

Neural Networks

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1 Motivation

2 Perceptron

3 Neural Networks

4 Backpropagation

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- Brain functions (thoughts) 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' plasticity: they exhibit long-term changes in connection strength
- There are about 10^{11} neurons and about 10^{14} synapses in the human brain

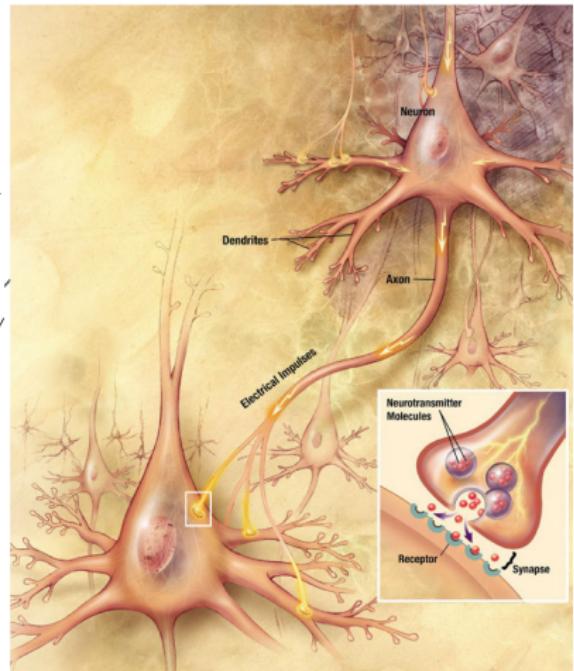
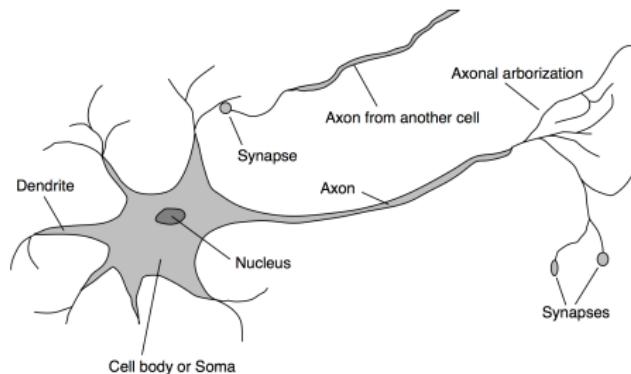
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Neurons II



- 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)
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The “one learning algorithm” hypothesis

- There is some evidence that the human brain uses essentially the same algorithm to understand many different input modalities
- Example: Ferret experiments, in which the “input” for vision was plugged into auditory part of brain, and the auditory cortex learns to “see”

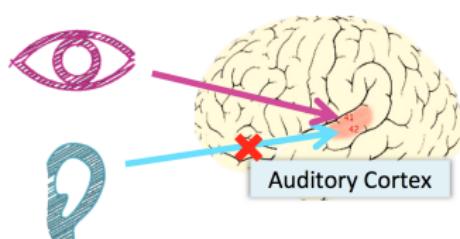


Figure – Auditory cortex learns to see

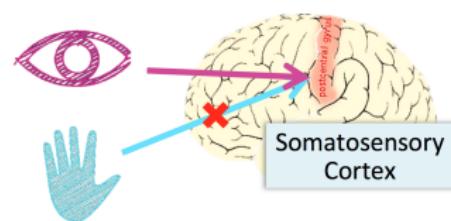


Figure – Somatosensory cortex learns to see

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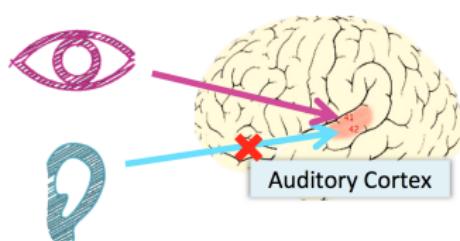


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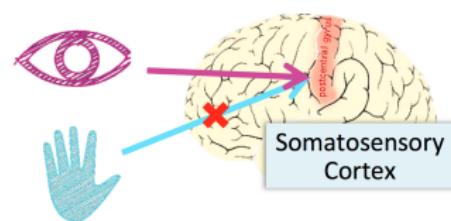


Figure – Somatosensory cortex learns to see



Figure – Seeing with your tongue



Figure – Haptic belt: direction sense

- Computers are way faster than neurons, e.g.: cycle time is 10^{-9} sec for a computer vs. 10^{-3} sec for a human brain
- But there are a lot more neurons (10^{11} neurons, 10^{14} synapses) than we can reasonably model in modern digital computers, and they all fire in parallel (bandwidth is 10^9 bits/sec for a computer vs. 10^{14} bits/sec for a human brain)
- Neural networks are designed to be massively parallel
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- Origins: Algorithms that try to mimic the brain
- Very widely used in 80s and early 90s; popularity diminished in late 90s
- Recent renaissance: state-of-the-art technique for many applications
- Artificial neural networks are not nearly as complex or intricate as the actual brain structure

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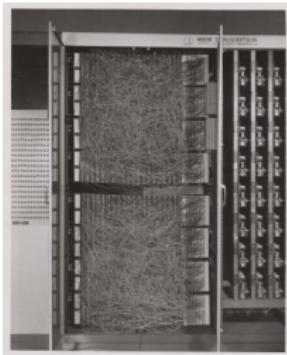
Cornell Aeronautical Laboratory



Figure – Rosenblatt & Mark I Perceptron: the first machine that could “learn” to recognize and identify optical patterns

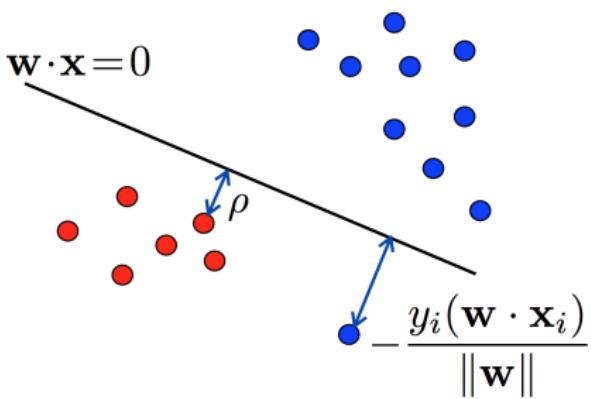
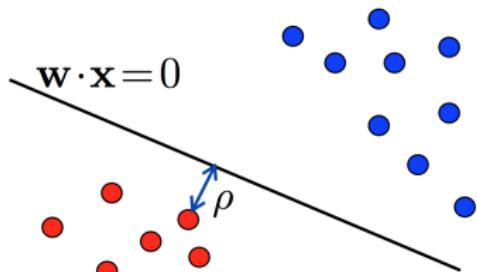
- Invented by F. Rosenblatt in 1957 in an attempt to understand human memory, learning and cognitive processes
- The first neural network model by computation, with a remarkable learning algorithm
- Became the foundation of pattern recognition research

