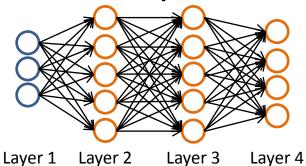


#### Machine Learning

## Neural Networks: Learning

### Cost function



#### Binary classification

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

1 output unit

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

L= total no. of layers in network

 $s_l = 1$  no. of units (not counting bias unit) in layer l

#### Multi-class classification (K classes)

$$y \in \mathbb{R}^K$$
 E.g.  $\left[ \begin{smallmatrix} 1 \\ 0 \\ 0 \\ 0 \end{smallmatrix} \right]$ ,  $\left[ \begin{smallmatrix} 0 \\ 1 \\ 0 \\ 0 \end{smallmatrix} \right]$ ,  $\left[ \begin{smallmatrix} 0 \\ 0 \\ 1 \\ 0 \end{smallmatrix} \right]$ ,  $\left[ \begin{smallmatrix} 0 \\ 0 \\ 0 \\ 1 \end{smallmatrix} \right]$  pedestrian car motorcycle truck

K output units

#### **Cost function**

#### Logistic regression:

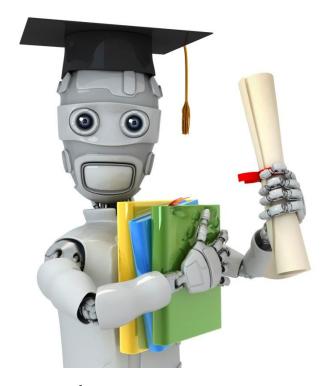
$$J(\theta) = -\frac{1}{m} \left[ \sum_{i=1}^{m} y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \right] + \frac{\lambda}{2m} \sum_{i=1}^{n} \theta_{j}^{2}$$

#### Neural network:

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

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

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



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:

- 
$$J(\Theta)$$

$$-J(\Theta)$$

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

#### **Gradient computation**

Given one training example (x, y):

#### Forward propagation:

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

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

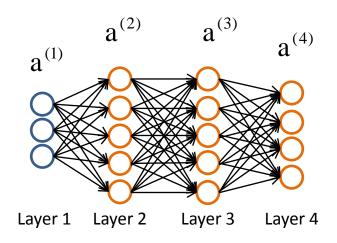
$$a^{(2)} = g(z^{(2)}) \text{ (add } a_0^{(2)})$$

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

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

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

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



#### **Gradient computation: Backpropagation algorithm**

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

$$\delta_j^{(4)} = a_j^{(4)} - y_j \qquad (h_\theta(x))_j$$

Layer 1 Layer 2 Layer 3 
$$a^{(3)}$$
.\* $(1-a^{(3)})$ 

Layer 4

$$\delta^{(3)} = (\Theta^{(3)})^T \delta^{(4)} \cdot * g'(z^{(3)}) \longleftarrow a^{(3)} \cdot * (1 - a^{(3)})$$

$$\delta^{(2)} = (\Theta^{(2)})^T \delta^{(3)} \cdot *g'(z^{(2)}) \leftarrow a^{(2)} \cdot *(1 - a^{(2)})$$

$$\frac{\partial}{\partial \theta_{i}^{l}} J(\theta) = a_{j}^{l} \delta_{i}^{l+1}$$

