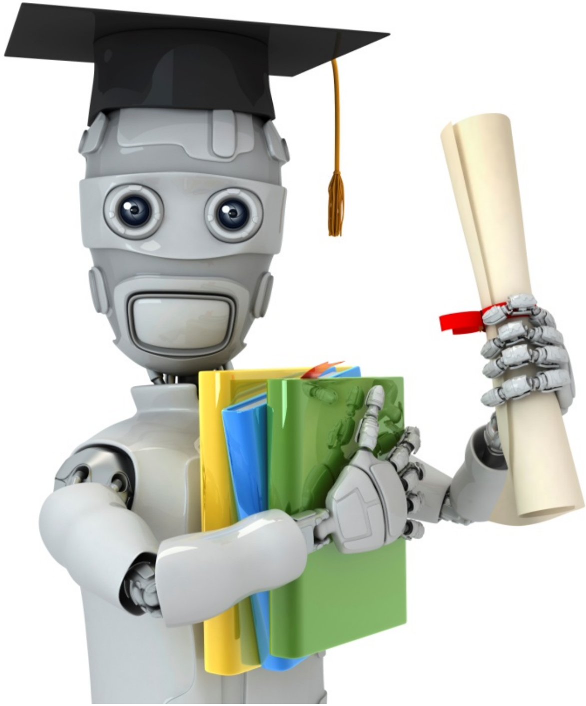
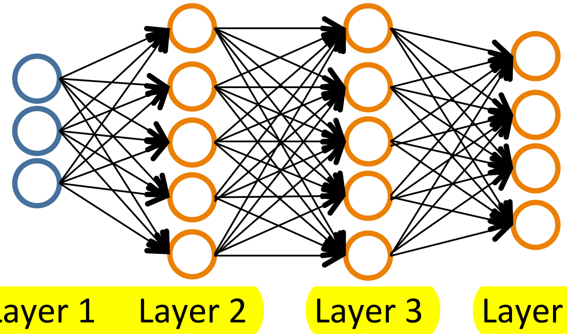


Machine Learning

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

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

Cost function

Logistic regression:

j:權重的編號
從1開始:忽略bias

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

Neural network:

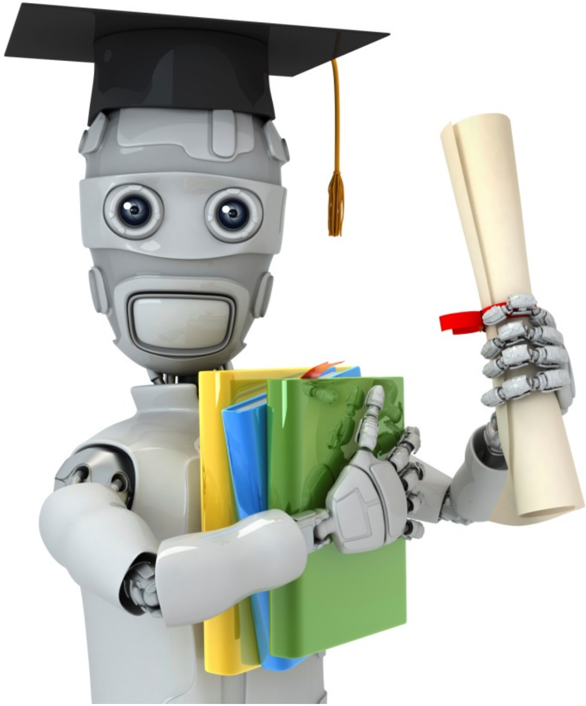
$$h_\Theta(x) \in \mathbb{R}^K \quad (h_\Theta(x))_i = i^{th} \text{ output}$$

對每個sample來說,都要求其k個輸出要與label一致

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

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

從1->2,2->3,...L-1->L 從l射到l+1層的權重，index都從1開始



Machine Learning

Neural Networks: Learning

Backpropagation algorithm

Gradient computation

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

$$\min_\Theta J(\Theta)$$

Need code to compute:

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

在l層的jth神經元射到l+1層的ith神經元的權重

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

Gradient computation

Given one training example (x, y):

Forward propagation:

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

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

注意theta(1)是連接第1和第2層的weight

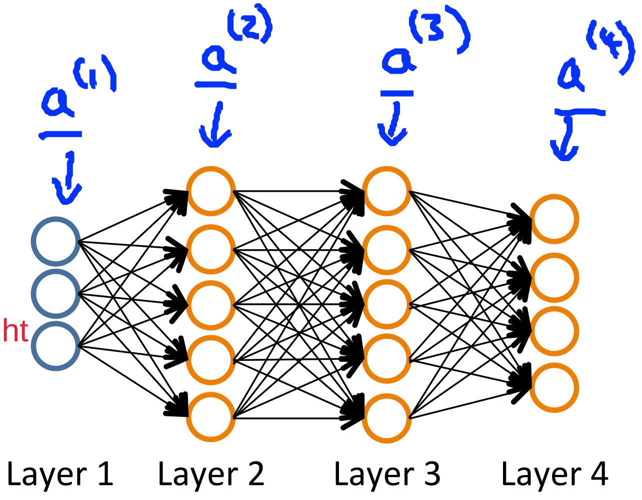
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$

