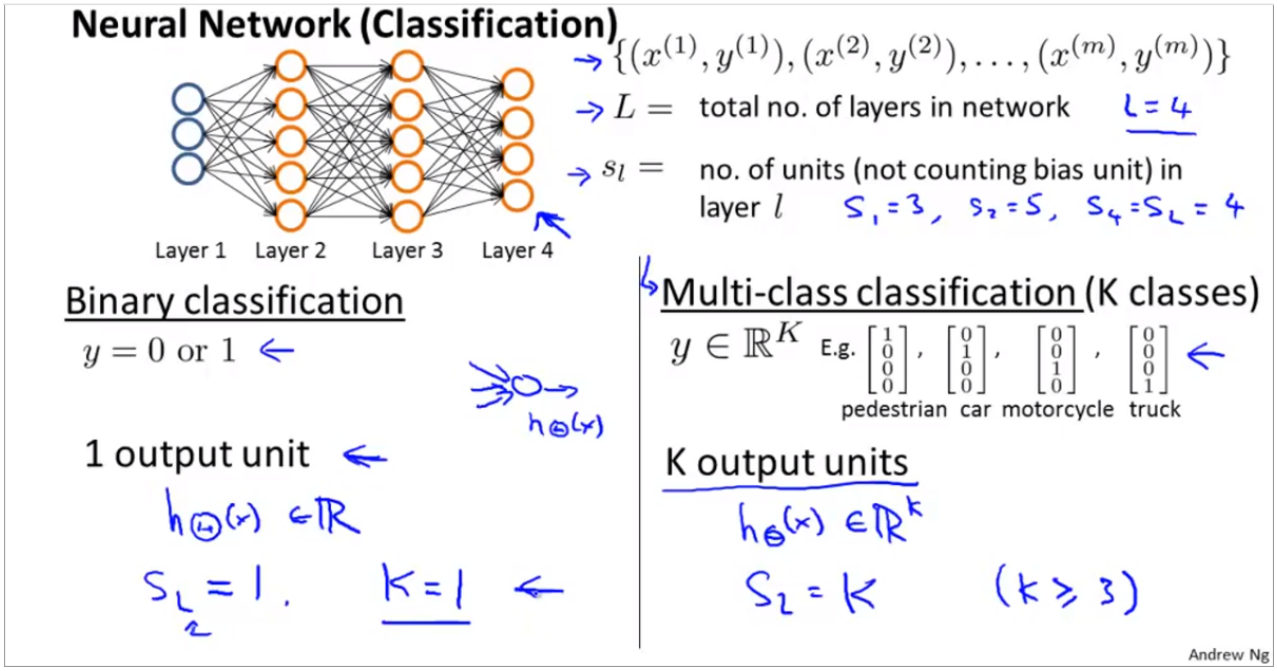
Week_5

CostFunction

Let's first define a few variables that we will need to use:

- L = total number of layers in the network
- s_l = number of units (not counting bias unit) in layer l
- K = number of output units/classes



Our cost function for neural networks is going to be a generalization of the one we used for logistic regression. Recall that the cost function for regularized logistic regression was:

Cost function

Logistic regression:

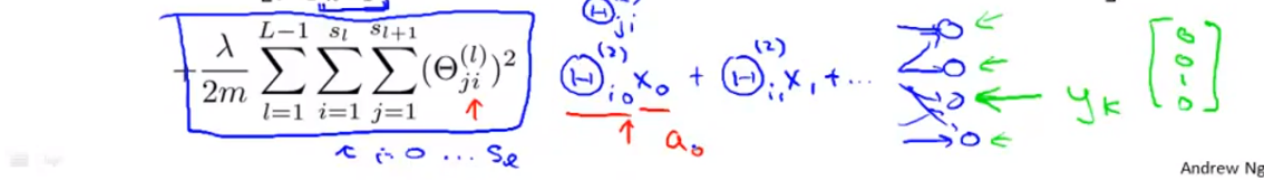
$$J(\theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1-y^{(i)}) \log(1-h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$$

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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Note:

- the double sum simply adds up the logistic regression costs calculated for each cell in the output layer
- the triple sum simply adds up the squares of all the individual Θs in the entire network.
- the i in the triple sum does **not** refer to training example i

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:

