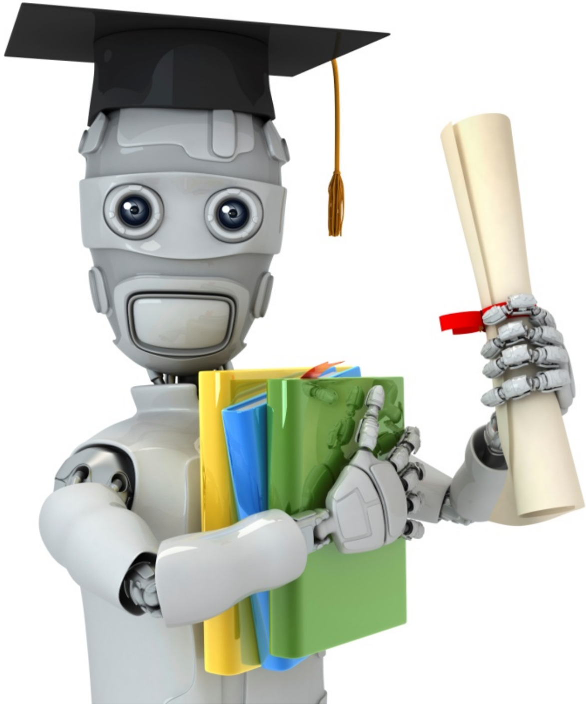


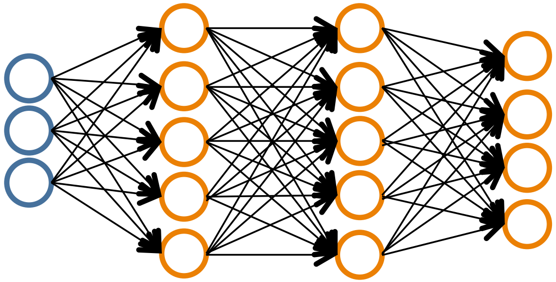
Machine Learning

Neural Networks: Learning

Cost function

Neural Network (Classification)

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$$



$L =$ total no. of layers in network

$s_l =$ no. of units (not counting bias unit) in layer l

Binary classification

$$y = 0 \text{ or } 1$$

1 output unit

sL4 = 1

Multi-class classification (K classes)

$y \in \mathbb{R}^K$ 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

sL(of output layer) = K where K >= 3

Cost function

We have added a few nested summations to account for our multiple output nodes. In the first part of the equation, before the square brackets, we have an additional nested summation that loops through the number of output nodes.In the regularization part, after the square brackets, we must account for multiple theta matrices. The number of columns in our current theta matrix is equal to the number of nodes in our current layer (including the bias unit). The number of rows in our current theta matrix is equal to the number of nodes in the next layer (excluding the bias unit). As before with logistic regression, we square every term.

Logistic regression:

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

Neural network:

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

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)})\log(1-(h_\Theta(x^{(i)}))_k)\right]$$

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

the i in the triple sum does not refer to training example i

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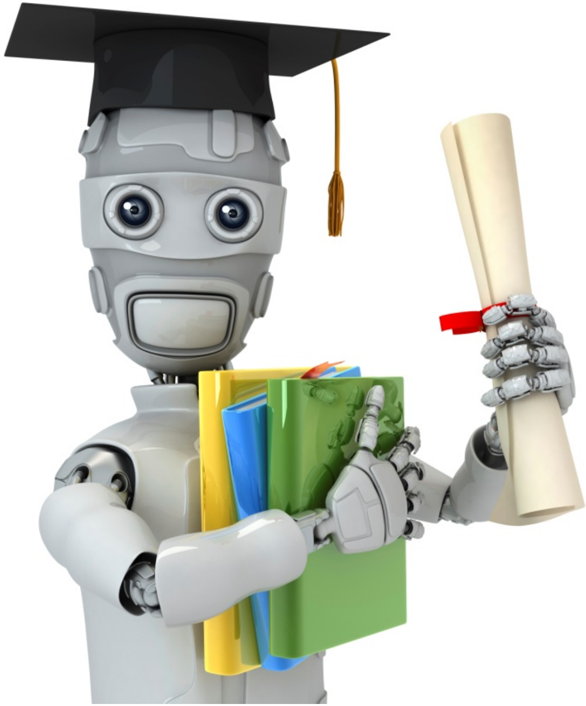


Machine Learning

Neural Networks: Learning

Backpropagation algorithm

Gradient computation

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log h_\theta(x^{(i)})_k + (1-y_k^{(i)}) \log(1-h_\theta(x^{(i)})_k)\right]$$
$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_j^{(l)})^2$$

$$\min_{\Theta} J(\Theta)$$

Need code to compute:

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

$\Theta_{ij}^{(l)} \in \mathbb{R}$

Gradient computation

Given one training example (x, y):

Forward propagation:

$$a^{(1)} = x$$

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

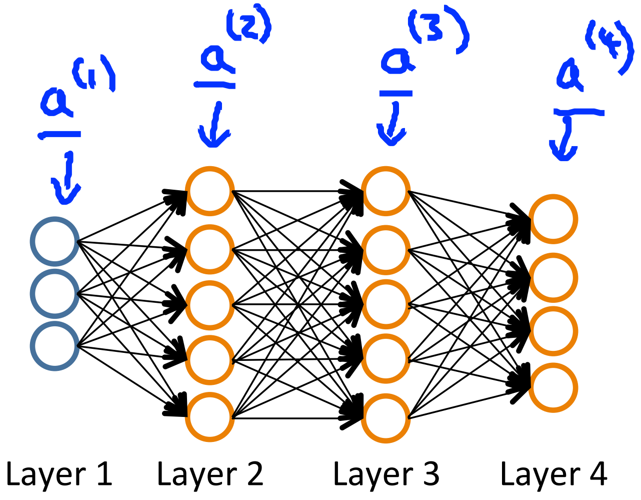
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$