#### Compound expressions: f(x, y, z) = (x + y)z

$$f(x,y,z) = (x+y)$$

$$q=x+y \qquad rac{\partial q}{\partial x}=1, rac{\partial q}{\partial y}=1$$

$$f=qz$$
  $rac{\partial f}{\partial q}=z, rac{\partial f}{\partial z}=q$ 

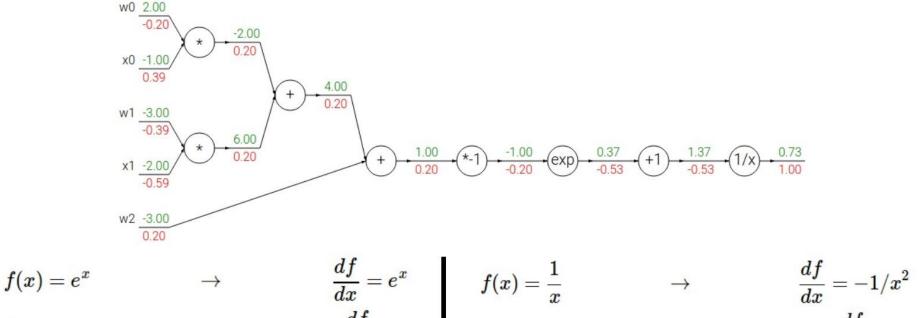
#### Chain rule:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

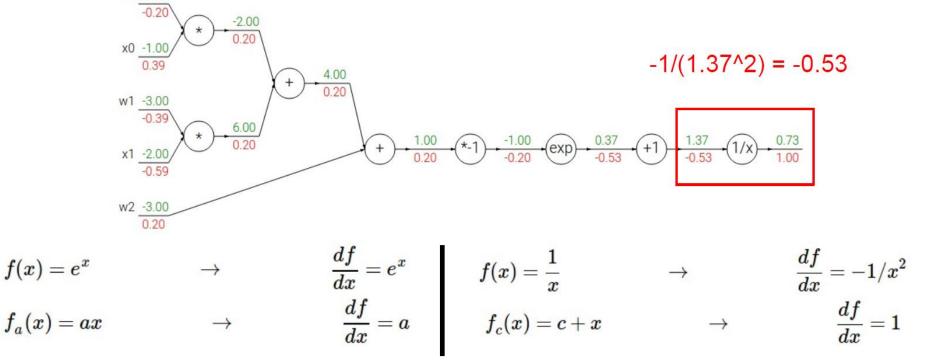
```
# set some inputs
x = -2; y = 5; z = -4
# perform the forward pass
q = x + y # q becomes 3
f = q * z # f becomes -12
# perform the backward pass (backpropagation) in reverse order:
# first backprop through f = q * z
dfdz = q # df/fz = q, so gradient on z becomes 3
dfdq = z # df/dq = z, so gradient on q becomes -4
\# now backprop through q = x + y
dfdx = 1.0 * dfdq # dq/dx = 1. And the multiplication here is the chain rule!
dfdy = 1.0 * dfdq # dq/dy = 1
```

 $f_a(x) = ax$ 

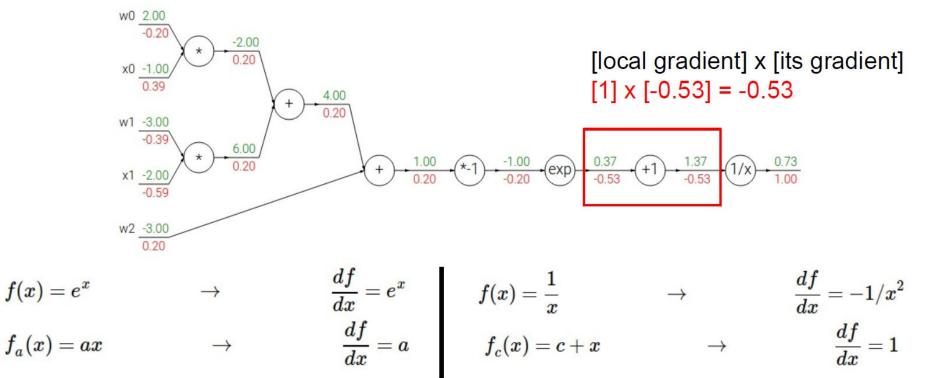
$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