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

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

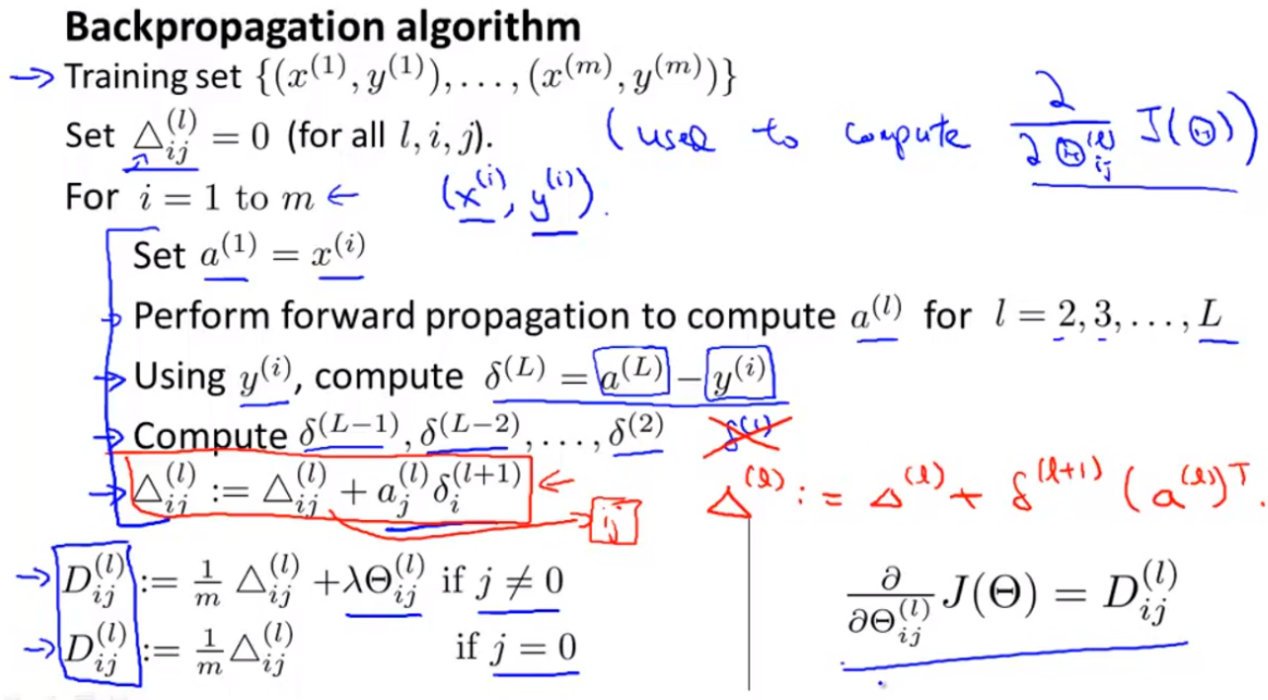
"Backpropagation" is neural-network terminology for minimizing our cost function, just like what we were doing with gradient descent in logistic and linear regression. Our goal is to compute:

$\min_\Theta J(\Theta)$

That is, we want to minimize our cost function J using an optimal set of parameters in theta. In this section we'll look at the equations we use to compute the partial derivative of J(Θ):

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

To do so, we use the following algorithm:



Back propagation Algorithm

Given training set $\{(x^{(1)}, y^{(1)}) \cdots (x^{(m)}, y^{(m)})\}$

- Set $\Delta_{i,j}^{(l)}$:= 0 for all (l,i,j), (hence you end up having a matrix full of zeros)

For training example t =1 to m:

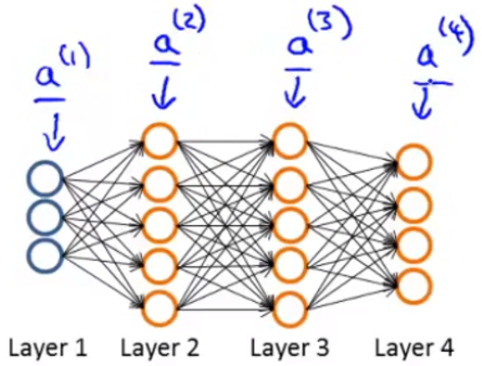
1. Set $a^{(1)} := x^{(t)}$
2. Perform forward propagation to compute $a^{(l)}$ for l=2,3,...,L

Gradient computation

Given one training example (x, y):

Forward propagation:

$$a^{(1)} = x$$
$$z^{(2)} = \Theta^{(1)} a^{(1)}$$
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$
$$z^{(3)} = \Theta^{(2)} a^{(2)}$$
$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$
$$z^{(4)} = \Theta^{(3)} a^{(3)}$$
$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