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

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

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

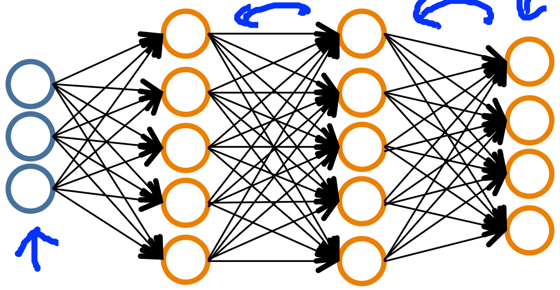
$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



Gradient computation: Backpropagation algorithm

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

$\delta^{(2)}$ $a_j^{(l)}$ $\delta^{(3)}$ $\delta^{(4)}$



For each output unit (layer L = 4)

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

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

theta3 transpose的維度:(s_3,s_4)

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

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

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

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

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

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

(ignoring λ; if $\lambda = 0$)

Backpropagation algorithm

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

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

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

For $i = 1$ to m

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

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 $\delta^{(L-1)}, \delta^{(L-2)}, \ldots, \delta^{(2)}$ ~~$\delta^{(1)}$~~

只算到layer2的error就好,layer1不需更新權重所以不算

$\boxed{\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}}$

這裡delta的下標i應該不是代表sample id的i

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

矩陣

column vector

row vector

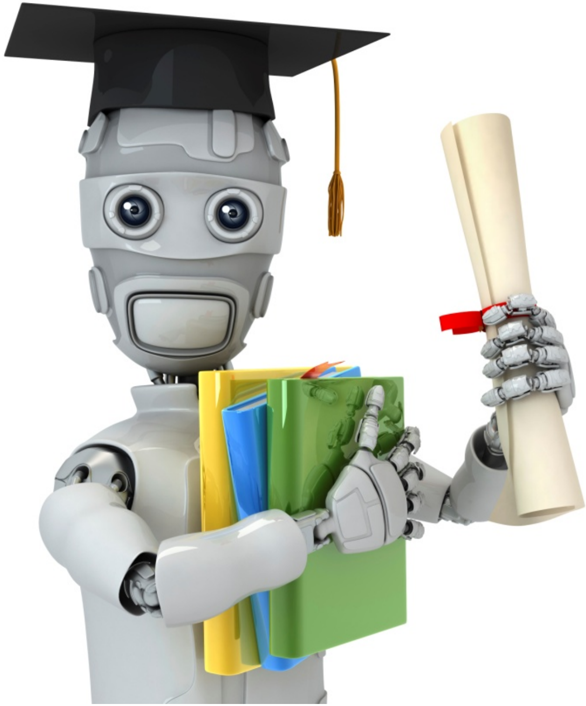
$D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)}$ if $j \neq 0$