One of the earliest and most influential neural networks: an important milestone in AI



- The Mark I Perceptron machine was connected to a camera with 20×20 cadmium sulfide photocells to produce a 400-pixel image. The main visible feature is a patchboard that allowed experimentation with different combinations of input features. To the right of that are arrays of potentiometers, implementing the adaptive weights
- The New York Times wrote that it was "the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence". In short, artificial intelligence

- Margin and errors



Perceptron(\mathbf{w}_0)

1. $\mathbf{w}_1 \leftarrow \mathbf{w}_0$ (typically $\mathbf{w}_0 = 0$)
2. **for** $t \leftarrow 1$ **to** T **do**
3. Receive(\mathbf{x}_t)
4. $\hat{y}_t \leftarrow \text{sgn}(\mathbf{w}_t \cdot \mathbf{x}_t)$
5. Receive(y_t)
6. **if** ($\hat{y}_t \neq y_t$) **then**
7. $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + y_t \mathbf{x}_t$ (or $\leftarrow \mathbf{w}_t + \eta y_t \mathbf{x}_t$, $\eta > 0$)
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- **Objective function:** convex but not differentiable

$$F(\mathbf{w}) = \frac{1}{T} \sum_{t=1}^T \max(0, -y_t(\mathbf{w} \cdot \mathbf{x}_t)) = \mathbb{E}_{\mathbf{x} \sim \hat{D}}[f(\mathbf{w}, \mathbf{x})]$$

with $f(\mathbf{w}, \mathbf{x}) = \max(0, -y(\mathbf{w} \cdot \mathbf{x}))$

- **Stochastic gradient:** for each \mathbf{x}_t , the update is

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where η is a learning rate parameter

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- A margin-based upper bound on the number of mistakes or updates made by the Perceptron algorithm when processing a sequence of T points that can be linearly separated by a hyperplane with margin $\rho > 0$

- **Theorem:**

- Let $x_1, \dots, x_T \in \mathbb{R}^d$ be a sequence of T points with $\|x_t\| \leq R$ for all $t \in [1, T]$, for some $R > 0$.
 - Assume that there exists $\rho > 0$ and $v \in \mathbb{R}^d$ such that for all $t \in [1, T]$, $\rho \leq \frac{y_t(v \cdot x_t)}{\|v\|}$.
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- bound independent of dimension and tight
- convergence can be slow for small margin, the number of updates made by the algorithm can be in $\Omega(2^N)$
- among the many variants: voted perceptron algorithm. Predict according to

$$\text{sign} \left(\left(\sum_{t \in I} c_t \mathbf{w}_t \right) \cdot \mathbf{x} \right),$$

where c_t is the number of iterations \mathbf{w}_t survives

- $\{\mathbf{x}_t : t \in I\}$ are the support vectors for the perceptron algorithm, since $\mathbf{w}_T = \sum_{t \in I} y_t \mathbf{x}_t$
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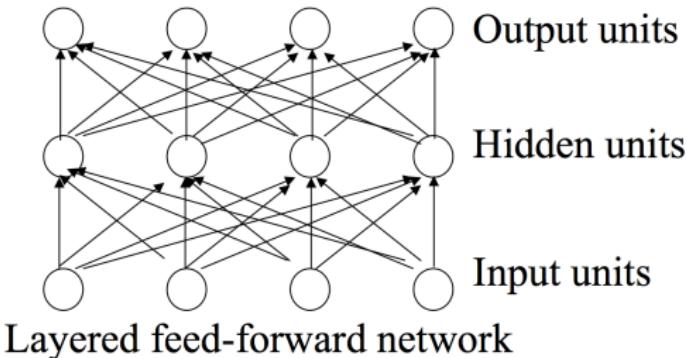
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1 Motivation