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

$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$

$$z^{(4)} = \Theta^{(3)} a^{(3)}$$

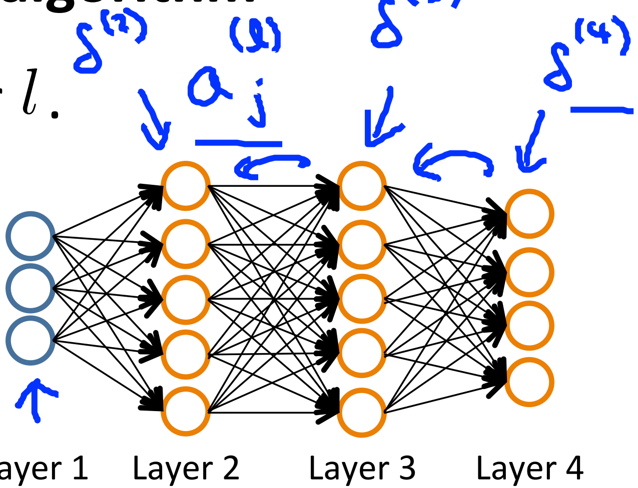
$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



Gradient computation: Backpropagation algorithm

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

Vector whose dimensions is equal to the output units in our network



For each output unit (layer L = 4)

$$\boxed{\delta_j^{(4)} = \boxed{a_j^{(4)}} - y_j}$$

$(h_\Theta(x))_j$ $\quad \delta^{(4)} = a^{(4)} - y$

$$\delta^{(3)} = (\Theta^{(3)})^T\delta^{(4)} .* g'(z^{(3)})$$

Derivative of a(3)

$a^{(3)} .* (1 - a^{(3)})$

$$\delta^{(2)} = (\Theta^{(2)})^T\delta^{(3)} .* g'(z^{(2)})$$

$a^{(2)} .* (1 - a^{(2)})$

(No $\delta^{(1)}$)

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

(ignoring λ; if $\lambda = 0$)

(hence you end up having a matrix full of zeros)

1-For training example t =1 to m: Set a^(1) := x^(t) .

2-Perform forward propagation to compute a^(l) for l=2,3,…,L

Using y^(t), compute **δ** (L) =a (L) y (t)

Backpropagation algorithm

Training set $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$

Set $\triangle_{ij}^{(l)} = 0$ (for all l, i, j).

$\left(\text{use to compute } \frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) \right)$

For $i = 1$ to m $(x^{(i)}, y^{(i)})$

Where L is our total number of layers and a^(L) is the vector of outputs of the activation units for the last layer. So our "error values" for the last layer are simply the differences of our actual results in the last layer and the correct outputs in y. To get the delta values of the layers before the last layer, we can use an equation that steps us back from right to left:

- Set $a^{(1)} = x^{(i)}$
- Perform forward propagation to compute $a^{(l)}$ for $l = 2, 3, \ldots, L$
- Using $y^{(i)}$, compute $\delta^{(L)} = \boxed{a^{(L)}} - \boxed{y^{(i)}}$
- Compute $\delta^{(L-1)}, \delta^{(L-2)}, \ldots, \delta^{(2)}$ $\cancel{\delta^{(1)}}$
- $\boxed{\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}}$

Compute delta^{(L-1)}, delta^{(L-2)} ... **δ** (L1) ,**δ** (L2) ,…,**δ** (2) using delta^(l) = ((Θ (l))T * **δ** (l+1)) .* a (l) .* (1 - a^(l))

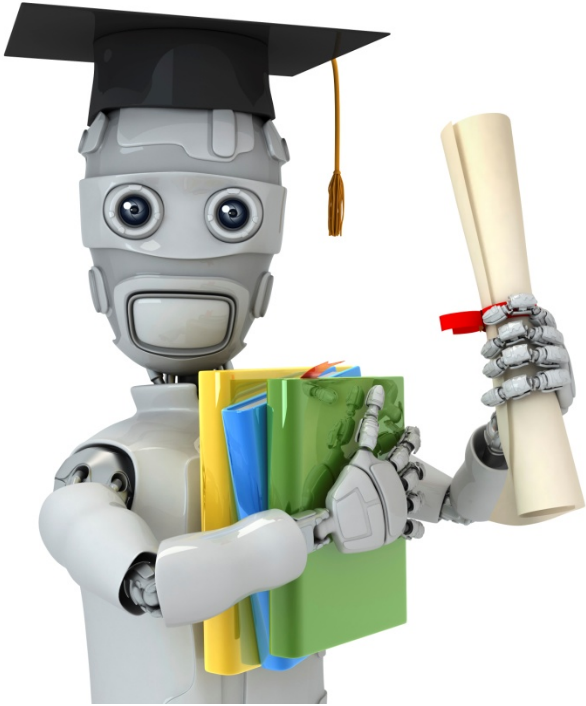
$$\triangle^{(l)} := \triangle^{(l)} + \delta^{(l+1)} (a^{(l)})^T$$

$$D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)} \quad \text{if } j \neq 0$$

$$D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} \quad \text{if } j = 0$$

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

The capital-delta matrix D is used as an "accumulator" to add up our values as we go along and eventually compute our partial derivative.

