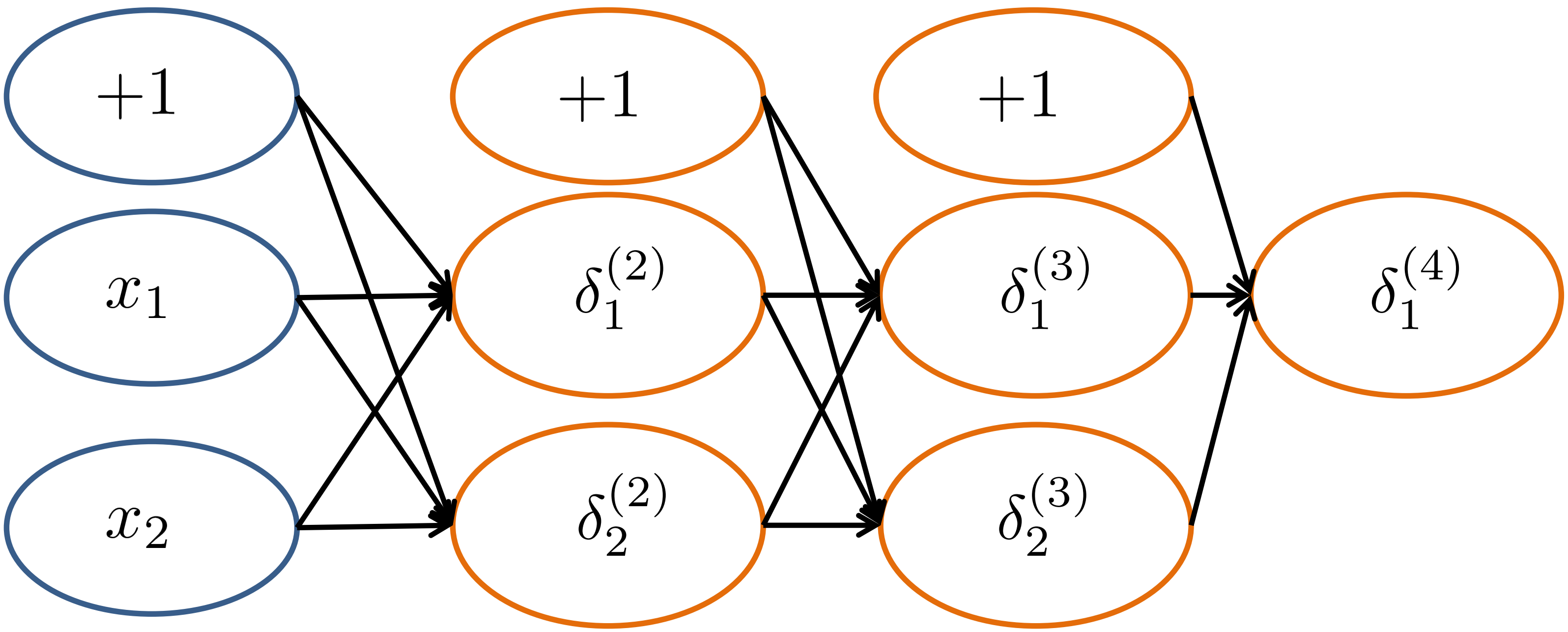
Problems:

- 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

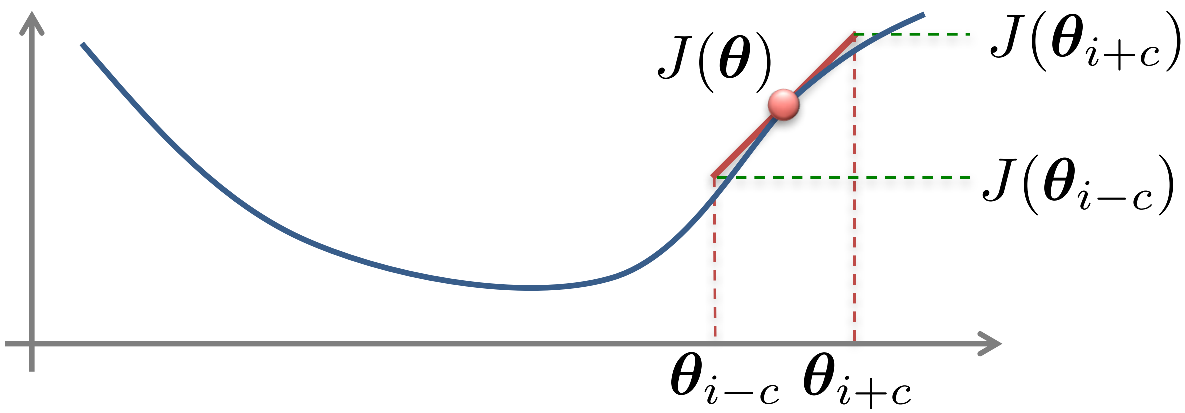
- For convenience, compress all parameters into $\boldsymbol{\theta}$
  - "unroll" $\Theta^{(1)}, \Theta^{(2)}, \ldots, \Theta^{(L-1)}$ into one long vector $\boldsymbol{\theta}$
    - E.g., if $\Theta^{(1)}$ is 10 x 10, then the first 100 entries of $\boldsymbol{\theta}$ contain the value in $\Theta^{(1)}$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

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

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

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

$$\vdots$$

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

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. Using backprop code for learning.

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

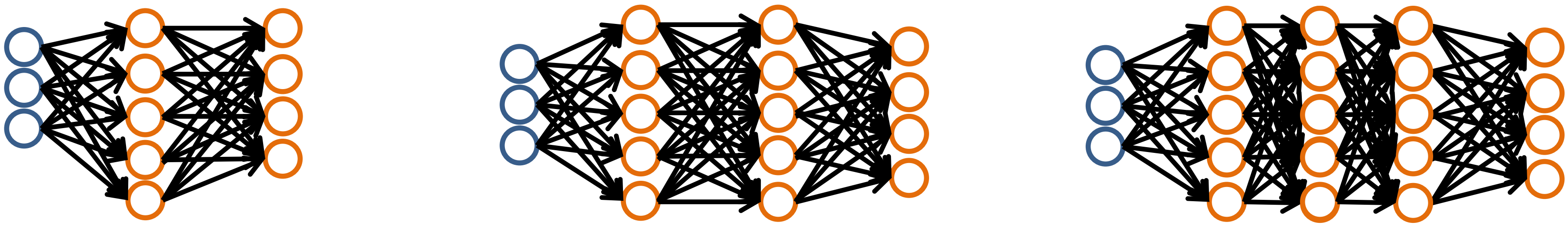
- If you run the numerical gradient computation on every iteration of gradient descent, your code will be very slow

Based on slide by Andrew Ng

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