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

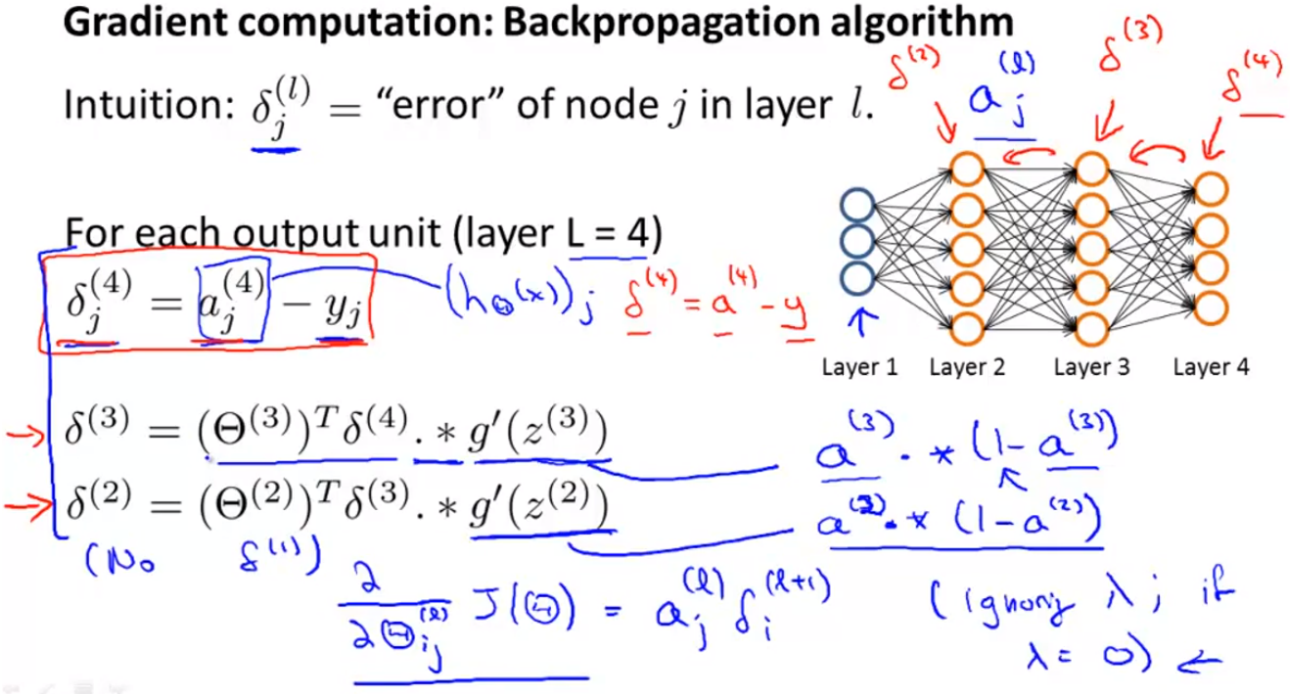
Where L is our total number of layers and $a^{(L)}$ is the vector of outputs of the activation units for the last layer. So our "error values" for the last layer are simply the differences of our actual results in the last layer and the correct outputs in y. To get the delta values of the layers before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

4. Compute $\delta^{(L-1)}, \delta^{(L-2)}, \dots, \delta^{(2)}$ using $\delta^{(l)} = ((\Theta^{(l)})^T \delta^{(l+1)}) .* a^{(l)} .* (1 - a^{(l)})$

The delta values of layer l are calculated by multiplying the delta values in the next layer with the theta matrix of layer l. We then element-wise multiply that with a function called g', or g-prime, which is the derivative of the activation function g evaluated with the input values given by $z^{(l)}$.

The g-prime derivative terms can also be written out as:

$$g'(z^{(l)}) = a^{(l)} .* (1 - a^{(l)})$$



5. $\Delta_{i,j}^{(l)} := \Delta_{i,j}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ or with vectorization, $\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