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

對m個sample做平均

j表示從某層的第j個神經元射入,非零表示非bias

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

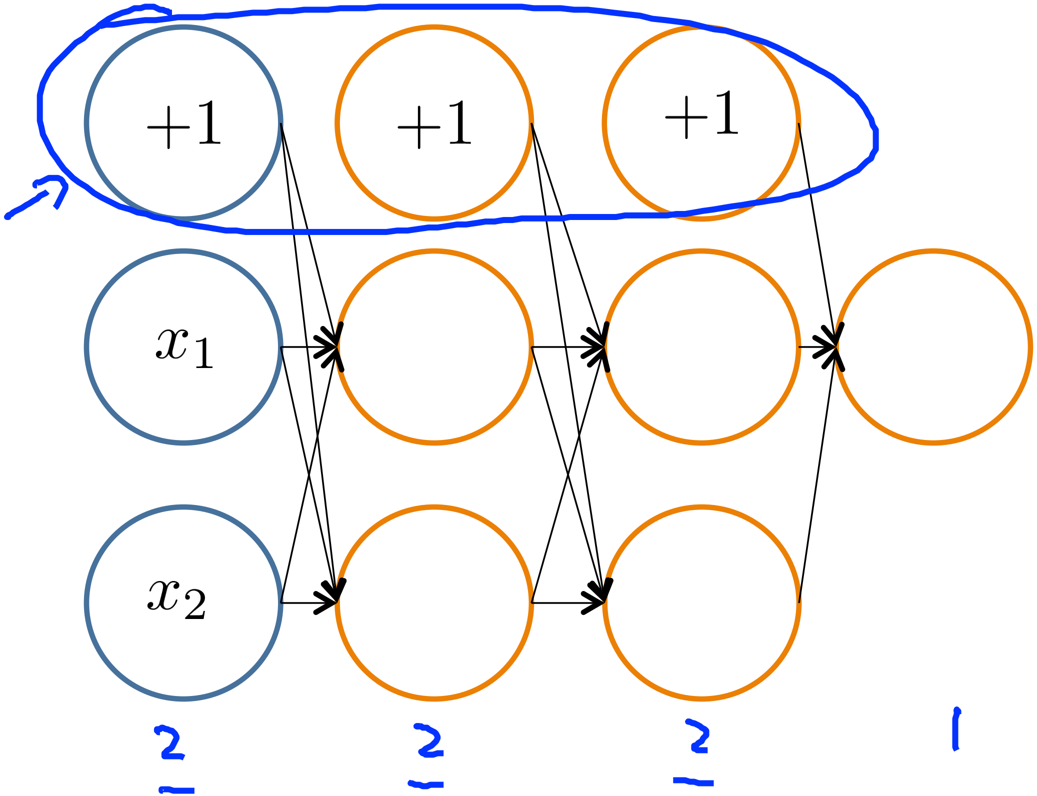


Machine Learning

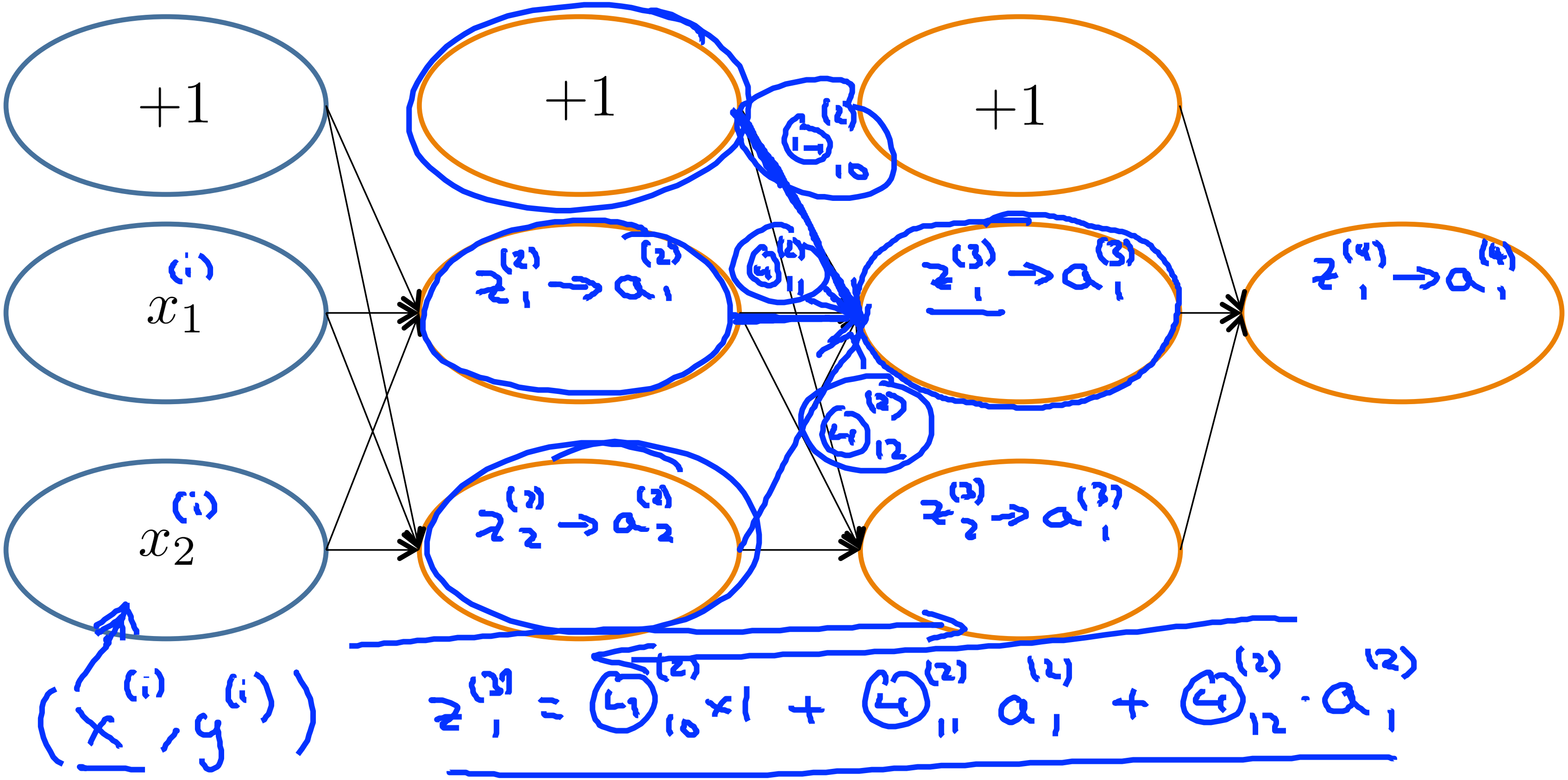
Neural Networks: Learning

Backpropagation intuition

Forward Propagation



Forward Propagation



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

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).

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

cost function是負的?