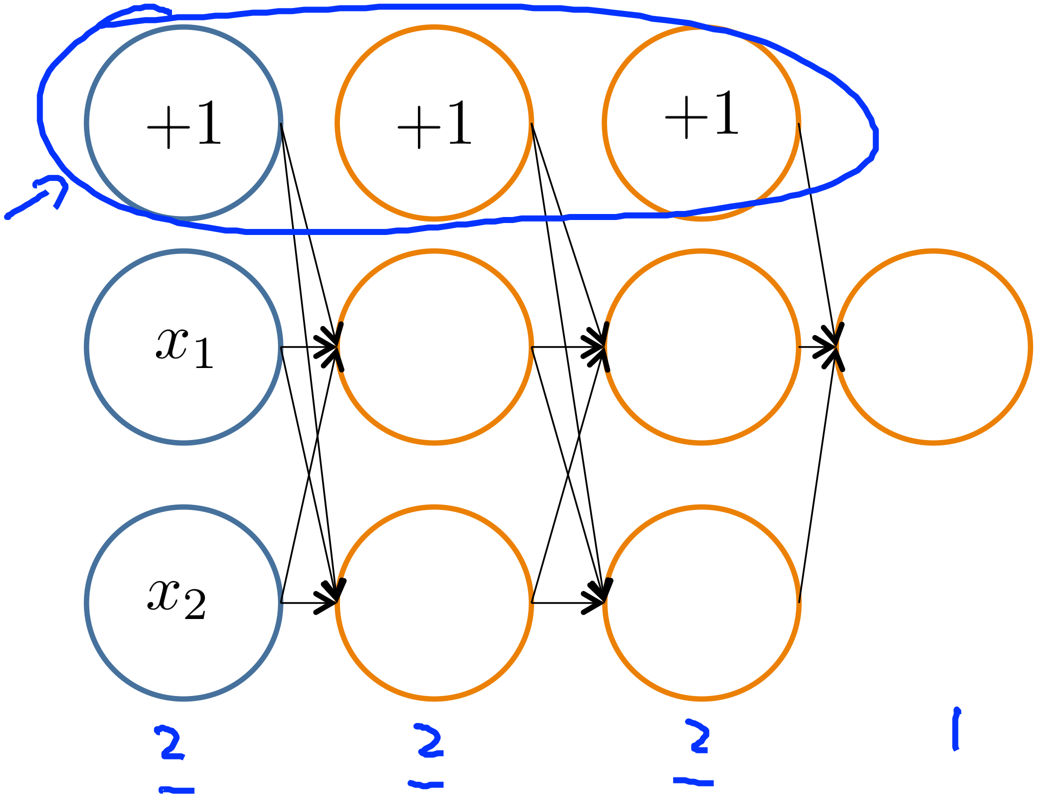


Machine Learning

Neural Networks: Learning

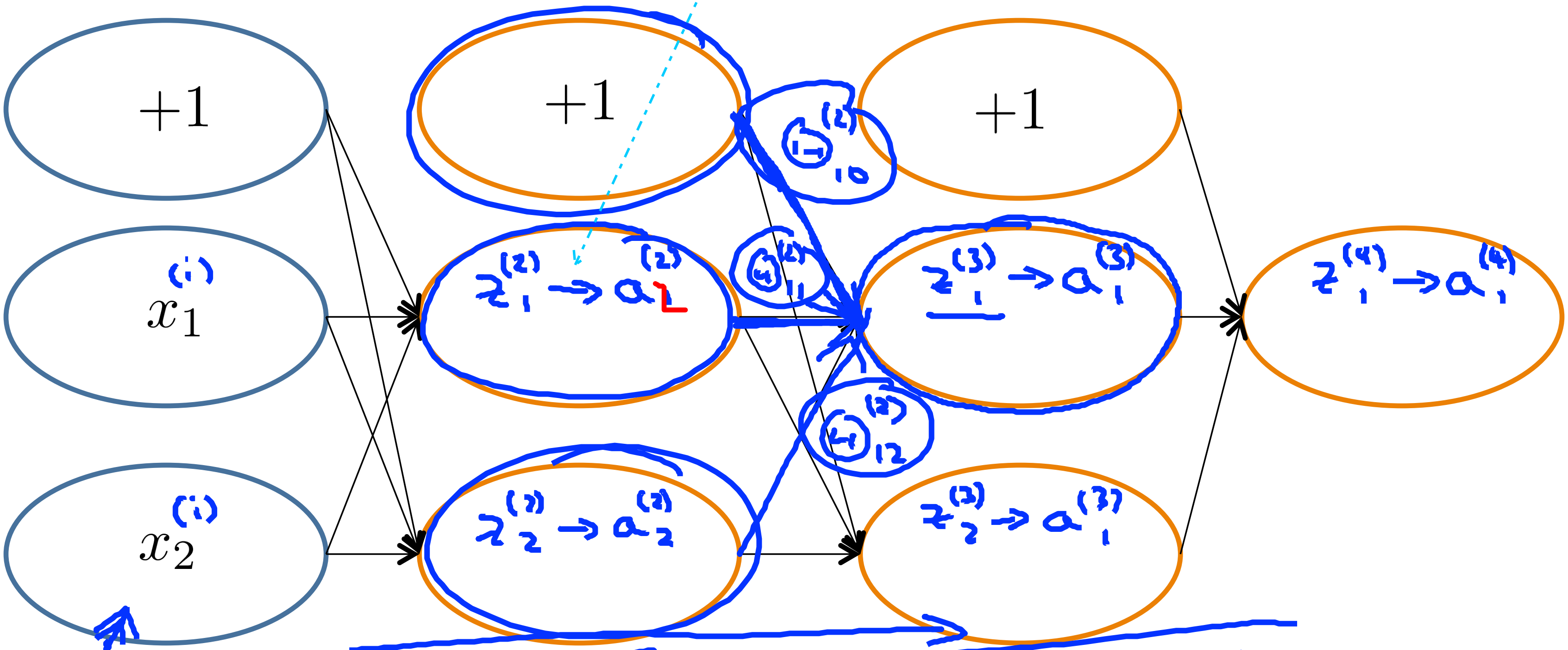
Backpropagation intuition

Forward Propagation



Forward Propagation

Applying sigmoid to get a1^(2)



$(x^{(i)}, y^{(i)})$

$$z_1^{(3)} = \Theta_{10}^{(2)} \times 1 + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} \cdot a_2^{(2)}$$

What is backpropagation doing?

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} \underbrace{y^{(i)}\log(h_\Theta(x^{(i)})) + (1-y^{(i)})\log(1-(h_\Theta(x^{(i)})))}_{(x^{(i)},\, y^{(i)})}\right]$$

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

Focusing on a single example $x^{(i)}$, $y^{(i)}$, the case of 1 output unit, and ignoring regularization ($\lambda = 0$),

Note: Mistake on lecture, it is supposed to be 1-h(x).

$$\text{cost(i)} = y^{(i)}\log h_\Theta(x^{(i)}) + (1-y^{(i)})\boxed{\log \overset{1-}{h_\Theta}(x^{(i)})}$$

$y^{(i)}$

(Think of $\text{cost(i)} \approx (h_\Theta(x^{(i)}) - y^{(i)})^2$)

I.e. how well is the network doing on example i?