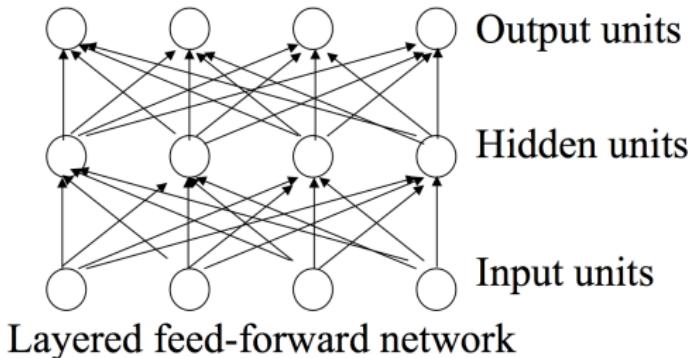
2 Perceptron

3 Neural Networks

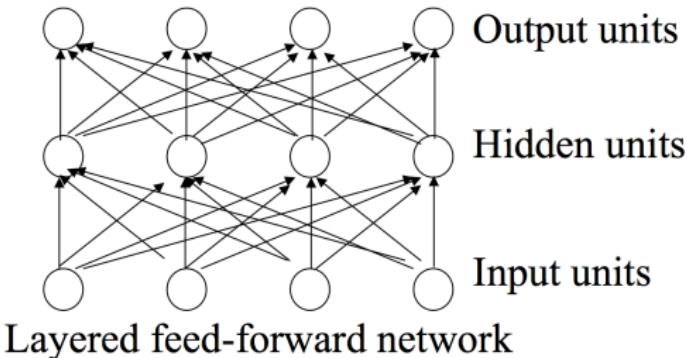
4 Backpropagation



- 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**

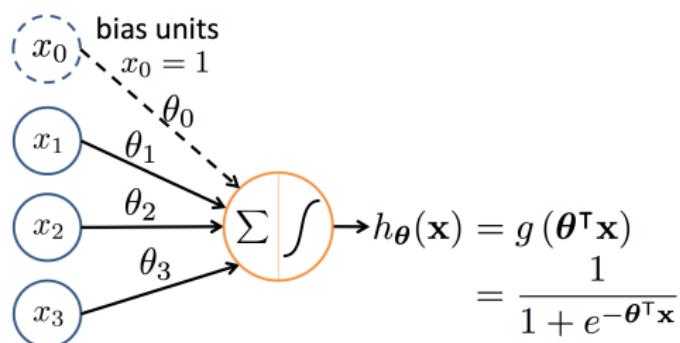


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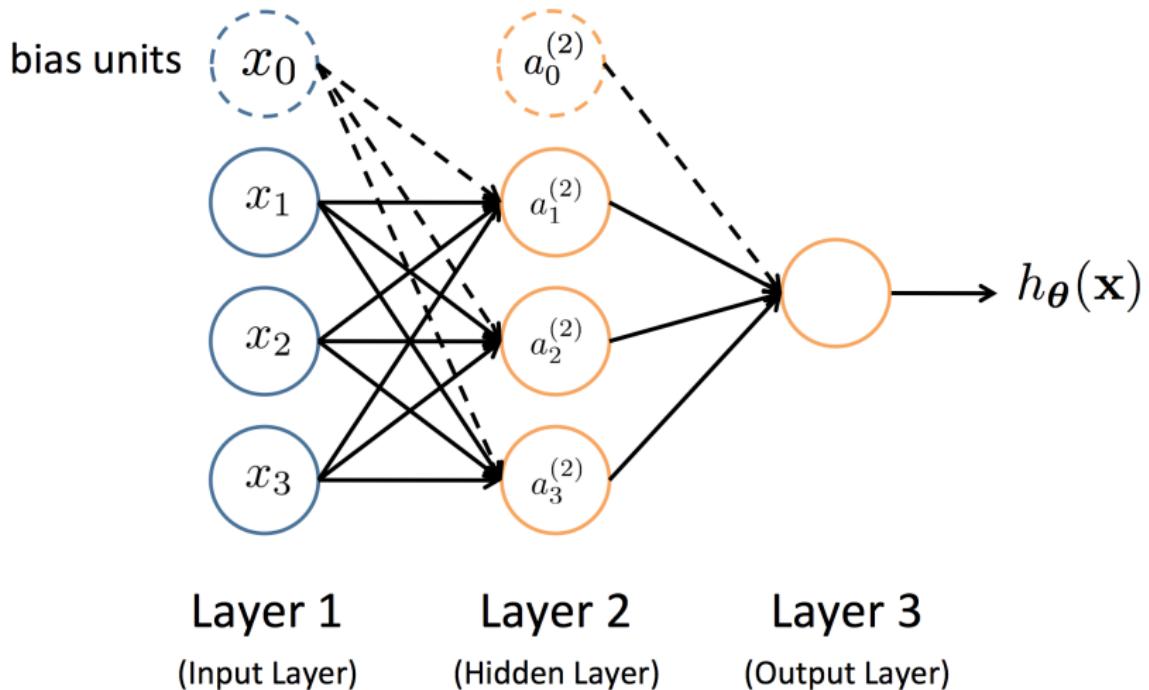


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- Let us define $\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}$ and $\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$



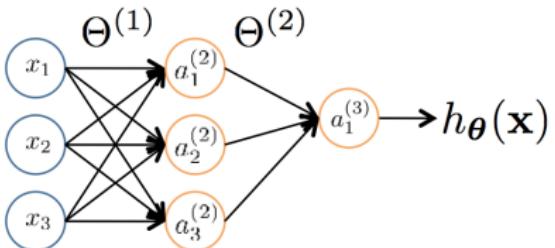
- Sigmoid (logistic) activation function $g(z) = \frac{1}{1+e^{-z}}$



- Input layer units are set by some exterior function, 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

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- $a_i^{(j)}$ = “activation” of unit i in layer j
- $\Theta^{(j)}$ = weight matrix controlling function mapping from layer j to layer $j + 1$

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

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

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

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

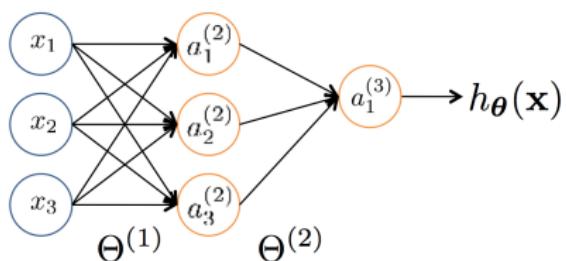
If network has s_j units in layer j and s_{j+1} units in layer $j + 1$, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j + 1)$: $\Theta^{(1)} \in \mathbb{R}^{3 \times 4}$, $\Theta^{(2)} \in \mathbb{R}^{1 \times 4}$

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

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

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



Feed-forward Steps:

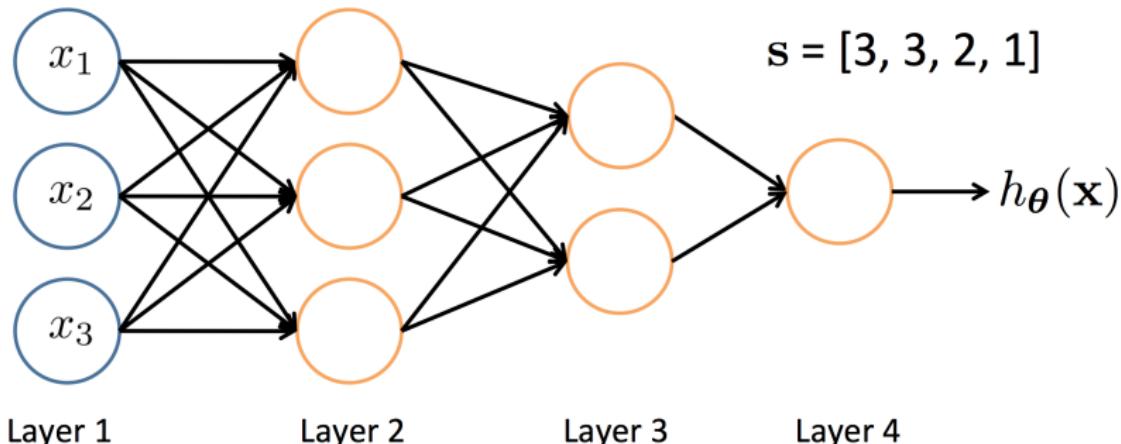
- $\mathbf{z}^{(2)} = \Theta^{(1)} \mathbf{x}$