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

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

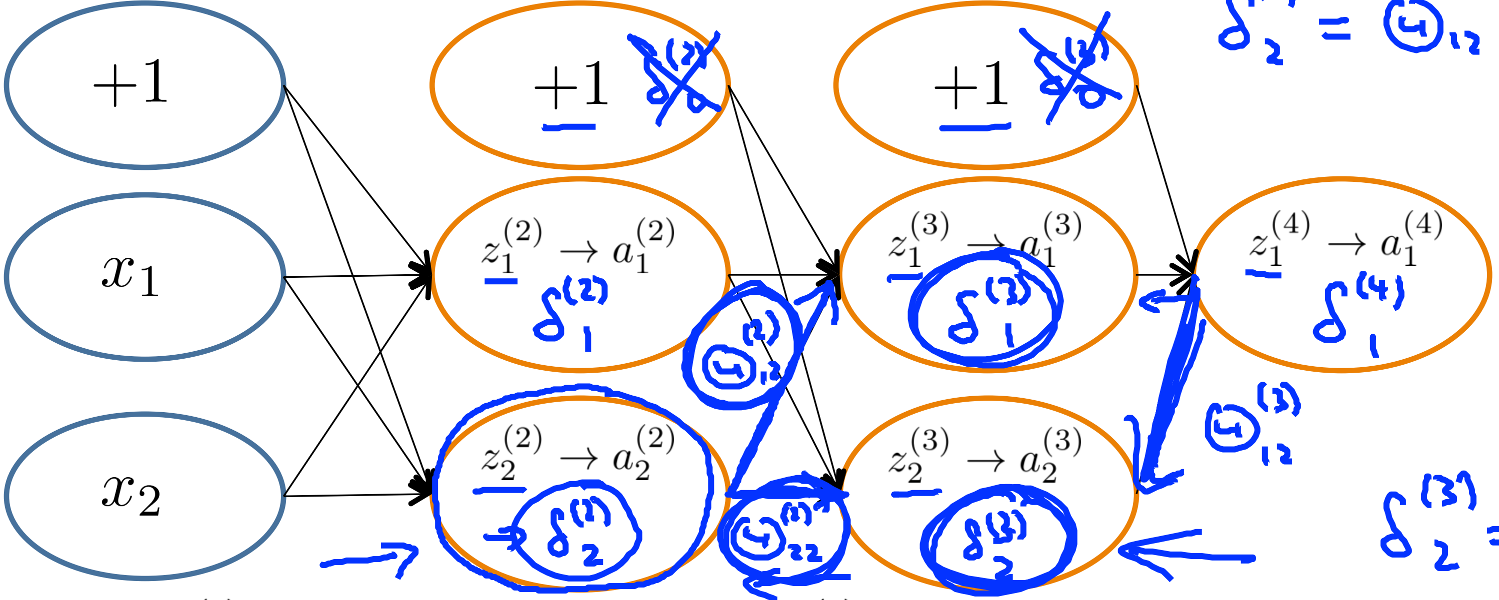
$y^{(i)}$

當y(i)與h_theta(x(i))一樣時,cost=0
不一樣時,cost=負無限大?

Forward Propagation

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

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

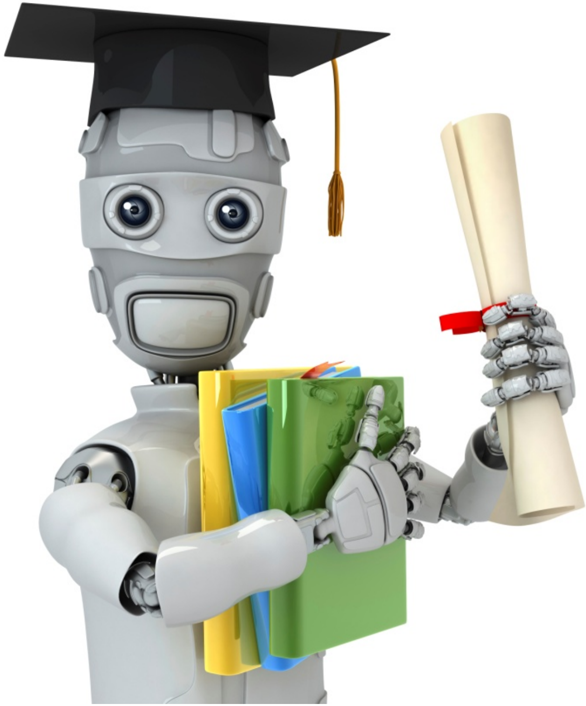


$$\delta_2^{(3)} = \Theta_{12}^{(3)} \cdot \delta_1^{(4)}.$$

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

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

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



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):

$\rightarrow$ $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$ - matrices (`Theta1`, `Theta2`, 連接第3,4層 `Theta3`)

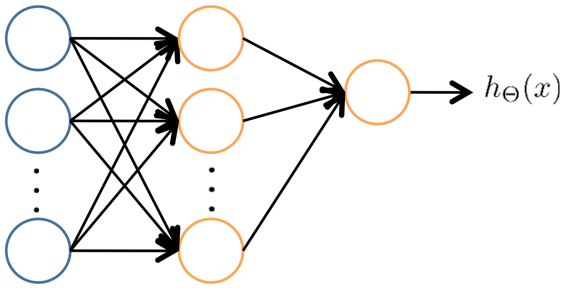
$\rightarrow$ $D^{(1)}, D^{(2)}, D^{(3)}$ - matrices (`D1`, `D2`, `D3`)