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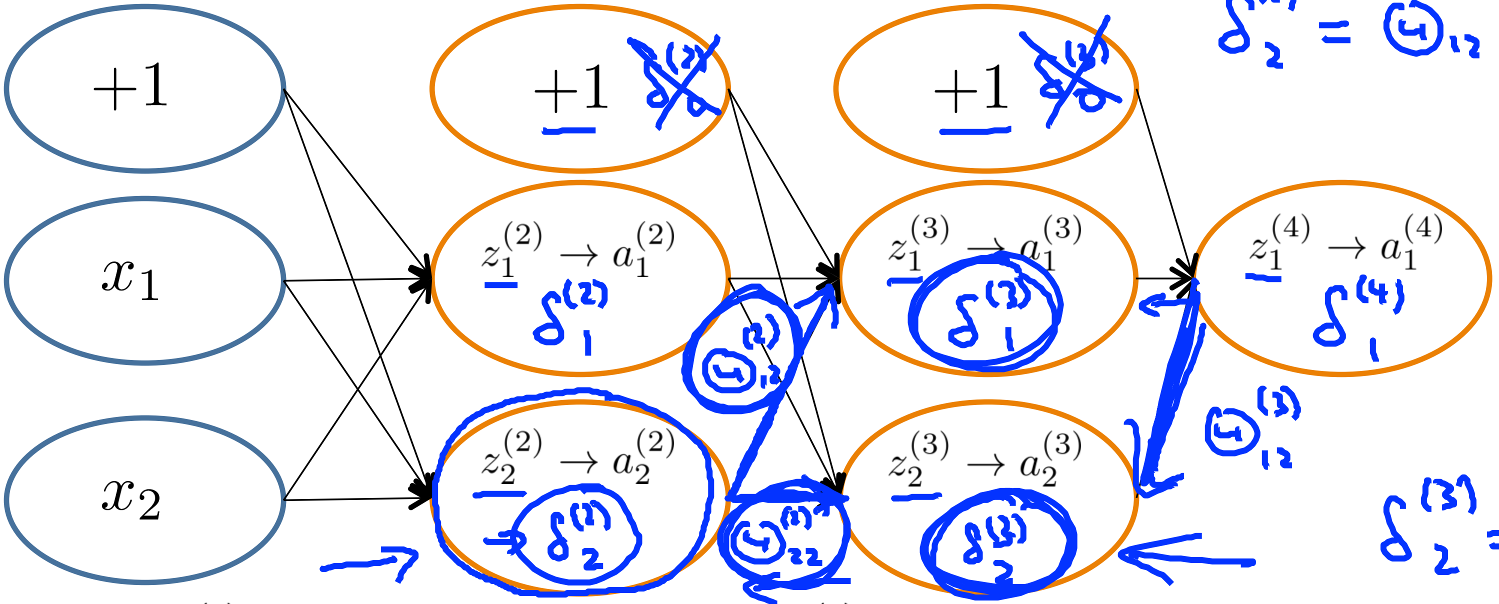
Forward Propagation

Delta = actual value a1^(4) - predicted value on example i

$$\delta_1^{(4)} = y^{(i)} - a_1^{(4)}$$

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



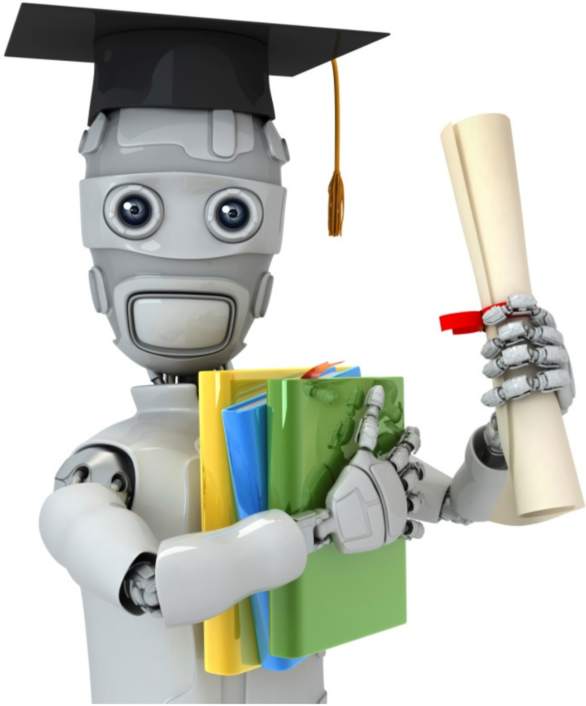
$$\delta_2^{(3)} = \Theta_{12}^{(3)} \cdot \delta_1^{(4)}.$$

$\delta_j^{(l)} =$ "error" of cost for $a_j^{(l)}$ (unit j in layer l).

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \mathrm{cost}(\mathrm{i})$ (for $j \geq 0$), where

$$\mathrm{cost}(\mathrm{i}) = y^{(i)} \log h_\Theta(x^{(i)}) + (1 - y^{(i)}) \log h_\Theta(x^{(i)})$$

Partial derivatives of the cost function



Machine Learning

Neural Networks: Learning

Implementation note: Unrolling parameters

Advanced optimization

```
function [jVal, gradient] = costFunction(theta)
  ...
optTheta = fminunc(@costFunction, initialTheta, options)
```

$\mathbb{R}^{n+1}$ $\mathbb{R}^{n+1}$ (vectors)

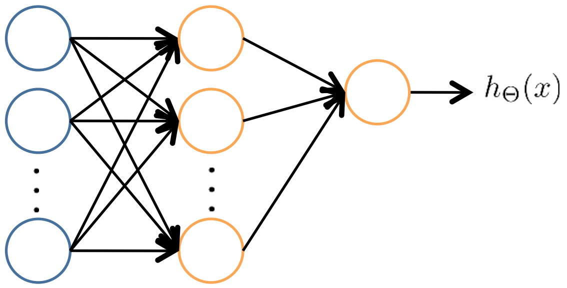
Neural Network (L=4):

→ $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$ - matrices (`Theta1`, `Theta2`, `Theta3`)

→ $D^{(1)}, D^{(2)}, D^{(3)}$ - matrices (`D1`, `D2`, `D3`)

"Unroll" into vectors

Example



$s_1 = 10, s_2 = 10, s_3 = 1$

$\boxed{\Theta^{(1)} \in \mathbb{R}^{10\times 11}}, \Theta^{(2)} \in \mathbb{R}^{10\times 11}, \Theta^{(3)} \in \mathbb{R}^{1\times 11}$

$D^{(1)} \in \mathbb{R}^{10\times 11}, D^{(2)} \in \mathbb{R}^{10\times 11}, D^{(3)} \in \mathbb{R}^{1\times 11}$

$\Theta^{(1)}$ $\Theta^{(2)}$ $\Theta^{(3)}$

```
thetaVec = [ Theta1(:); Theta2(:); Theta3(:)];
DVec = [D1(:); D2(:); D3(:)];

Theta1 = reshape(thetaVec(1:110),10,11);
Theta2 = reshape(thetaVec(111:220),10,11);
Theta3 = reshape(thetaVec(221:231),1,11);
```