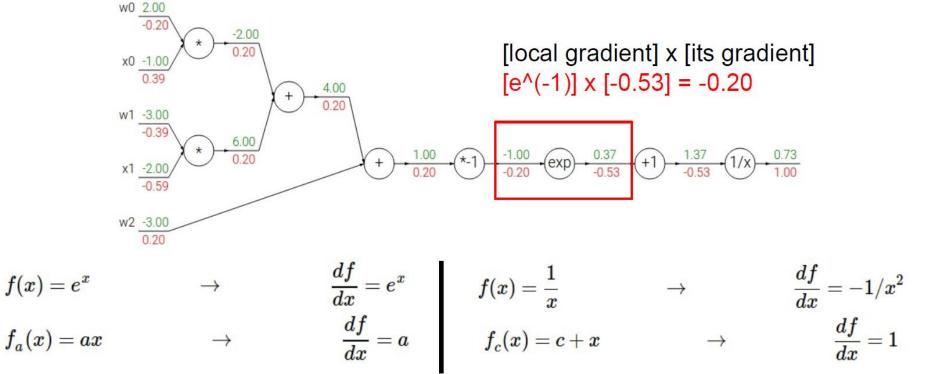
$$f(w,x) = rac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$



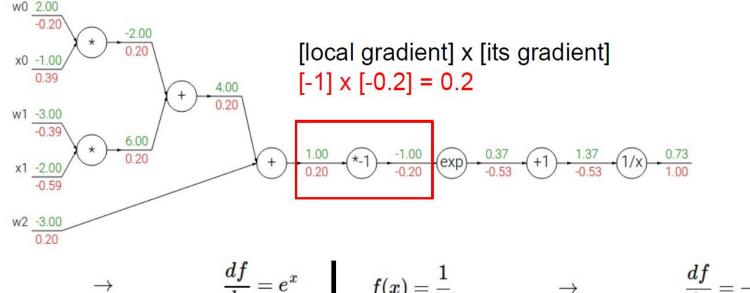
$$f(w,x) = rac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$



$$f(w,x) = rac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

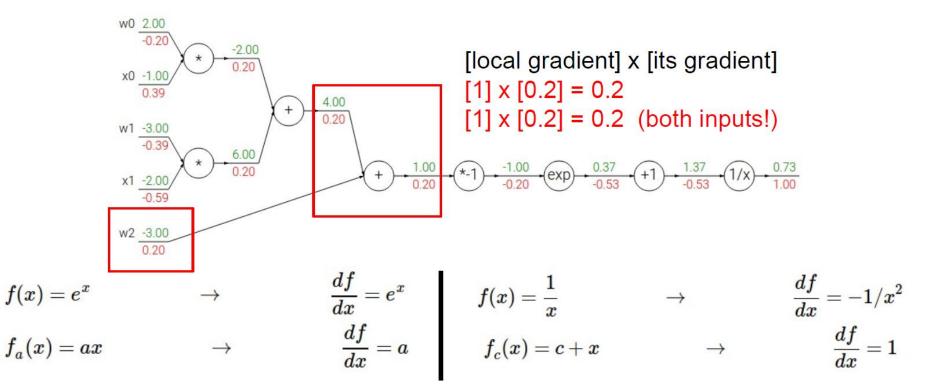


$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

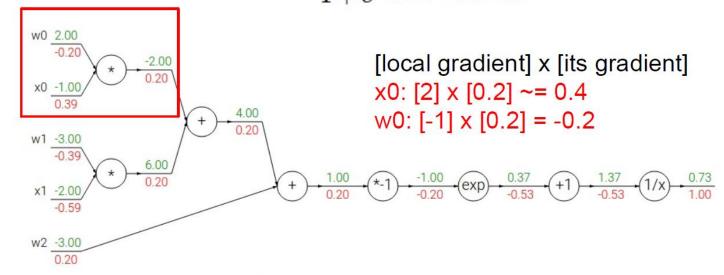


$$egin{array}{lll} f(x)=e^x & 
ightarrow & rac{df}{dx}=e^x & f(x)=rac{1}{x} & 
ightarrow & \ f_a(x)=ax & 
ightarrow & rac{df}{dx}=a & f_c(x)=c+x & 
ightarrow & 
ightarrow$$