"Unroll" into vectors

Example

s_3=10, s_4=1

$s_1 = 10, s_2 = 10, \cancel{s_3 = 1}$



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

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

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

```
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)`

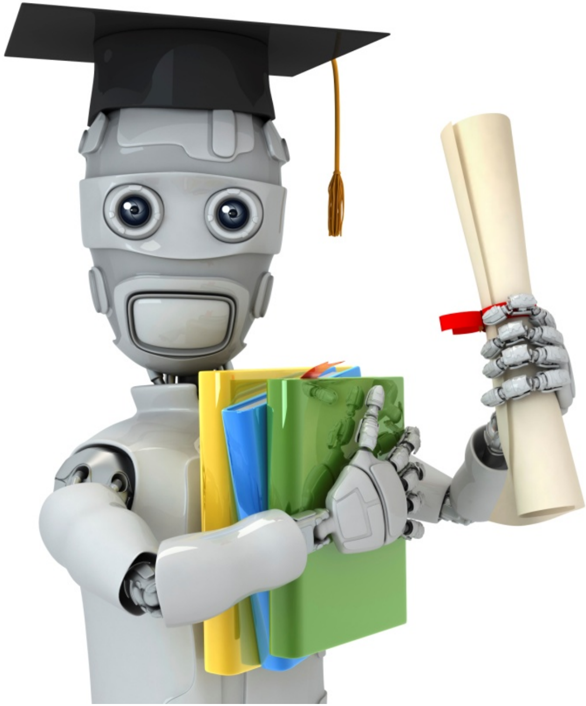
`function [jval, gradientVec] = costFunction(thetaVec)`

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

formular in p.8

Unroll $D^{(1)}, D^{(2)}, D^{(3)}$ to get `gradientVec`.

Unroll D(1),D(2),D(3) to get gradientVec

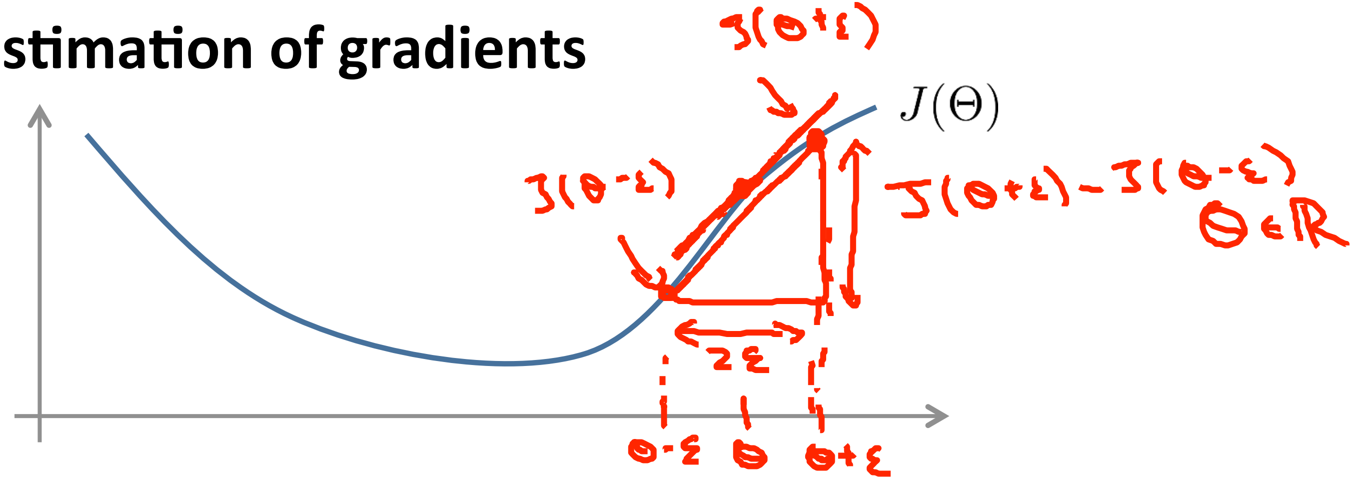


Machine Learning

Neural Networks: Learning

Gradient checking

Numerical estimation of gradients



$$\frac{d}{d\theta} J(\theta) \approx \underbrace{\frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}}$$

$\varepsilon = 10^{-4}$

$$\cancel{\frac{J(\theta+\varepsilon) - J(\theta)}{\varepsilon}}$$

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

Parameter vector θ

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

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

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

$$\vdots$$

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

```
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 $\boxed{\texttt{gradApprox}}$ ≈ $\boxed{\texttt{DVec}}$

From backprop.

