



Machine Learning

# Neural Networks: Learning

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## Cost function

# Neural Network (Classification)



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

$L =$  total no. of layers in network

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

## Binary classification

$y = 0$  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:

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

Neural network:

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

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



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## Backpropagation algorithm

## Gradient computation

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

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

Need code to compute:

$$\rightarrow - \underline{J(\Theta)}$$

$$\rightarrow - \underline{\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)} \quad \leftarrow$$

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

# Gradient computation

Given one training example  $(x, y)$ :

Forward propagation:

$$\begin{aligned} &\rightarrow \underline{a^{(1)}} = \underline{x} \\ &\rightarrow z^{(2)} = \Theta^{(1)} a^{(1)} \\ &\rightarrow a^{(2)} = g(z^{(2)}) \quad (\text{add } \underline{a_0^{(2)}}) \\ &\rightarrow z^{(3)} = \Theta^{(2)} a^{(2)} \\ &\rightarrow a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)}) \\ &\rightarrow z^{(4)} = \Theta^{(3)} a^{(3)} \\ &\rightarrow \underline{a^{(4)}} = \underline{h_{\Theta}(x)} = g(z^{(4)}) \end{aligned}$$



# Gradient computation: Backpropagation algorithm

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

For each output unit (layer  $L = 4$ )

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

*(handwritten note:  $(\text{activation})_j$   $\delta_j^{(4)} = a_j^{(4)} - y_j$ )*



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

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

*(handwritten notes for  $g'(z)$ ):*  
 $a^{(3)} \cdot (1 - a^{(3)})$   
 $a^{(2)} \cdot (1 - a^{(2)})$

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

(ignoring  $\lambda$ ; if  $\lambda = 0$ )

# Backpropagation algorithm

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

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

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

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

Set  $\underline{a^{(1)}} = \underline{x^{(i)}}$

→ Perform forward propagation to compute  $\underline{a^{(l)}}$  for  $l = \underline{2}, \underline{3}, \dots, \underline{L}$

→ Using  $\underline{y^{(i)}}$ , compute  $\underline{\delta^{(L)}} = \underline{a^{(L)}} - \underline{y^{(i)}}$

→ Compute  $\underline{\delta^{(L-1)}}, \underline{\delta^{(L-2)}}, \dots, \underline{\delta^{(2)}}$  ~~set~~

→  $\underline{\Delta_{ij}^{(l)}} := \underline{\Delta_{ij}^{(l)}} + \underline{a_j^{(l)}} \underline{\delta_i^{(l+1)}}$

$\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + \delta_i^{(l+1)} (a_j^{(l)})^T$

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

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

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





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## Backpropagation intuition

# Forward Propagation



# Forward Propagation



# What is backpropagation doing?

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

(x<sup>(i)</sup>, y<sup>(i)</sup>)

Focusing on a single example x<sup>(i)</sup>, y<sup>(i)</sup>, the case of 1 output unit, and ignoring regularization (λ = 0),

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

(Think of cost(i) ≈ (h<sub>Θ</sub>(x<sup>(i)</sup>) - y<sup>(i)</sup>)<sup>2</sup>)

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

# Forward Propagation



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

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

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



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Implementation  
note: Unrolling  
parameters

## Advanced optimization

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

Handwritten annotations:  $\mathbb{R}^{n+1}$  (twice) and  $\mathbb{R}^{n+1}$  (vectors) with arrows pointing to gradient, theta, and initialTheta respectively.

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

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

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

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



$$\rightarrow \text{thetaVec} = [ \text{Theta1}(:); \text{Theta2}(:); \text{Theta3}(:) ] ;$$

$$\rightarrow \text{DVec} = [ \text{D1}(:); \text{D2}(:); \text{D3}(:) ] ;$$

$$\text{Theta1} = \text{reshape}(\text{thetaVec}(1:110), 10, 11) ;$$

$$\rightarrow \text{Theta2} = \text{reshape}(\text{thetaVec}(111:220), 10, 11) ;$$

$$\rightarrow \text{Theta3} = \text{reshape}(\text{thetaVec}(221:231), 1, 11) ;$$



## 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  $D^{(1)}, D^{(2)}, D^{(3)}$   $J(\Theta)$   
and  $D^{(1)}, D^{(2)}, D^{(3)}$   
Unroll \_\_\_\_\_ to get gradientVec.



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## Gradient checking

## Numerical estimation of gradients



$$\frac{d}{d\Theta} J(\Theta) \approx$$

$$\frac{J(\Theta + \epsilon) - J(\Theta - \epsilon)}{2\epsilon}$$

$\epsilon = 10^{-4}$

~~$$\frac{J(\Theta + \epsilon) - J(\Theta)}{\epsilon}$$~~

Implement: gradApprox = (J(theta + EPSILON) - J(theta - EPSILON)) / (2\*EPSILON)

## Parameter vector $\theta$

→  $\theta \in \mathbb{R}^n$  (E.g.  $\theta$  is “unrolled” version of  $\underline{\Theta^{(1)}}$ ,  $\underline{\Theta^{(2)}}$ ,  $\underline{\Theta^{(3)}}$  )

→  $\theta = [\theta_1, \theta_2, \theta_3, \dots, \theta_n]$

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

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

⋮

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

```

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 gradApprox  $\approx$  DVec ←

↑  
From back prop.

## 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.  


## 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.



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## Random initialization

## Initial value of $\Theta$

For gradient descent and advanced optimization method, need initial value for  $\Theta$ .

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

Consider gradient descent

Set initialTheta = zeros(n,1) ?



## Zero initialization



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

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

$$\frac{\partial}{\partial \Theta_{0,1}^{(1)}} J(\Theta) = \frac{\partial}{\partial \Theta_{0,2}^{(1)}} J(\Theta)$$

$$\underline{\Theta_{0,1}^{(1)}} = \underline{\Theta_{0,2}^{(1)}}$$

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

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

## 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 10x11 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;`



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# 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)

$y \in \{1, 2, 3, \dots, 10\}$   
 ~~$y = 5$~~

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

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

→ 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  $l = 2, \dots, L$ ).

→  $\Delta^{(2)} := \Delta^{(2)} + \delta^{(L)} (a^{(2)})^T$

...

}

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



## Training a neural network

- 5. Use gradient checking to compare  $\frac{\partial}{\partial \Theta_{ik}^{(l)}} J(\Theta)$  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  $\Theta$

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

$J(\Theta)$  — non-convex.





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Backpropagation  
example: Autonomous  
driving (optional)