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

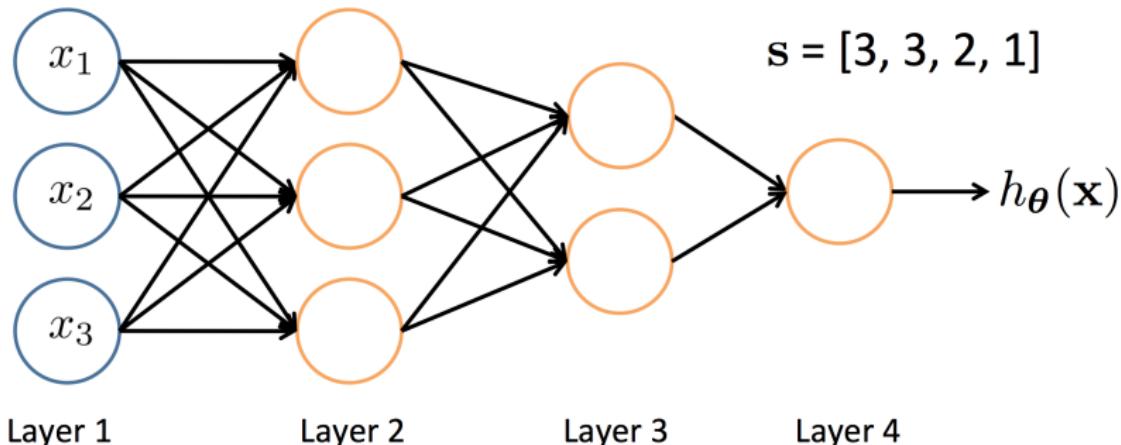
Add $a_0^{(2)} = 1$

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

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

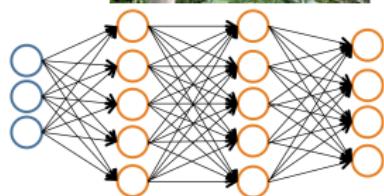


- L denotes the number of layers
- $\mathbf{s} \in (\mathbb{N}_+)^L$ contains the number of nodes at each layer
 - Not counting bias units
 - Typically, $s_0 = N$ (number of input features) and $s_{L-1} = K$ (number of classes)



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Multiple Output Units: One-vs-Rest I



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

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

when cat

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

when dog

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

when car

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

when driver



Figure – Cat



Figure – Dog



Figure – Car

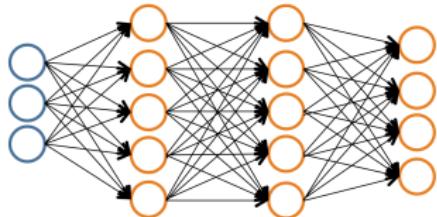


Figure – Driver

- Given $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)\}$

- Convert labels to 1-of- K repr., e.g. $y_i = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when car, etc.

$$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$



Given

- $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)\}$
- $\mathbf{s} \in (\mathbb{N}_+)^L$ contains number of nodes at each layer, $s_0 = N$ (number of features)

Multi-class classification (K classes)

Binary classification:

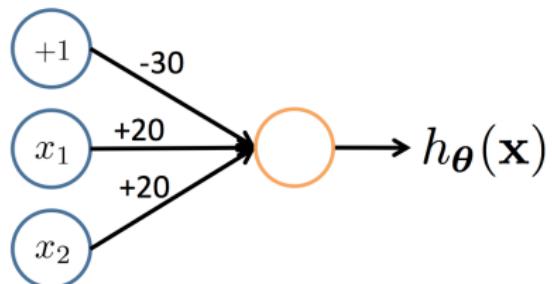
- $y = 0$ or 1
- 1 output unit ($s_{L-1} = 1$)

- $y \in \mathbb{R}^K$, e.g. $y = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when car
- K output units ($s_{L-1} = K$)

Simple example: AND

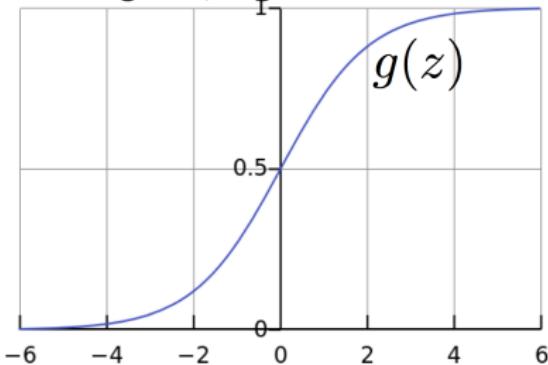
$$x_1, x_2 \in \{0, 1\}$$

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

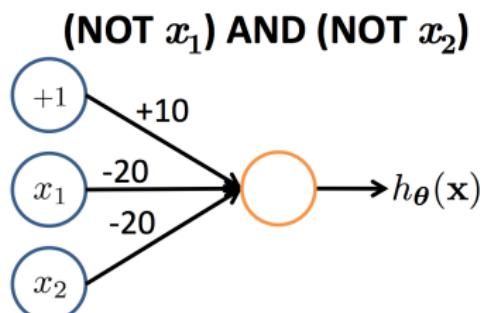
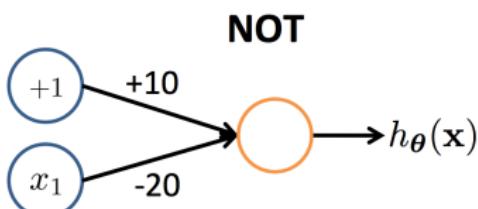
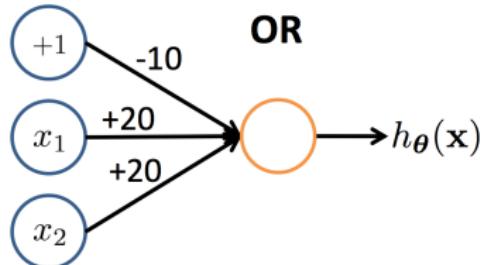
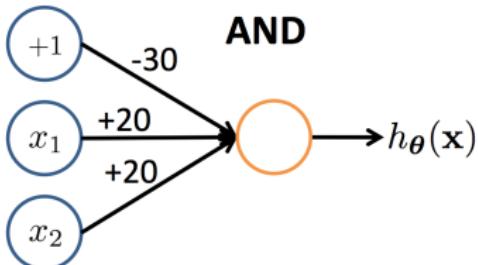