Implementation Note:

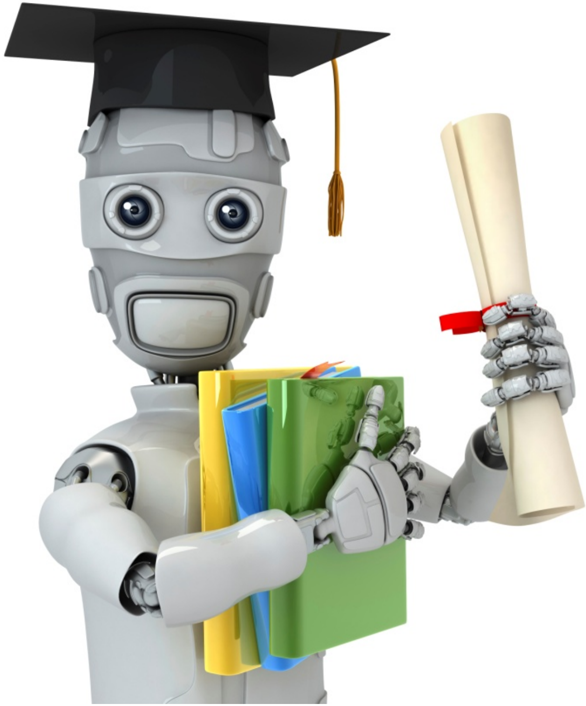
- Implement backprop to compute `DVec` (unrolled $D^{(1)}, D^{(2)}, D^{(3)}$).
- Implement numerical gradient check to compute `gradApprox`.
- Make sure they give similar values.
- Turn off gradient checking. Using backprop code for learning.

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 <u>very</u> slow.



Neural Networks: Learning

Random initialization

Machine Learning

Initial value of Θ

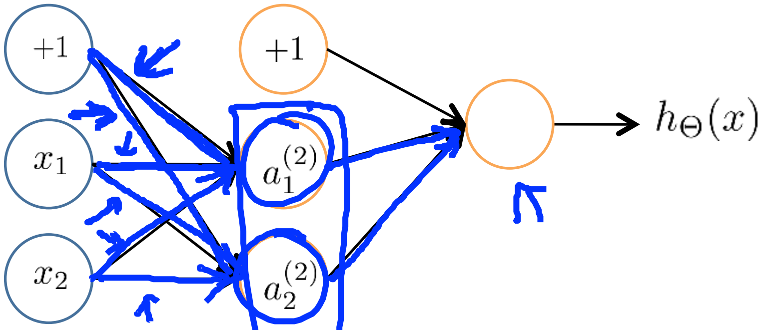
For gradient descent and advanced optimization method, need initial value for Θ.

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

Consider gradient descent

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

Zero initialization



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

delta(2)_1,delta(2)_2是由delta(3)_1跟theta(2)做運算得來
因為theta(2)裡的每個元素都被初始化成一樣的值,所以算出來的
delta(2)_1跟delta(2)_2也一樣

$a^{(2)}_1 = a^{(2)}_2$. Also $\delta^{(2)}_1 = \delta^{(2)}_2$.

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

$$\Theta^{(1)}_{01} = \Theta^{(1)}_{02}$$

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

$a^{(2)}_1 = a^{(2)}_2$

Random initialization: Symmetry breaking

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

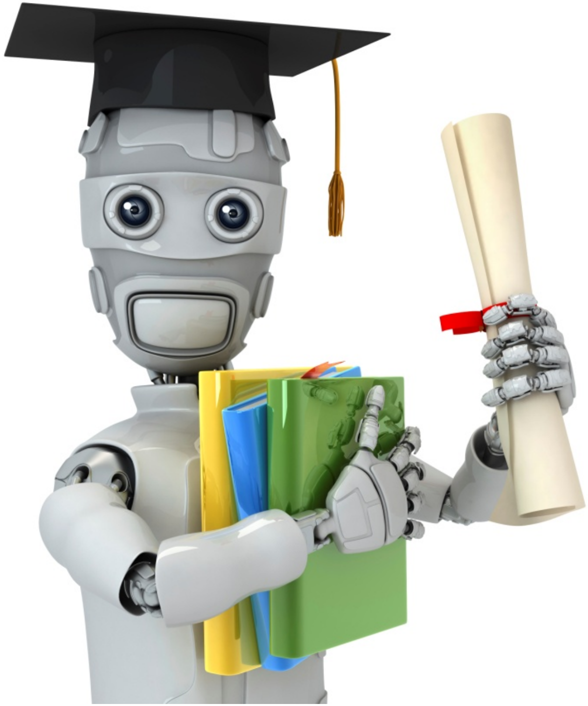
E.g.