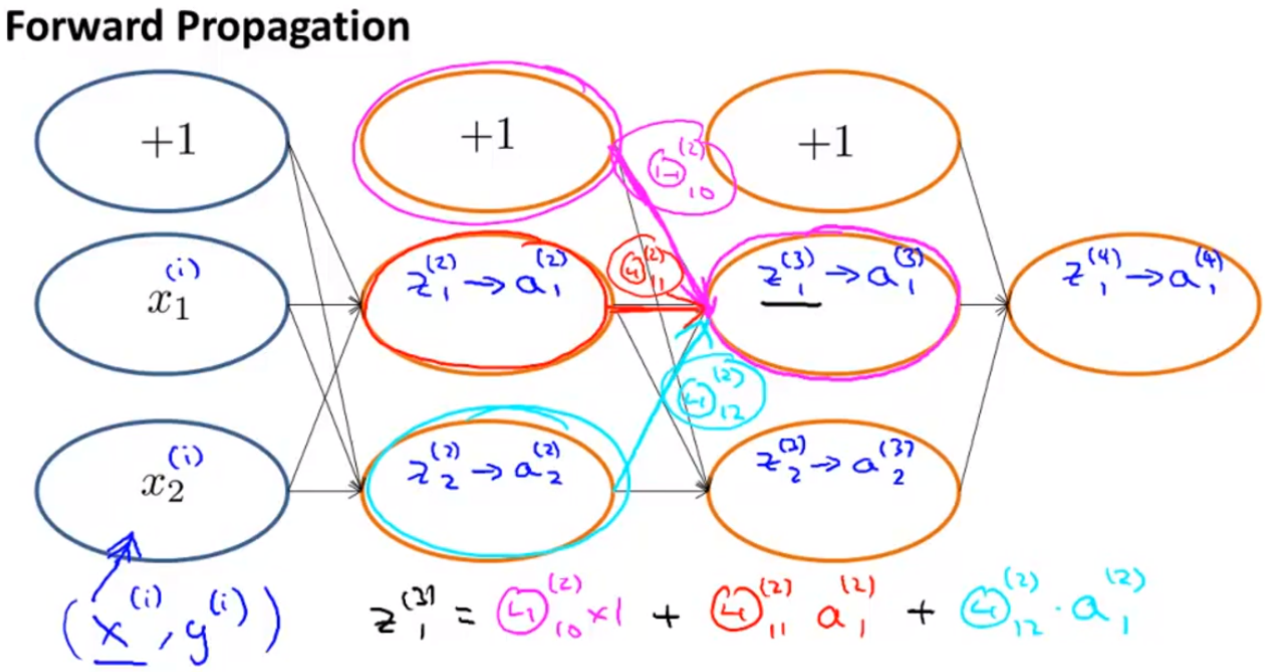
Hence we update our new Δ matrix.

- $D_{i,j}^{(l)} := \frac{1}{m} \left(\Delta_{i,j}^{(l)} + \lambda \Theta_{i,j}^{(l)} \right)$, if j≠0.
- $D_{i,j}^{(l)} := \frac{1}{m} \Delta_{i,j}^{(l)}$ If j=0

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

Backpropagation Intuition

Note: [4:39, the last term for the calculation for z_1^3 (three-color handwritten formula) should be a_2^2 instead of a_1^2. 6:08 - the equation for cost(i) is incorrect. The first term is missing parentheses for the log() function, and the second term should be $(1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$. 8:50 - $\delta^{(4)} = y - a^{(4)}$ is incorrect and should be $\delta^{(4)} = a^{(4)} - y$.]



Recall that the cost function for a neural network is:

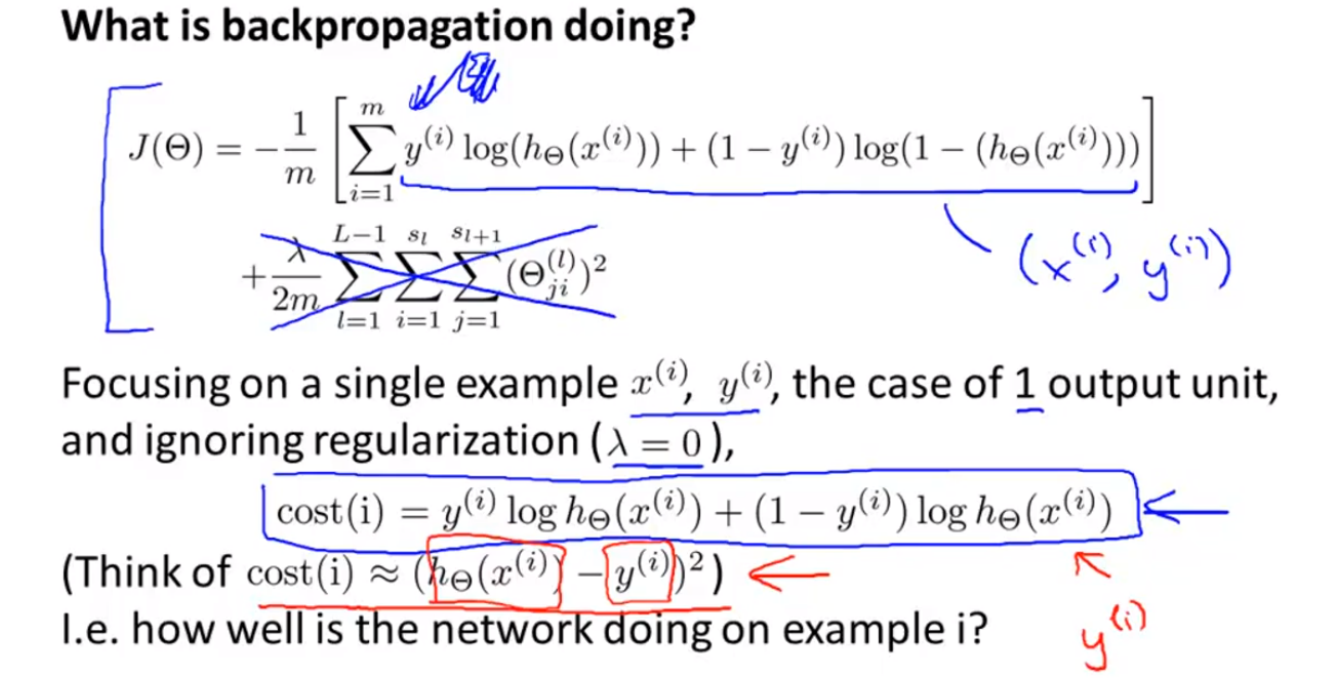
$$J(\Theta) = -\frac{1}{m}\sum_{t=1}^{m}\sum_{k=1}^{K}\left[y_k^{(t)}\ \log(h_\Theta(x^{(t)}))_k + (1-y_k^{(t)})\ \log(1-h_\Theta(x^{(t)})_k)\right] + \frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_l+1}(\Theta_{j,i}^{(l)})^2$$