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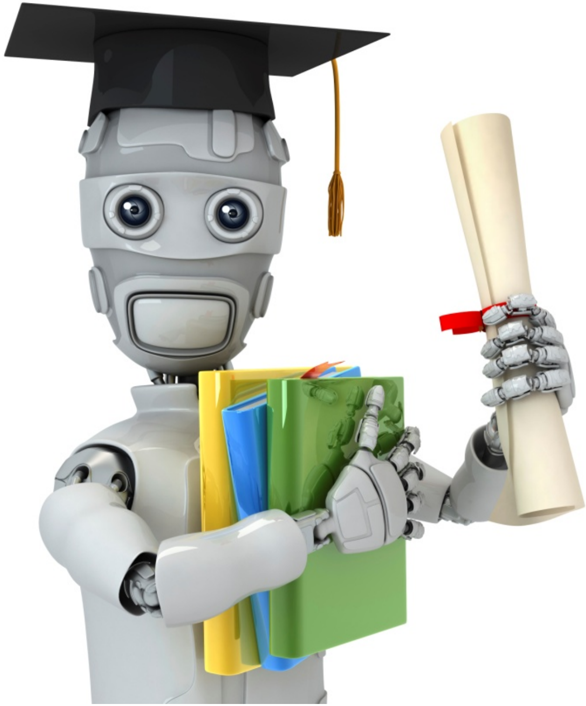
Learning Algorithm

- Have initial parameters $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$.
- Unroll to get `initialTheta` to pass to
- `fminunc(@costFunction, initialTheta, options)`

```
function [jval, gradientVec] = costFunction(thetaVec)
```

- From `thetaVec`, get $\boxed{\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}}$. reshape
- Use forward prop/back prop to compute $D^{(1)}, D^{(2)}, D^{(3)}$ and $J(\Theta)$
  Unroll $D^{(1)}, D^{(2)}, D^{(3)}$ to get `gradientVec`.

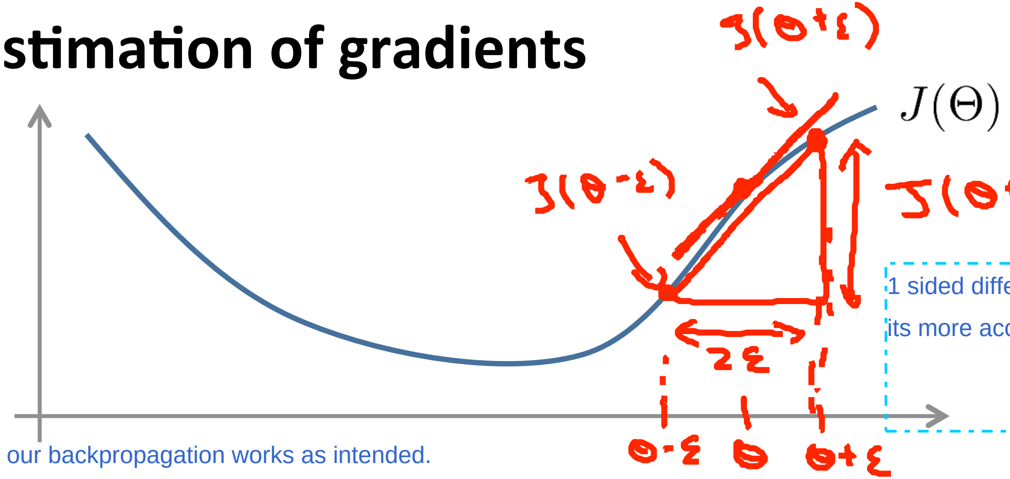


Machine Learning

Neural Networks: Learning

Gradient checking

Numerical estimation of gradients



$J(\theta+\varepsilon) - J(\theta-\varepsilon)$

$\theta \in \mathbb{R}$

1 sided difference equation, we use 2 sided bec
its more accurate

Gradient checking will assure that our backpropagation works as intended.

We can approximate the derivative of our cost function with:

$$\frac{d}{d\theta} J(\theta) \approx \underbrace{\frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}}_{} \quad \leftarrow \quad \Bigg| \quad \cancel{\frac{J(\theta+\varepsilon) - J(\theta)}{\varepsilon}}$$

$\varepsilon = 10^{-4} \leftarrow$

A small value for ϵ = 10^-(4) , guarantees that the math works out properly. If the value for ϵ is too small, we can end up with numerical problems.

Implement: `gradApprox = (J(theta + EPSILON) – J(theta – EPSILON))/(2*EPSILON)`

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Parameter vector θ

- $\theta \in \mathbb{R}^n$ (E.g. θ is "unrolled" version of $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$)
- $\theta = [\theta_1, \theta_2, \theta_3, \dots, \theta_n]$

$$\frac{\partial}{\partial \theta_1} J(\theta) \approx \frac{J(\boxed{\theta_1+\epsilon},\theta_2,\theta_3,\dots,\theta_n) - J(\boxed{\theta_1-\epsilon},\theta_2,\theta_3,\dots,\theta_n)}{2\epsilon}$$

$$\frac{\partial}{\partial \theta_2} J(\theta) \approx \frac{J(\theta_1,\boxed{\theta_2+\epsilon},\theta_3,\dots,\theta_n) - J(\theta_1,\boxed{\theta_2-\epsilon},\theta_3,\dots,\theta_n)}{2\epsilon}$$

Numerical approximation of the partial derivative of J w.r.t theta(i)

$\vdots$

$$\frac{\partial}{\partial \boxed{\theta_n}} J(\theta) \approx \frac{J(\theta_1,\theta_2,\theta_3,\dots,\boxed{\theta_n+\epsilon}) - J(\theta_1,\theta_2,\theta_3,\dots,\boxed{\theta_n-\epsilon})}{2\epsilon}$$

```
for i = 1:n,
  thetaPlus = theta;
  thetaPlus(i) = thetaPlus(i) + EPSILON;
  thetaMinus = theta;
  thetaMinus(i) = thetaMinus(i) - EPSILON;
  gradApprox(i) = (J(thetaPlus) - J(thetaMinus))
                  /(2*EPSILON);
end;
```

$\begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_i + \epsilon \\ \vdots \\ \theta_n \end{bmatrix} \rightarrow \theta_i - \epsilon$

$\frac{\partial}{\partial \theta_i} J(\theta)$.