$$h_{\theta}(\mathbf{x}) = g(-30 + 20x_1 + 20x_2)$$

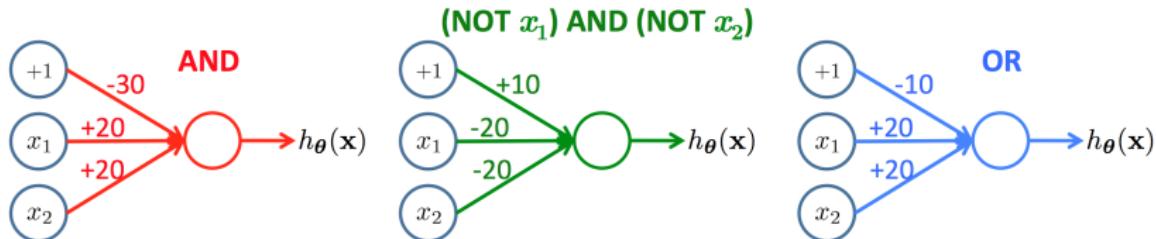
Logistic / Sigmoid Function



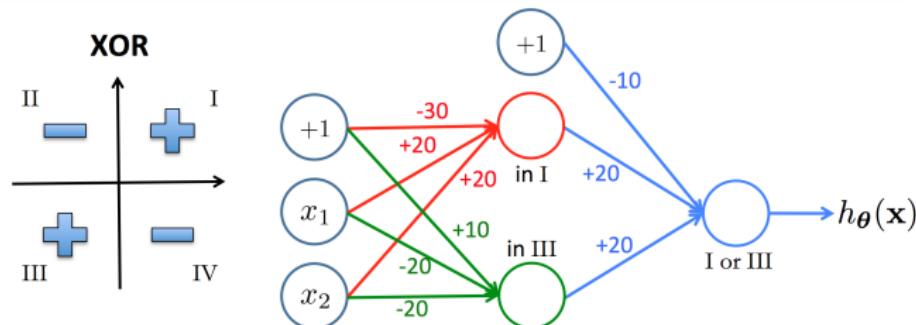
x_1	x_2	$h_{\theta}(\mathbf{x})$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$



Building blocks:



XOR function:

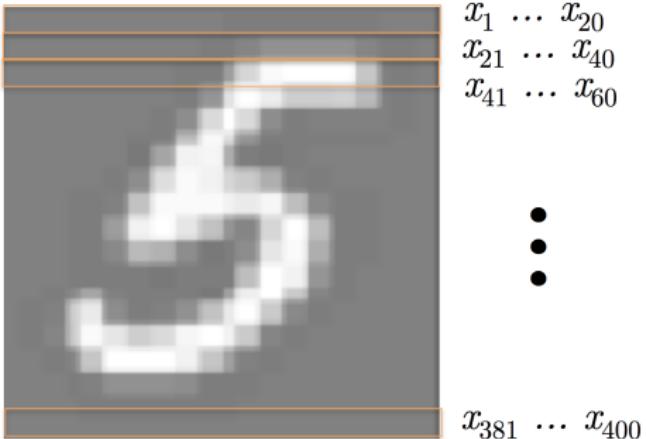


Representation of Layers I

7	9	6	5	8	7	4	4	1	0
0	7	3	3	2	4	8	4	5	1
6	6	3	2	9	2	3	3	2	6
1	3	7	1	5	6	5	2	4	4
7	0	9	8	7	5	8	9	5	4
4	6	6	5	0	2	1	3	6	9
8	5	1	8	9	3	8	7	3	6
1	0	2	8	2	3	0	5	1	5
6	7	8	2	5	3	9	7	0	0
7	9	3	9	8	5	7	2	9	8

20×20 pixel images

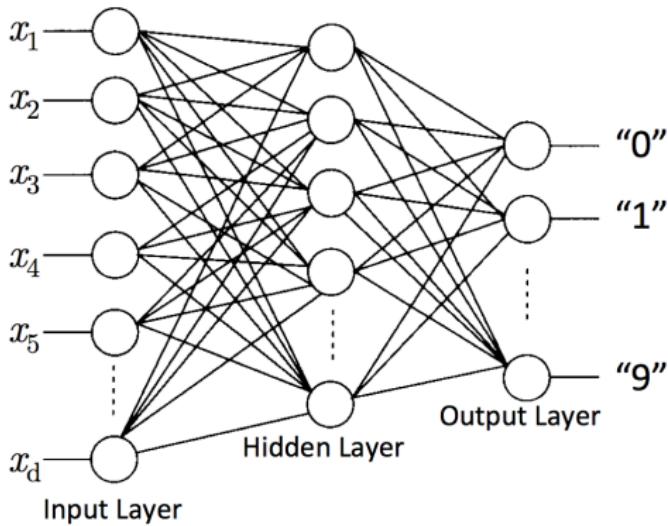
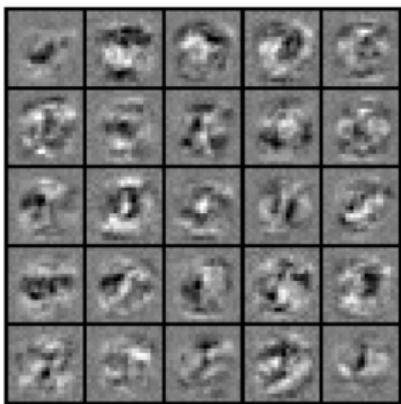
$d = 400$ 10 classes