If we consider simple non-multiclass classification (k = 1) and disregard regularization, the cost is computed with:

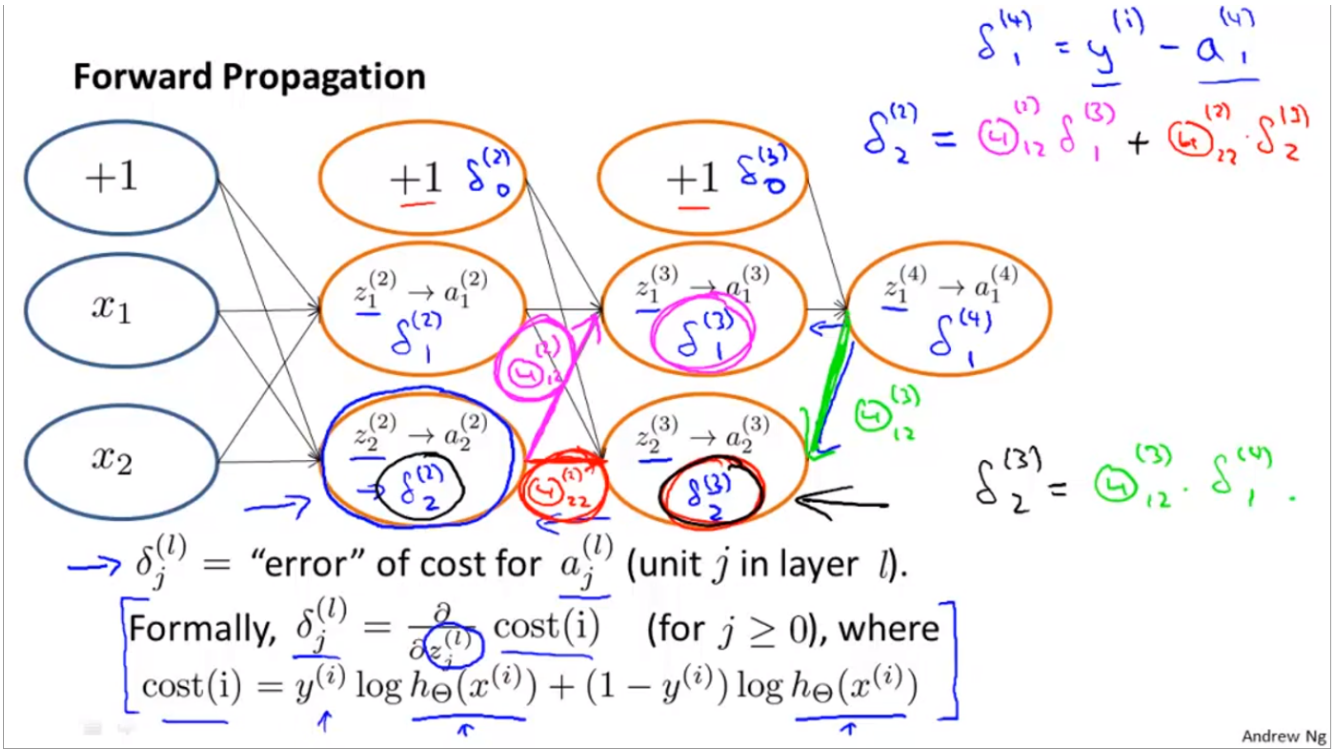
$$cost(t) = y^{(t)}\ \log(h_\Theta(x^{(t)})) + (1-y^{(t)})\ \log(1-h_\Theta(x^{(t)}))$$

Intuitively, $\delta_j^{(l)}$ is the "error" for $a_j^{(l)}$ (unit j in layer l). More formally, the delta values are actually the derivative of the cost function:

$$\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} cost(t)$$



Recall that our derivative is the slope of a line tangent to the cost function, so the steeper the slope the more incorrect we are. Let us consider the following neural network below and see how we could calculate some $\delta_j^{(l)}$:



In the image above, to calculate $\delta_2^{(2)}$, we multiply the weights $\Theta_{12}^{(2)}$ and $\Theta_{22}^{(2)}$ by their respective δ values found to the right of each edge. So we get $\delta_2^{(2)} = \Theta_{12}^{(2)} * \delta_1^{(3)} + \Theta_{22}^{(2)} * \delta_2^{(3)}$. To calculate every single possible $\delta_j^{(l)}$, we could start from the right of our diagram. We can think of our edges as our Θ_{ij}. Going from right to left, to calculate the value of $\delta_j^{(l)}$, you can just take the over all sum of each weight times the δ it is coming from. Hence, another example would be $\delta_2^{(3)} = \Theta_{12}^{(3)} * \delta_1^{(4)}$.

Implementation Note:Unrolling Parameters

With neural networks, we are working with sets of matrices:

$\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}, \dots$
$D^{(1)}, D^{(2)}, D^{(3)}, \dots$

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

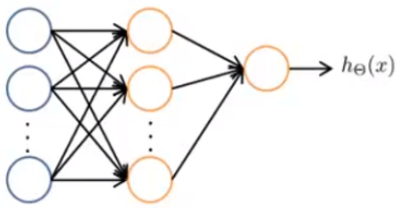
In order to use optimizing functions such as "fminunc()", we will want to "unroll" all the elements and put them into one long vector:

Example

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

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

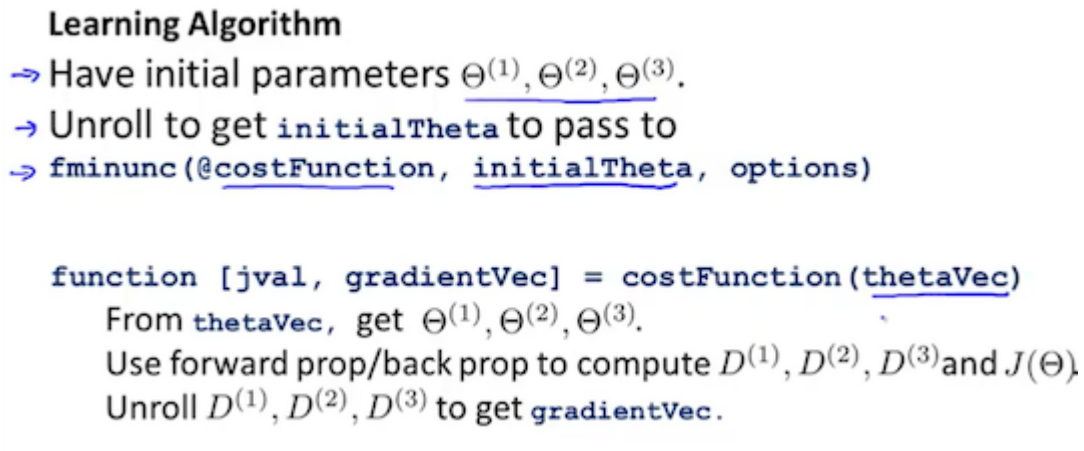
→ $D^{(1)} \in \mathbb{R}^{10\times 11}, D^{(2)} \in \mathbb{R}^{10\times 11}, D^{(3)} \in \mathbb{R}^{1\times 11}$




```
→ 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);
```

To summarize:

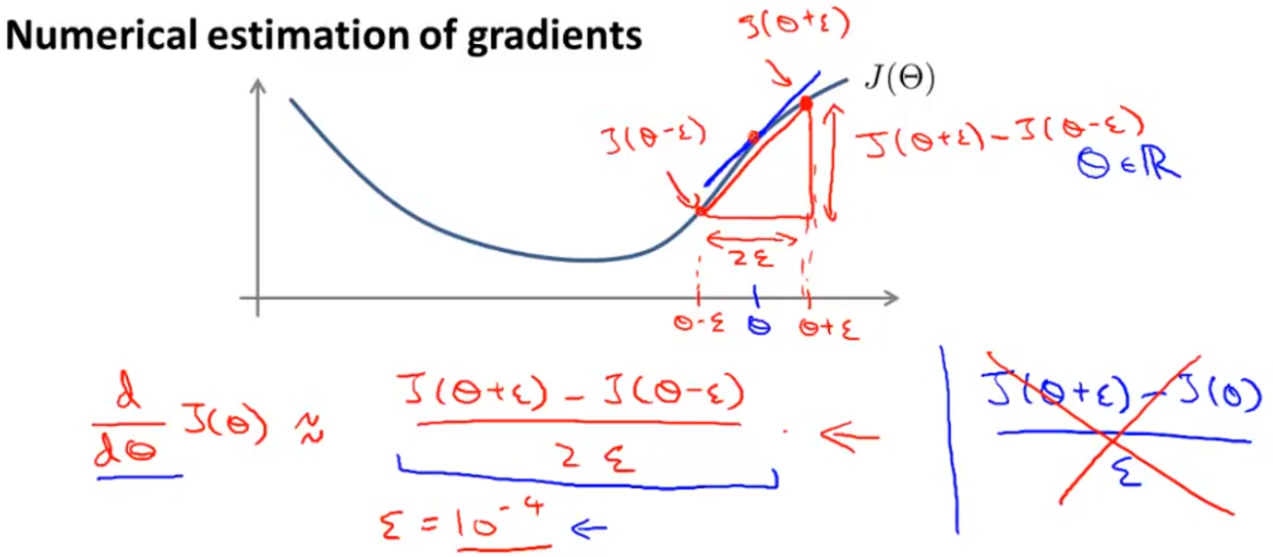


Gradient Checking

Gradient checking will assure that our backpropagation works as intended. We can approximate the derivative of our cost function with:

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

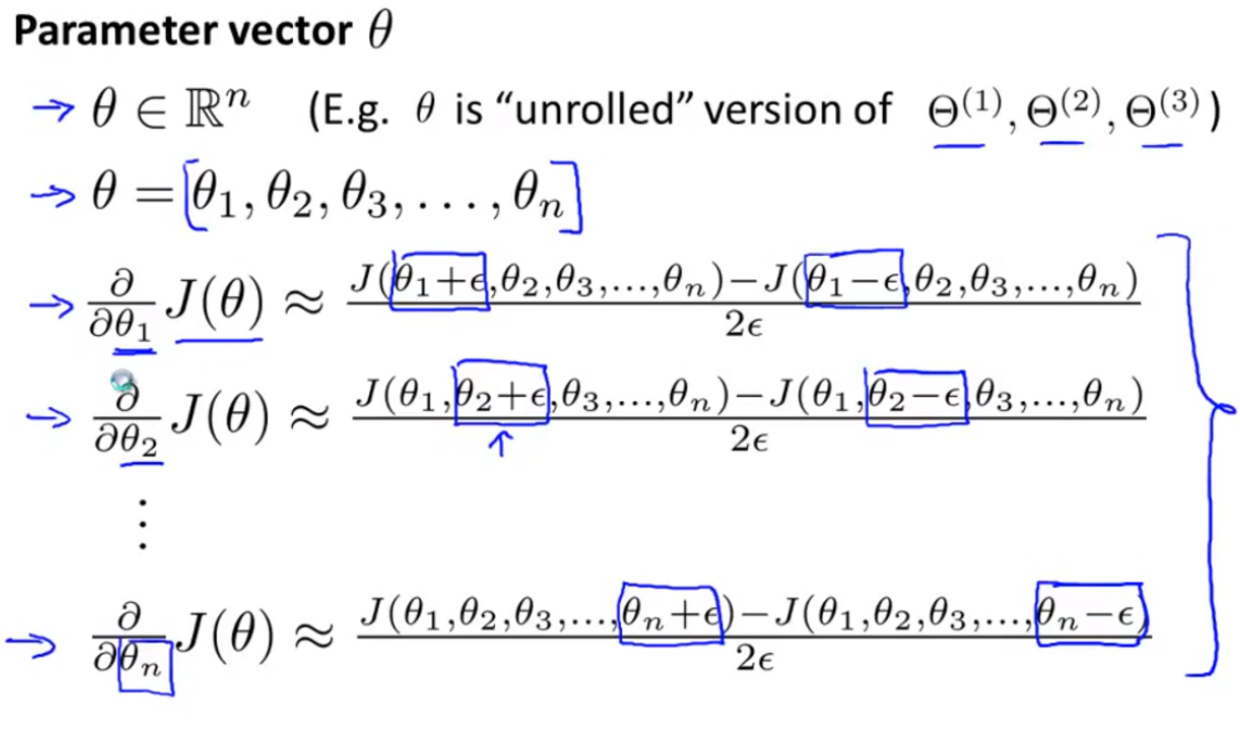
A small value for ϵ (epsilon) such as ϵ=10−4, guarantees that the math works out properly. If the value for ϵ is too small, we can end up with numerical problems.