Check that $\boxed{\texttt{gradApprox}} \approx \boxed{\texttt{DVec}}$

From backprop.

Implementation Note:

- Implement backprop to compute `DVec` (unrolled $D^{(1)}, D^{(2)}, D^{(3)}$).
- Implement numerical gradient check to compute `gradApprox`.
- Make sure they give similar values.
- Turn off gradient checking. Using backprop code for learning.

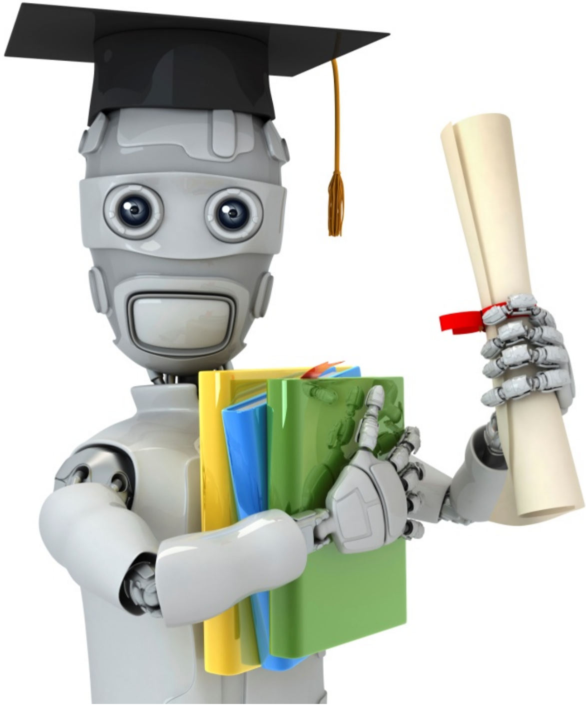
Computationally expensive

DVec

$\delta^{(4)}, \delta^{(3)}, \delta^{(2)}$

Important:

- Be sure to disable your gradient checking code before training your classifier. If you run numerical gradient computation on every iteration of gradient descent (or in the inner loop of `costFunction(…)`)your code will be very slow.



Machine Learning

Neural Networks: Learning

Random initialization

Initial value of Θ

For gradient descent and advanced optimization method, need initial value for Θ.

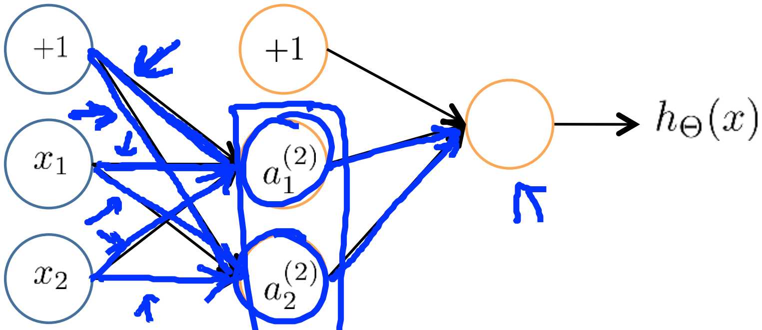
```
optTheta = fminunc(@costFunction,
               initialTheta, options)
```

Consider gradient descent

Set `initialTheta = zeros(n,1)` ?

Zero initialization

Initializing all theta weights to zero does not work with neural networks. When we backpropagate, all nodes will update to the same value repeatedly.



$$\Theta_{ij}^{(l)} = 0 \text{ for all } i, j, l.$$

$a_1^{(2)} = a_2^{(2)}$. Also $\delta_1^{(2)} = \delta_2^{(2)}$.

$$\frac{\partial}{\partial \Theta_{01}^{(1)}} J(\Theta) = \frac{\partial}{\partial \Theta_{02}^{(1)}} J(\Theta)$$

$\Theta_{01}^{(1)} = \Theta_{02}^{(1)}$

After each update, parameters corresponding to inputs going into each of two hidden units are identical.

$a_1^{(2)} = a_2^{(2)}$

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Random initialization: Symmetry breaking

No relation between this epsilon & gradient checking epsilon

→ Initialize each $\Theta_{ij}^{(l)}$ to a random value in $[-\epsilon, \epsilon]$
(i.e. $-\epsilon \leq \Theta_{ij}^{(l)} \leq \epsilon$)

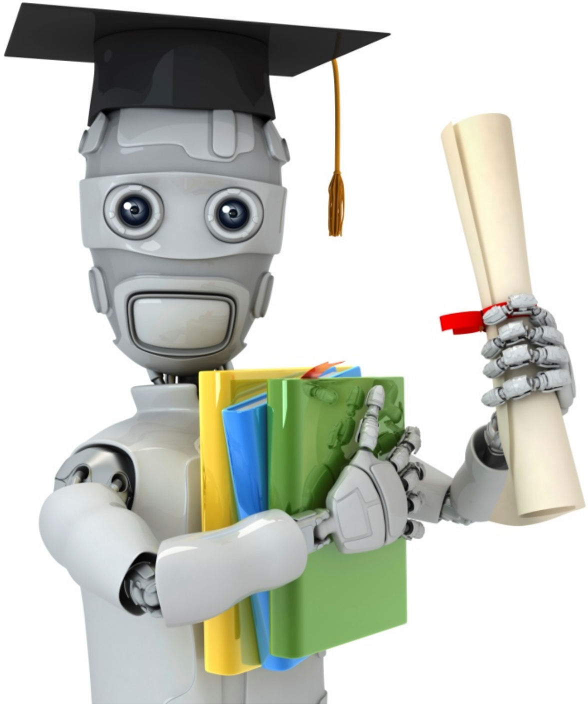
E.g.

random 10×11 matrix (betw. 0 and 1)

```
Theta1 =  rand(10,11)*(2*INIT_EPSILON)
          - INIT_EPSILON;
```

$[-\epsilon, \epsilon]$

```
Theta2 =  rand(1,11)*(2*INIT_EPSILON)
          - INIT_EPSILON;
```