$$f(w,x) = rac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2 x_1 + w_2 x_2 + w_2 x_2$$



$$f(w,x) = rac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$



$$f(x)=e^x$$

$$f_a(x) = ax$$

$$egin{aligned} rac{df}{dx} = e^x & f(x) = rac{1}{x} & 
ightarrow \ rac{df}{dx} = a & f_c(x) = c + x & 
ightarrow \end{aligned}$$

$$f(x) = \frac{1}{3}$$

$$(x) = \frac{1}{x}$$

$$(x) = c + c$$

$$\rightarrow$$

$$ightarrow rac{df}{dx}=$$

$$ightarrow rac{df}{dx}=$$

#### **Backpropagation algorithm**

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

Set  $\triangle_{ij}^{(l)}=0$  (for all l,i,j). use to compute  $\frac{C}{\partial \theta_{\cdot \cdot}^{l}}J(\theta)$ 

For i = 1 to m

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

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

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

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

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

$$\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_i^{(l)} \delta_i^{(l+1)} \longrightarrow \Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$$

$$f j \neq 0$$
if  $i = 0$ 

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

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

#### **Example for Regression**

Cost function:

tion: 
$$J(W, b; x, y) = \frac{1}{2} \|h_{W, b}(x) - y\|^2$$

That is 
$$J(W,b) = \left[ \frac{1}{m} \sum_{i=1}^{m} J(W,b;x^{(i)},y^{(i)}) \right] + \frac{\lambda}{2} \sum_{l=1}^{n_l-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} \left( W_{ji}^{(l)} \right)^2$$
$$= \left[ \frac{1}{m} \sum_{i=1}^{m} \left( \frac{1}{2} \left\| h_{W,b}(x^{(i)}) - y^{(i)} \right\|^2 \right) \right] + \frac{\lambda}{2} \sum_{l=1}^{n_l-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} \left( W_{ji}^{(l)} \right)^2$$

Gradient computation: 
$$W_{ij}^{(l)}=W_{ij}^{(l)}-\alpha\frac{\partial}{\partial W_{ij}^{(l)}}J(W,b)$$
 
$$b_i^{(l)}=b_i^{(l)}-\alpha\frac{\partial}{\partial b_i^{(l)}}J(W,b)$$

#### **Example for Regression**

Gradient computation:

$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$
$$b_i^{(l)} = b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W, b)$$

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b) = \left[ \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x^{(i)}, y^{(i)}) \right] + \lambda W_{ij}^{(l)}$$
$$\frac{\partial}{\partial b_i^{(l)}} J(W, b) = \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial b_i^{(l)}} J(W, b; x^{(i)}, y^{(i)})$$

#### **Example for Regression**

Gradient computation:

$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$
$$b_i^{(l)} = b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W, b)$$

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b) = \left[ \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x^{(i)}, y^{(i)}) \right] + \lambda W_{ij}^{(l)}$$
$$\frac{\partial}{\partial b_i^{(l)}} J(W, b) = \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial b_i^{(l)}} J(W, b; x^{(i)}, y^{(i)})$$

- 1. 进行前向传播,计算层 $L_2,L_3,...,L_{n_1}$ 的激活。
- 2. 对层n<sub>1</sub>(输出层)的每一个节点 i, 令。

$$\delta_{i}^{(n_l)} = \frac{\partial}{\partial z_{i}^{(n_l)}} J(W, b)$$

3. 对 $l = n_l - 1, n_l - 2, n_l - 3, ..., 2$ ,对第 1 层的每一个节点  $\underline{i}$ ,令。

$$\delta_{i}^{(l)} = \left(\sum_{i=1}^{s_{l+1}} W_{ji}^{(l)} \delta_{j}^{(l+1)}\right) g'(z_{i}^{(l)})$$