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;
```



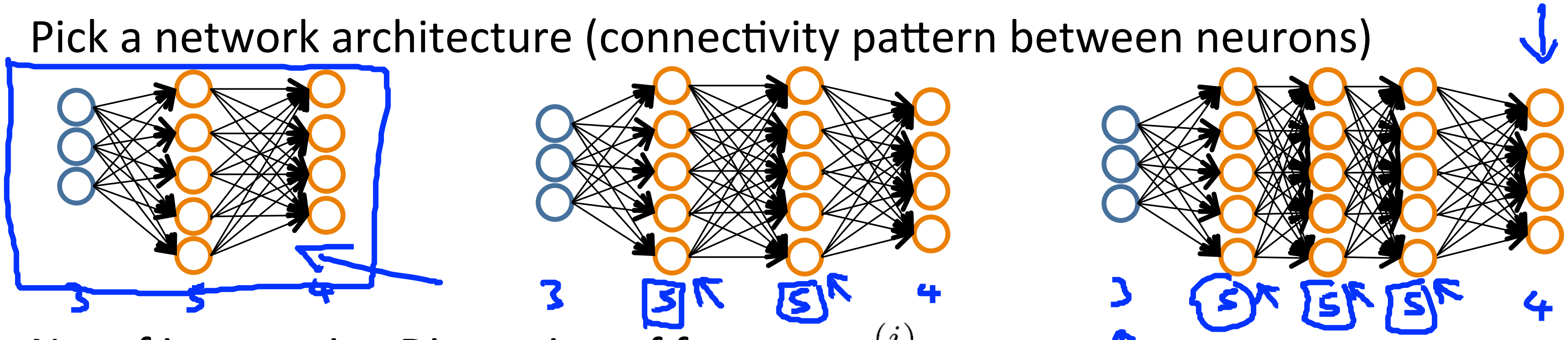
Machine Learning

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

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 $l = 2, \ldots, L$).

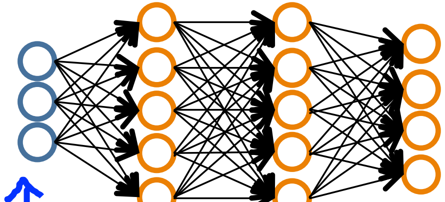
$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

....

}

...

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



$x^{(i)}$

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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 $J(\Theta)$.