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

Representation of Layers II

7	9	6	5	8	7	4	4	1	0
0	7	3	3	2	4	8	4	5	1
6	6	3	2	9	2	3	3	2	6
1	3	7	1	5	6	5	2	4	4
7	0	9	8	7	5	8	9	5	4
4	6	6	5	0	2	1	3	6	9
8	5	1	8	9	7	8	7	3	6
1	0	2	8	2	3	0	5	1	5
6	7	8	2	5	3	9	7	0	0
7	9	3	9	8	5	7	2	9	8



Visualization of
Hidden Layer

1 Motivation

2 Perceptron

3 Neural Networks

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

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Logistic Regression for binary {0, 1}-case:

$$\widehat{R}(\theta) = -\frac{1}{m} \sum_{i=1}^m [y_i \log h_\theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\theta(\mathbf{x}_i))] + \frac{\lambda}{2m} \sum_{j=1}^N \theta_j^2$$

Neural Network:

$$h_\theta \in \mathbb{R}^K, \quad (h_\theta(\mathbf{x}))_k = k^{\text{th}} \text{ output}$$

$$\begin{aligned}\widehat{R}(\theta) &= -\frac{1}{m} \left[\sum_{i=1}^m \sum_{k=1}^K y_{ik} \log(h_\theta(\mathbf{x}_i))_k + (1 - y_{ik}) \log(1 - (h_\theta(\mathbf{x}_i))_k) \right] \\ &\quad + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l-1} \sum_{j=1}^{s_l} \left(\theta_{ji}^{(l)} \right)^2\end{aligned}$$

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Neural Network:

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$$\begin{aligned}\widehat{R}(\theta) &= -\frac{1}{m} \left[\sum_{i=1}^m \sum_{k=1}^K y_{ik} \log(h_\theta(\mathbf{x}_i))_k + (1 - y_{ik}) \log(1 - (h_\theta(\mathbf{x}_i))_k) \right] \\ &\quad + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l-1} \sum_{j=1}^{s_l} \left(\theta_{ji}^{(l)} \right)^2\end{aligned}$$

Logistic Regression for binary {0, 1}-case:

$$\widehat{R}(\theta) = -\frac{1}{m} \sum_{i=1}^m [y_i \log h_\theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\theta(\mathbf{x}_i))] + \frac{\lambda}{2m} \sum_{j=1}^N \theta_j^2$$

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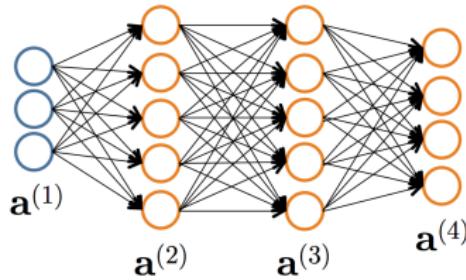
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- Given one labeled training instance (\mathbf{x}, y)

Forward Propagation

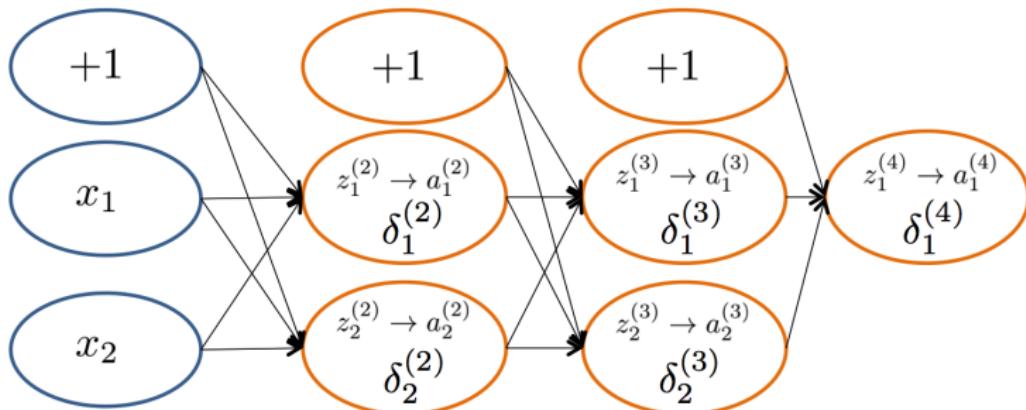
- $\mathbf{a}^{(1)} = \mathbf{x}$
- $\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{a}^{(1)}$
- $\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$ [add $a_0^{(2)}$]
- $\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$
- $\mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$ [add $a_0^{(3)}$]
- $\mathbf{z}^{(4)} = \Theta^{(3)}\mathbf{a}^{(3)}$
- $\mathbf{a}^{(4)} = h_{\Theta}(\mathbf{x}) = g(\mathbf{z}^{(4)})$



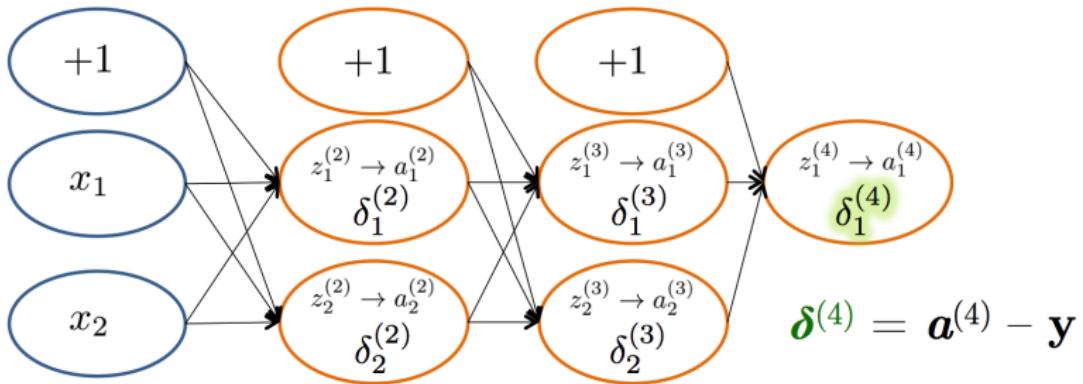
- Each hidden node j is “responsible” for some fraction of the error $\delta_j^{(l)}$ in each of the output nodes to which it connects
- $\delta_j^{(l)}$ is divided according to the strength of the connection between hidden node and the output node
- Then, the “blame” is propagated back to provide the error values for the hidden layer