根据以下公式计算偏导数:

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x, y) = a_j^{(l)} \delta_i^{(l+1)}$$

$$\frac{\partial}{\partial b_i^{(l)}} J(W, b; x, y) = \delta_i^{(l+1)}$$

算法 2: 后向传播算法向量化表达

- 1. 进行前向传播,计算层 $L_2,L_3,...,L_{n_l}$ 的激活。
- 2. 对输出层 (第n<sub>1</sub>层), 令。

$$\delta^{(n_l)} = \frac{\partial}{\partial z^{(n_l)}} J(W, b)$$

3.  $\forall l = n_1 - 1, n_1 - 2, n_1 - 3, ..., 2, \Leftrightarrow$ 

$$\delta^{(l)} = \left( \left( W^{(l)} \right)^T \delta^{(l+1)} \right) \bullet g'(z^{(l)}).$$

4. 计算偏导数: 4

$$abla_{W^{(l)}}J(W,b;x,y) = \delta^{(l+1)}(a^{(l)})^{T_{a}}$$

$$abla_{b^{(l)}}J(W,b;x,y) = \delta^{(l+1)}a^{(l)}$$

上述算法中•为按位相乘操作符,即如果 $a = b \cdot c$ ,那么有 $a_i = b_i c_i$ .

1.  $\phi \Delta W^{(1)} := 0$ .  $\Delta b^{(1)} := 0$  (这里的 0 分别代表全为 0 的矩阵和向量)。

a. 使用后向传播算法计算∇<sub>W(l)</sub>J(W, b; x, y)和∇<sub>b(l)</sub>J(W, b; x, y). √

b. 计算
$$\Delta W^{(l)} := \Delta W^{(l)} + \nabla_{W^{(l)}} J(W,b;x,y)$$
.

c. 计算
$$\Delta b^{(l)} := \Delta b^{(l)} + \nabla_{b^{(l)}} J(W, b; x, y)$$
.

3. 更新参数:

$$W^{(l)} = W^{(l)} - \alpha \left[ \left( \frac{1}{m} \Delta W^{(l)} \right) + \lambda W^{(l)} \right]_{a}^{a}$$
$$b^{(l)} = b^{(l)} - \alpha \left[ \frac{1}{m} \Delta b^{(l)} \right]_{a}^{a}$$