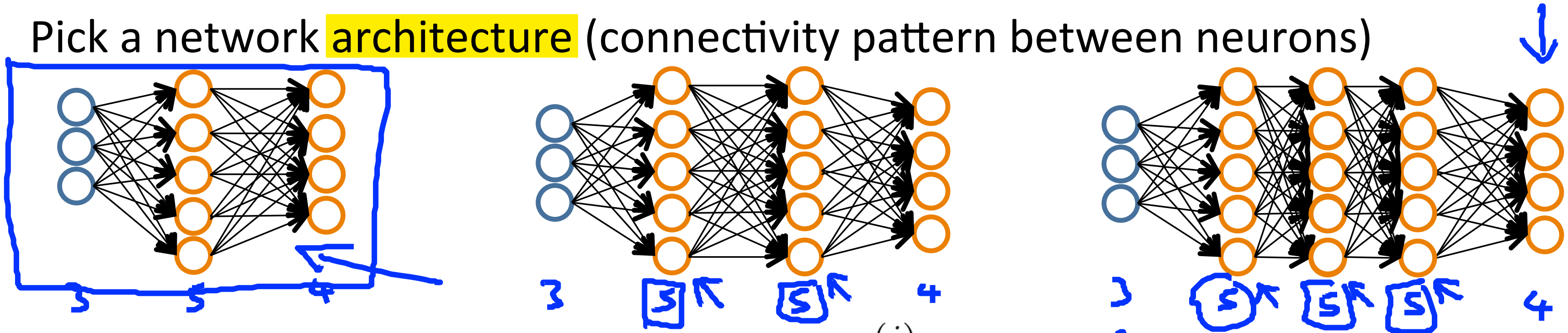
Machine Learning

Neural Networks: Learning

Putting it together

Training a neural network

Pick a network architecture (connectivity pattern between neurons)



→ No. of input units: Dimension of features $x^{(i)}$

→ No. output units: Number of classes

Reasonable default: 1 hidden layer, or if >1 hidden layer, have same no. of hidden units in every layer (usually the more the better)

$y \in \{1, 2, 3, \dots, 10\}$

$\cancel{y = 5}$

$y = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ or $\begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$

Training a neural network

1. Randomly initialize weights
2. Implement forward propagation to get $h_\Theta(x^{(i)})$ for any $x^{(i)}$
3. Implement code to compute cost function $J(\Theta)$
4. Implement backprop to compute partial derivatives $\boxed{\frac{\partial}{\partial\Theta^{(l)}_{jk}} J(\Theta)}$

`for i = 1:m {` $(x^{(1)}, y^{(1)})$ $(x^{(2)}, y^{(2)})$, ... $(x^{(m)}, y^{(m)})$

Perform forward propagation and backpropagation using example $(x^{(i)}, y^{(i)})$

(Get activations $a^{(l)}$ and delta terms $\delta^{(l)}$ for $l = 2, \ldots, L$).

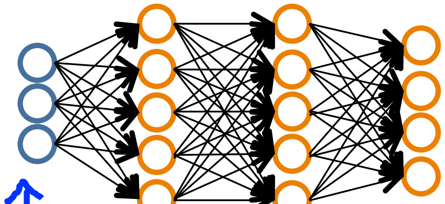
$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

....

}

...

compute $\frac{\partial}{\partial\Theta^{(l)}_{jk}} J(\Theta)$.



$x^{(i)}$

Training a neural network

5. Use gradient checking to compare $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$ computed using backpropagation vs. using numerical estimate of gradient of $J(\Theta)$.

   Then disable gradient checking code.

6. Use gradient descent or advanced optimization method with backpropagation to try to minimize $J(\Theta)$ as a function of parameters Θ

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

$J(\Theta)$ — non-convex.

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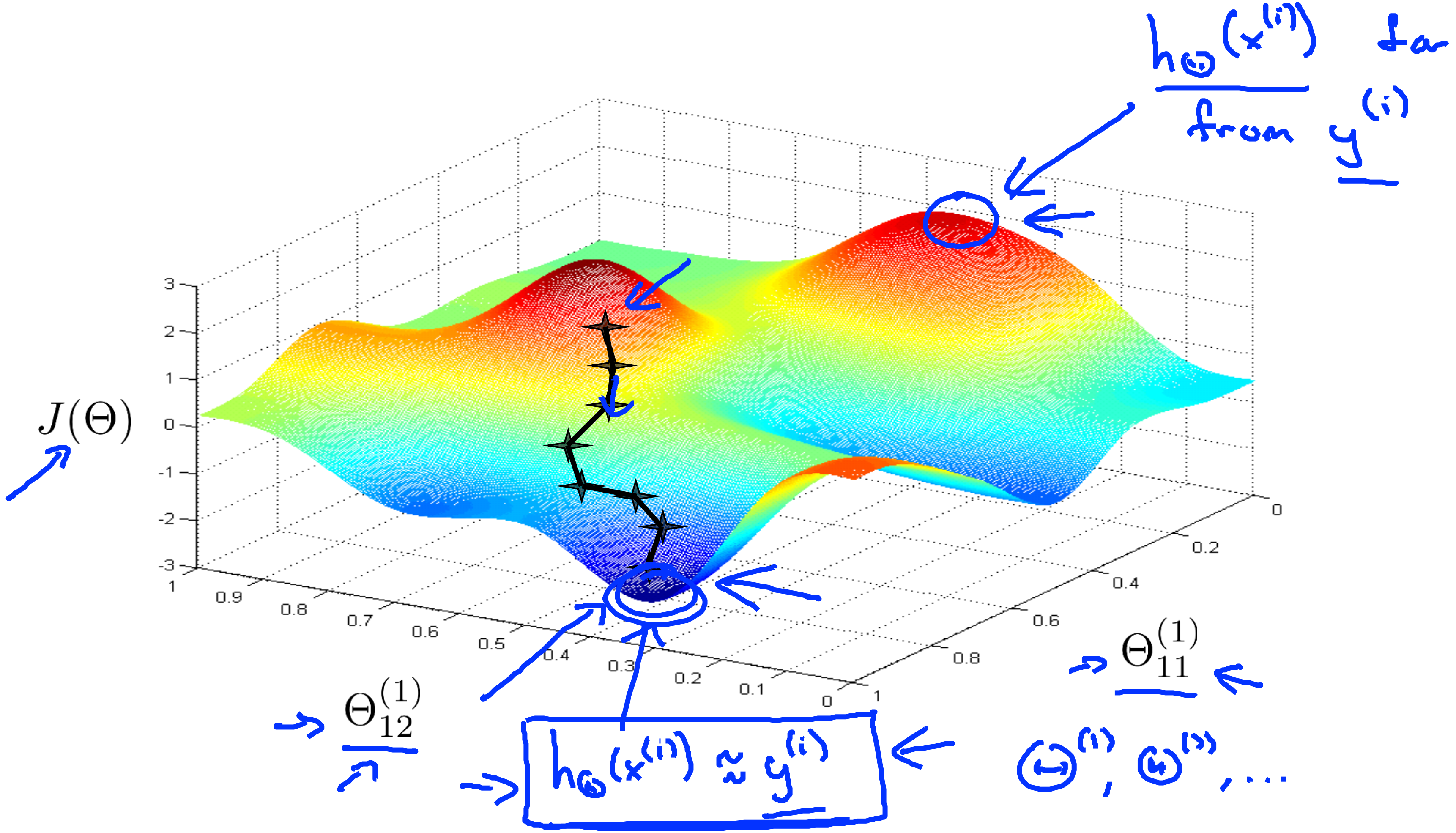