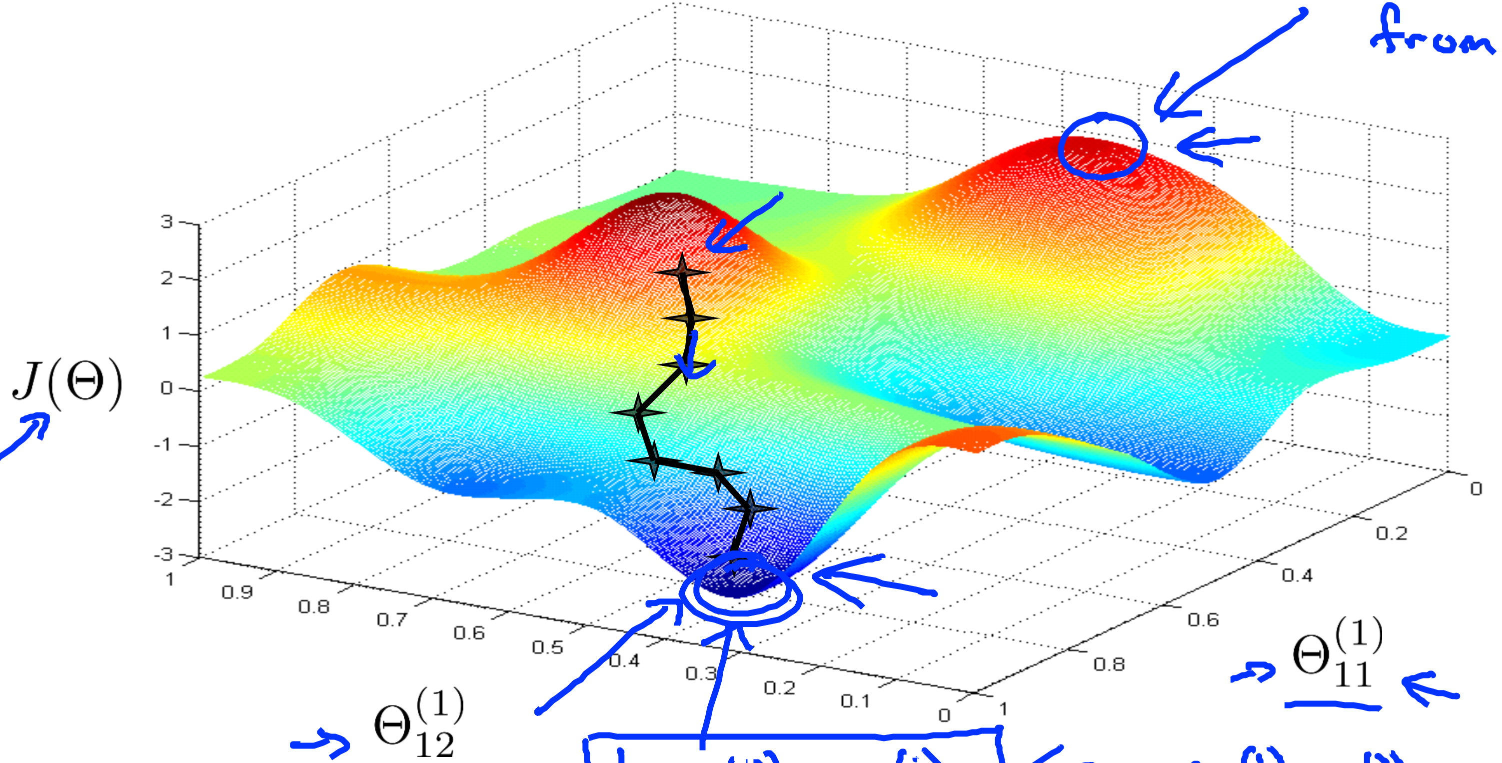
   Then disable gradient checking code.

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

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

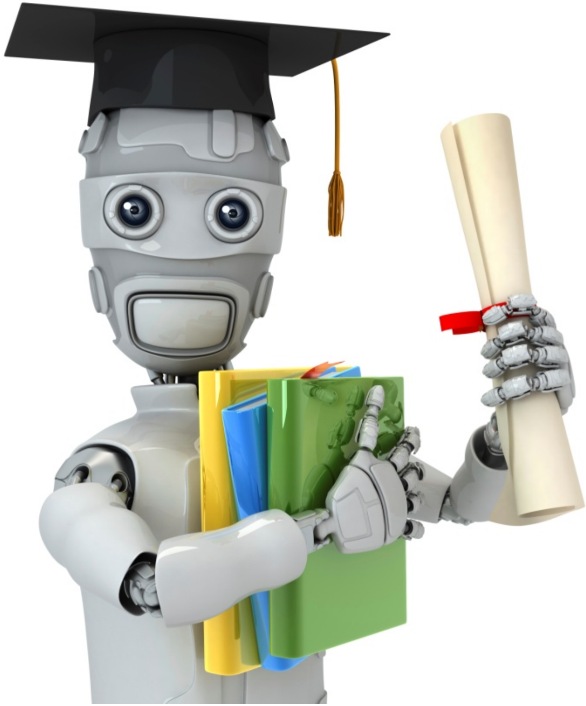
$J(\Theta)$ – non-convex.

$h_\Theta(x^{(i)})$ far from $y^{(i)}$



$\boxed{h_\Theta(x^{(i)}) \approx y^{(i)}}$

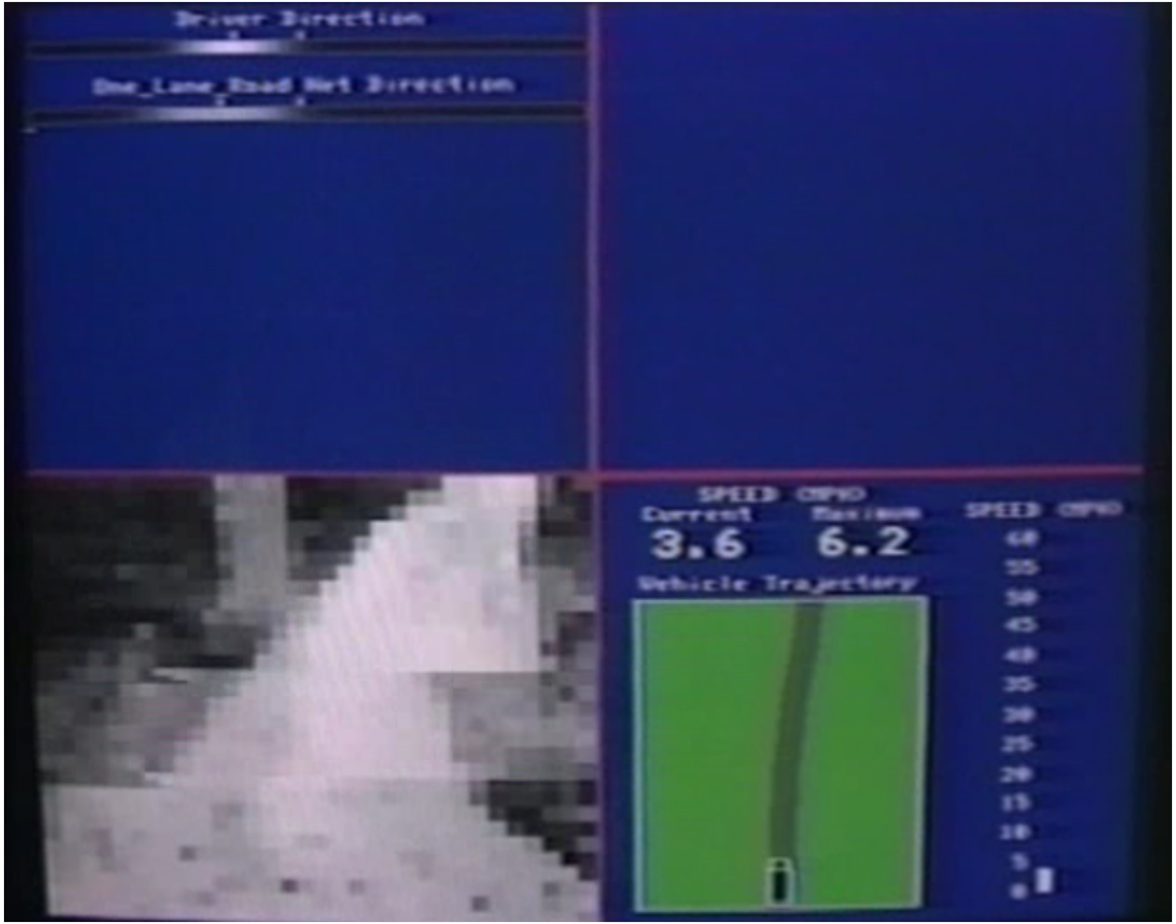
$\Theta^{(1)}, \Theta^{(2)}, \ldots$



Machine Learning

Neural Networks: Learning

Backpropagation example: Autonomous driving (optional)



[Courtesy of Dean Pomerleau]