4. 重复 1~3 直到满足迭代停止条件。』

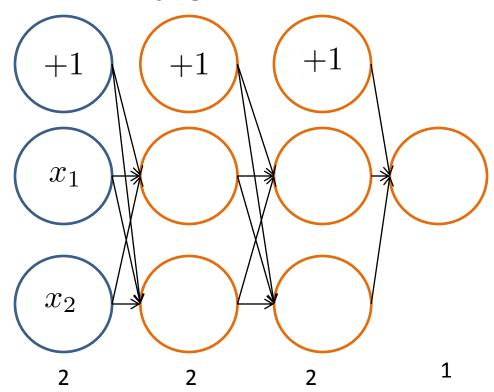


**Machine Learning** 

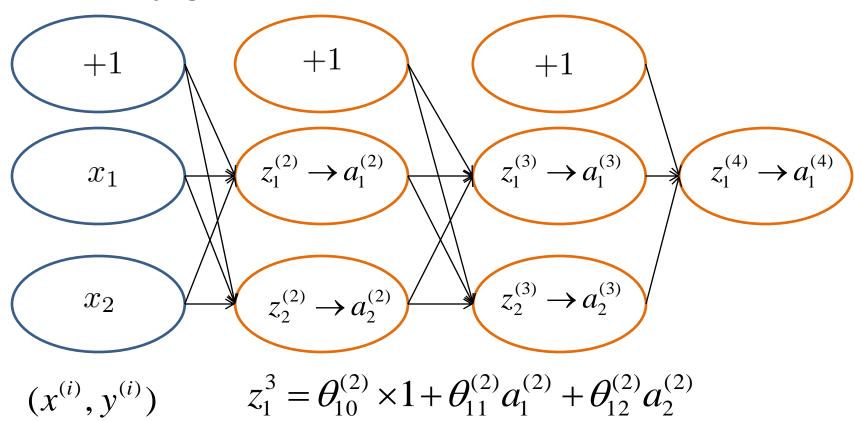
## Neural Networks: Learning

## Backpropagation intuition

#### **Forward Propagation**



#### **Forward Propagation**



#### What is backpropagation doing?

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

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

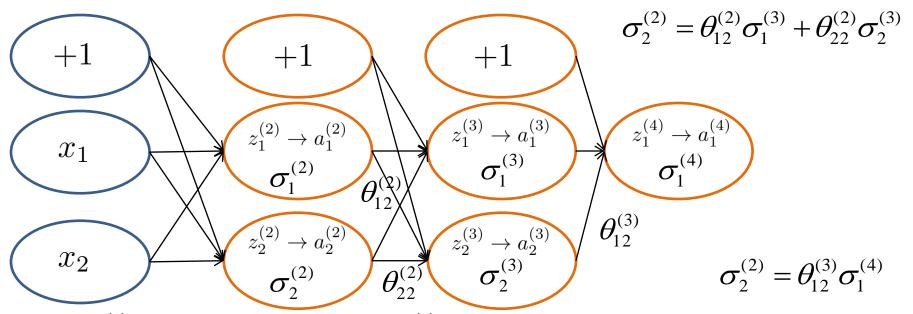
$$cost(i) = y^{(i)} \log h_{\Theta}(x^{(i)}) + (1 - y^{(i)}) \log h_{\Theta}(x^{(i)})$$

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

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

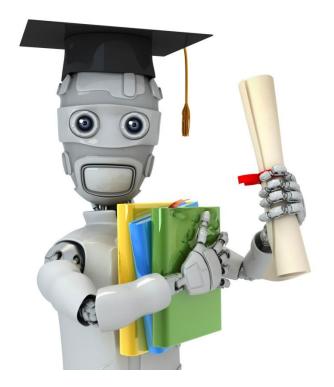
#### **Forward Propagation**

$$\sigma_1^{(4)} = y^{(i)} - a_1^{(4)}$$



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

Formally,  $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \cot(i)$  (for  $j \geq 0$ ), where  $\cot(i) = y^{(i)} \log h_{\Theta}(x^{(i)}) + (1 - y^{(i)}) \log h_{\Theta}(x^{(i)})$ 



Machine Learning

## Neural Networks: Learning

Implementation note: Unrolling parameters

#### **Advanced optimization**

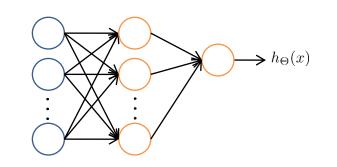
```
function [jVal, gradient] = costFunction(theta)
optTheta = fminunc(@costFunction, initialTheta, options)
Neural Network (L=4):
      \Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)} - matrices (Theta1, Theta2, Theta3)
      D^{(1)}, D^{(2)}, D^{(3)} - matrices (D1, D2, D3)
"Unroll" into vectors
```