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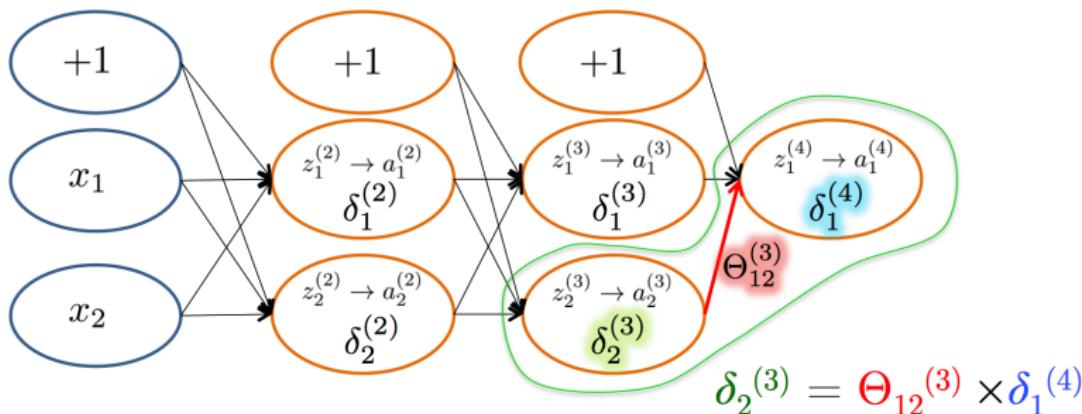
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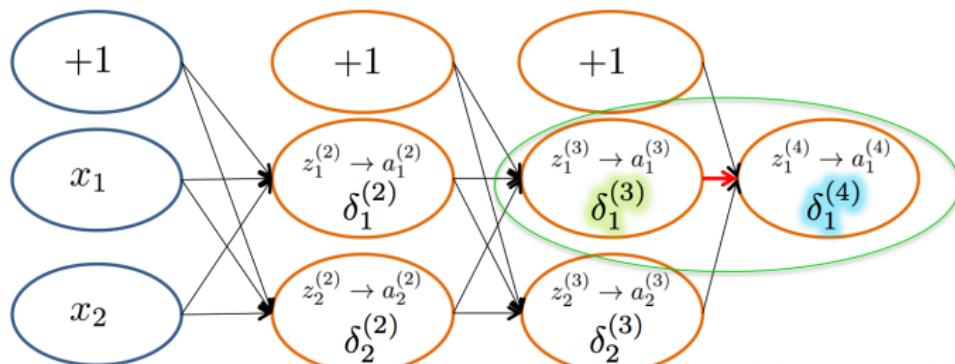
- $\delta_j^{(l)}$ = “error” of node j in layer l
 - Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$,
where $\text{cost}(\mathbf{x}_i) = y_i \log h_\theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\theta(\mathbf{x}_i))$



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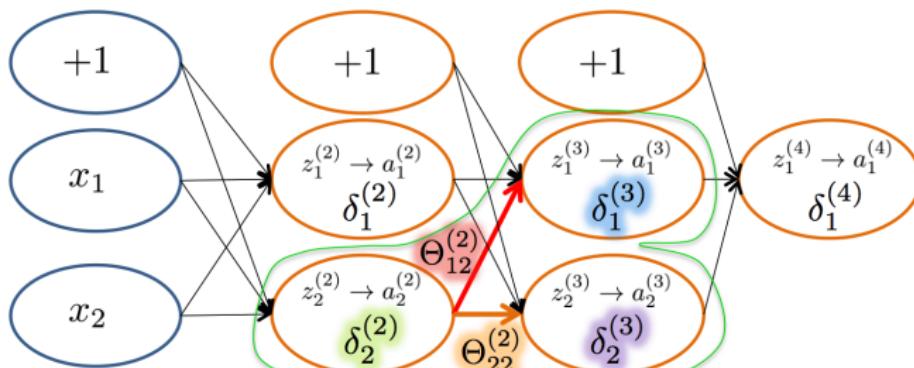
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$$\delta_2^{(3)} = \Theta_{12}^{(3)} \times \delta_1^{(4)}$$

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

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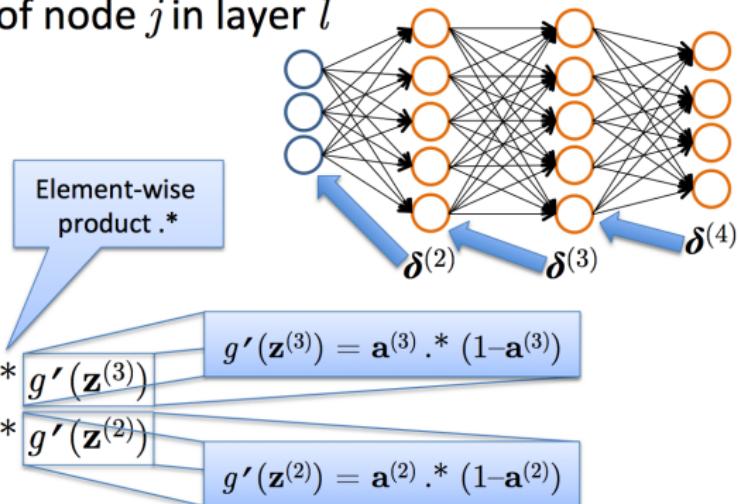
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Let $\delta_j^{(l)}$ = “error” of node j in layer l

(#layers $L = 4$)

Backpropagation

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



$$\frac{\partial}{\partial \theta_{ij}^{(l)}} \hat{R}(\theta) = a_j^{(l)} \delta_i^{(l+1)} \quad (\text{ignoring } \lambda; \text{ if } \lambda = 0)$$

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

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

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

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

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

- $\mathbf{D}^{(l)}$ is the matrix of partial derivatives of $\widehat{R}(\theta)$
- Note: can vectorize $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ as $\Delta^{(l)} = \Delta^{(l)} + \delta^{(l+1)} (\mathbf{a}^{(l)})^T$