$h_\Theta(x^{(i)})$ far from $y^{(i)}$
$J(\Theta)$
$\Theta_{12}^{(1)}$
$\Theta_{11}^{(1)}$
$h_\Theta(x^{(i)}) \approx y^{(i)}$
$\Theta^{(1)}, \Theta^{(2)}, \ldots$

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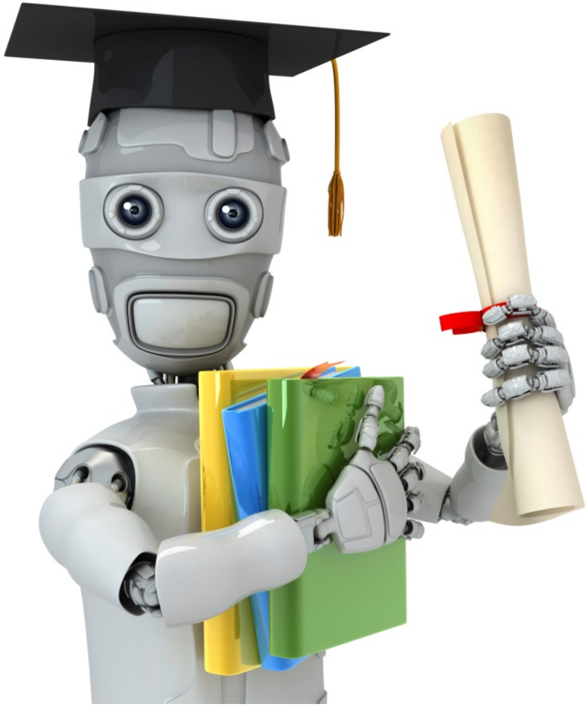
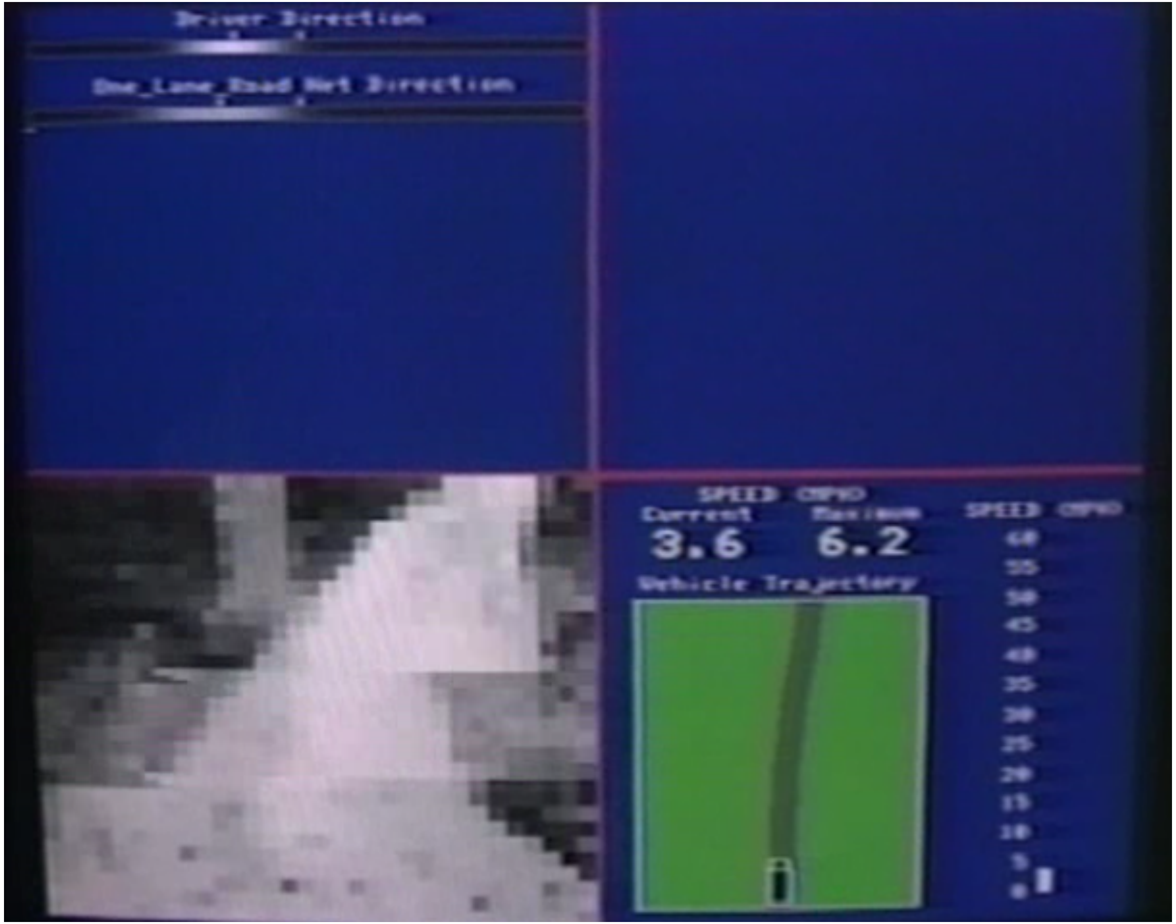


Machine Learning

Neural Networks: Learning

Backpropagation example: Autonomous driving (optional)



[Courtesy of Dean Pomerleau]