#### **Example**

```
s_1 = 10, s_2 = 10, s_3 = 1

\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}
```



```
thetaVec = [ Theta1(:); Theta2(:); Theta3(:)];

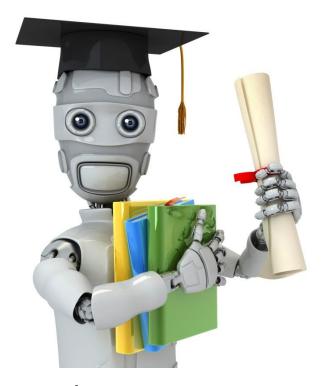
DVec = [D1(:); D2(:); D3(:)];

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

#### **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)}. 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 $J(\theta + \varepsilon)$

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

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

$$\theta - \varepsilon \quad \theta + \varepsilon$$

$$\frac{\partial}{\partial \theta} J(\theta) \approx \frac{J(\theta + \varepsilon) - J(\theta - \varepsilon)}{2\varepsilon}$$
$$\varepsilon = 10^{-4}$$

#### Parameter vector $\theta$

$$heta \in \mathbb{R}^n$$
 (E.g.  $heta$  is "unrolled" version of  $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$ )

$$\theta = \theta_1, \theta_2, \theta_3, \dots, \theta_n$$

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

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

•

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

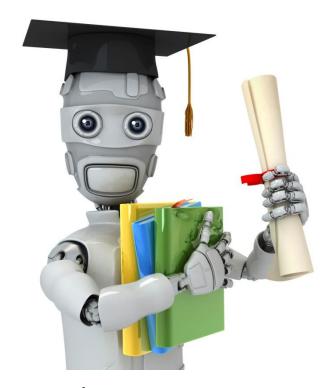
```
for i = 1:n,
   thetaPlus = theta;
   thetaPlus(i) = thetaPlus(i) + EPSILON;
   thetaMinus = theta;
   thetaMinus(i) = thetaMinus(i) - EPSILON;
   gradApprox(i) = (J(thetaPlus) - J(thetaMinus))
                     /(2*EPSILON);
end;
Check that gradApprox ≈ DVec
```

#### **Implementation Note:**

- Implement backprop to compute  $exttt{DVec}$  (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.



Machine Learning

## Neural Networks: Learning

# Random initialization

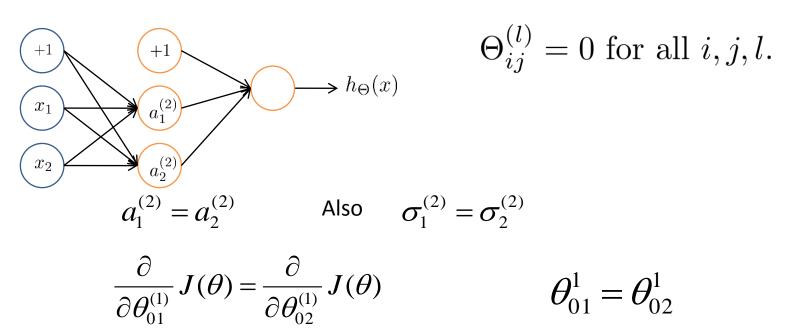
#### Initial value of $\Theta$

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



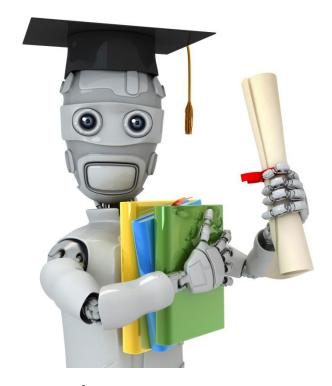
After each update, parameters corresponding to inputs going into each of two hidden units are identical.

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

#### 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.



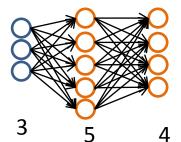
Machine Learning

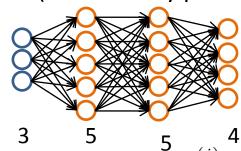
## Neural Networks: Learning

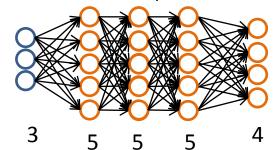
# Putting it together

#### 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)

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

$$y = \begin{bmatrix} 0 \\ 0 \\ \dots \end{bmatrix}$$

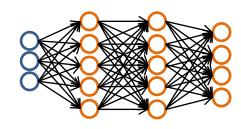
#### Training a neural network

- 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

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

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



#### 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  $\Theta$

$$rac{\partial}{\partial heta_{ii}^l} J( heta)$$

$$J( heta)$$
 —non-convex