Given: training set $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$

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

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

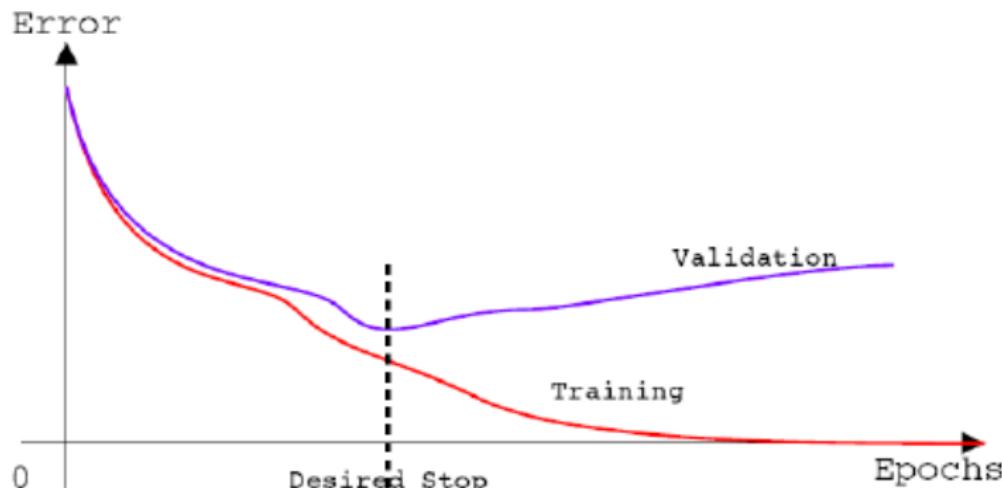
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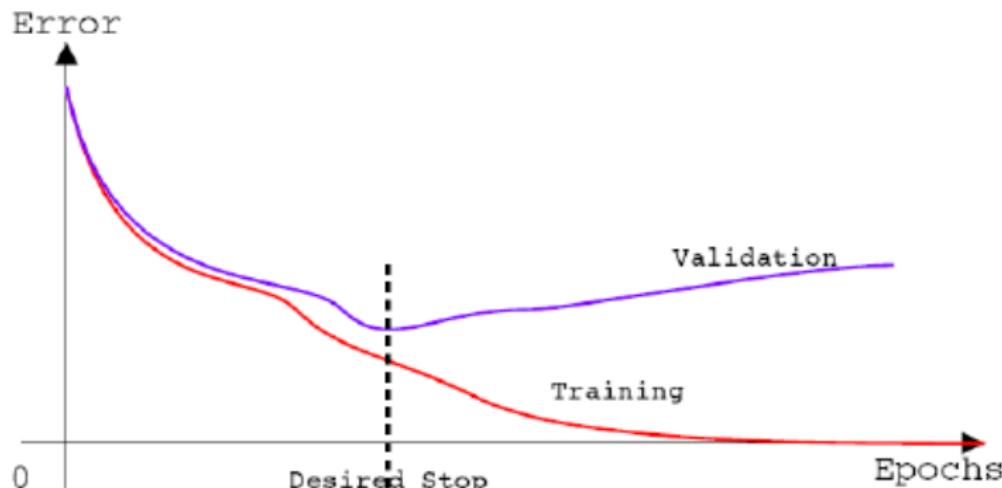
Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$

Until weights converge or max #epochs is reached

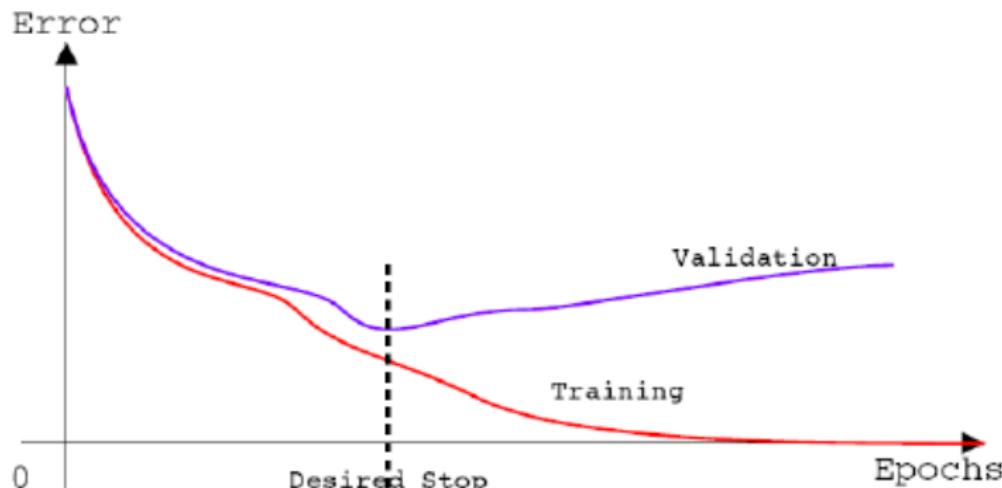
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- Random initialization
- Random division into train and validation sets
- Second order optimization methods
- Early stopping



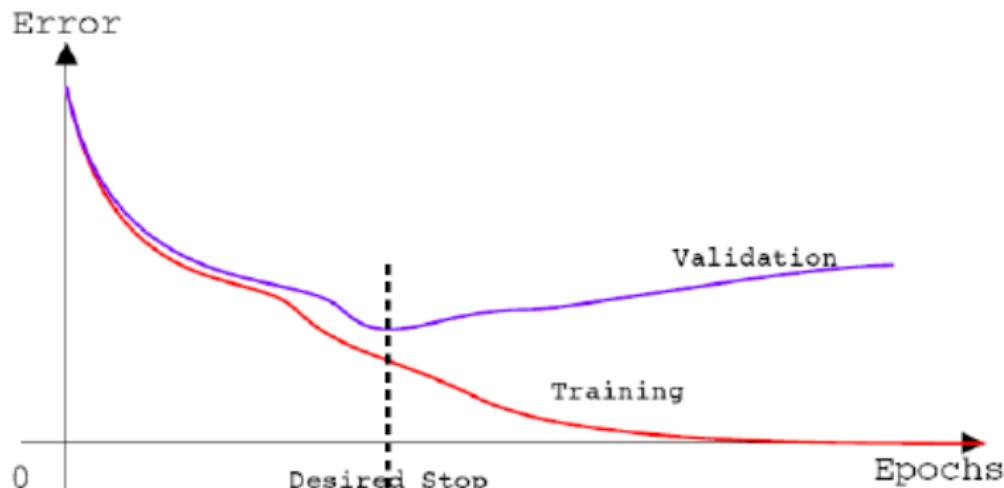
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