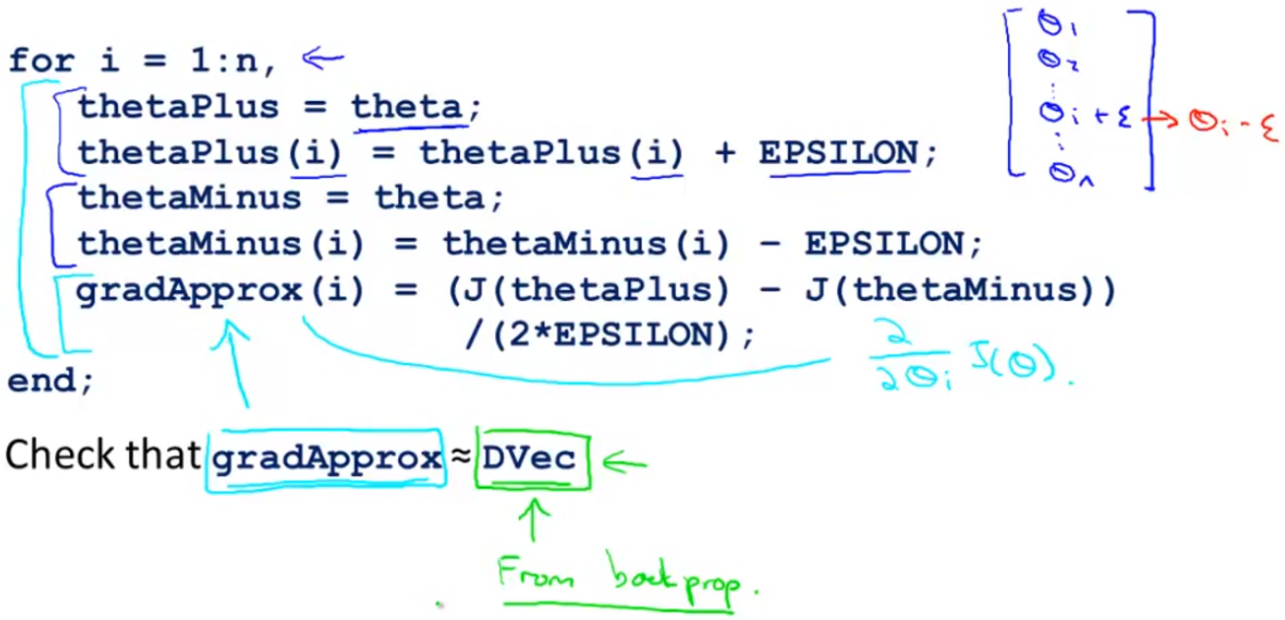
Implement: `gradApprox = (J(theta + EPSILON) - J(theta - EPSILON)) / (2*EPSILON)`

With multiple theta matrices, we can approximate the derivative **with respect to** Θ*j* as follows:

$$\frac{\partial}{\partial\Theta_j}J(\Theta) \approx \frac{J(\Theta_1,\ldots,\Theta_j+\epsilon,\ldots,\Theta_n)-J(\Theta_1,\ldots,\Theta_j-\epsilon,\ldots,\Theta_n)}{2\epsilon}$$



Hence, we are only adding or subtracting epsilon to the Θ*j* matrix. In octave we can do it as follows:



We previously saw how to calculate the deltaVector. So once we compute our gradApprox vector, we can check that gradApprox ≈ deltaVector.

Once you have verified **once** that your backpropagation algorithm is correct, you don't need to compute gradApprox again. The code to compute gradApprox can be very slow.

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.

Random 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. Instead we can randomly initialize our weights for our Θ matrices using the following method:

Initial value of Θ

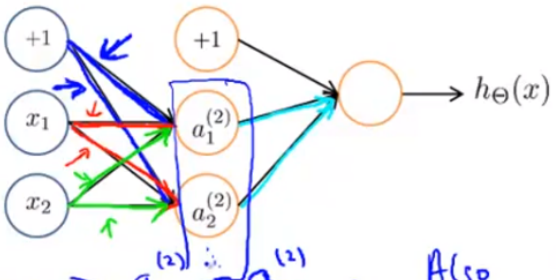
For gradient descent and advanced optimization method, need initial value for Θ.

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

Consider gradient descent

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

Zero initialization



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

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

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Hence, we initialize each $\Theta_{ij}^{(l)}$ to a random value between $[-\epsilon, \epsilon]$. Using the above formula guarantees that we get the desired bound. The same procedure applies to all the Θ's. Below is some working code you could use to experiment.

```
If the dimensions of Theta1 is 10x11, Theta2 is 10x11 and Theta3 is 1x11.

Theta1 = rand(10,11) * (2 * INIT_EPSILON) - INIT_EPSILON;
Theta2 = rand(10,11) * (2 * INIT_EPSILON) - INIT_EPSILON;
Theta3 = rand(1,11) * (2 * INIT_EPSILON) - INIT_EPSILON;

```

rand(x,y) is just a function in octave that will initialize a matrix of random real numbers between 0 and 1.

(Note: the epsilon used above is unrelated to the epsilon from Gradient Checking)

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;

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

$[-\epsilon, \epsilon]$