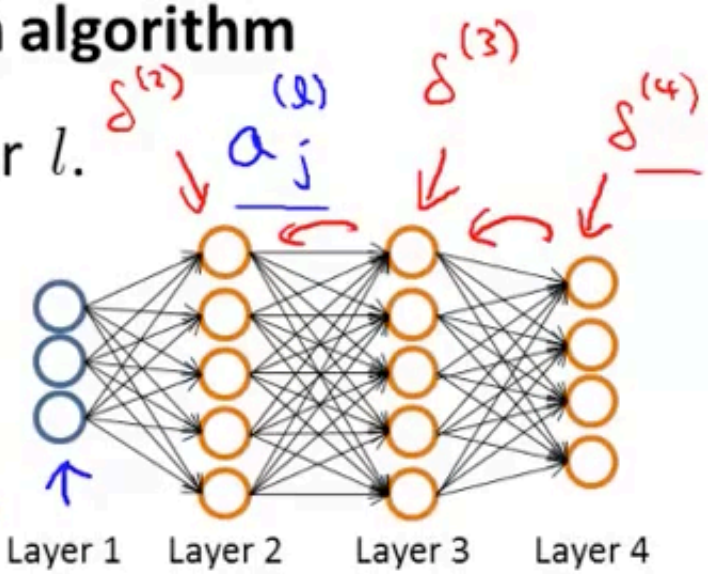
Gradient computation: Backpropagation algorithm

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



For each output unit (layer L = 4)

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

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

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

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

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

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

(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 $\Delta_{ij}^{(l)} = 0$ (for all l, i, j). (used to compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$)

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

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

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

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

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

$\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ ← i, j

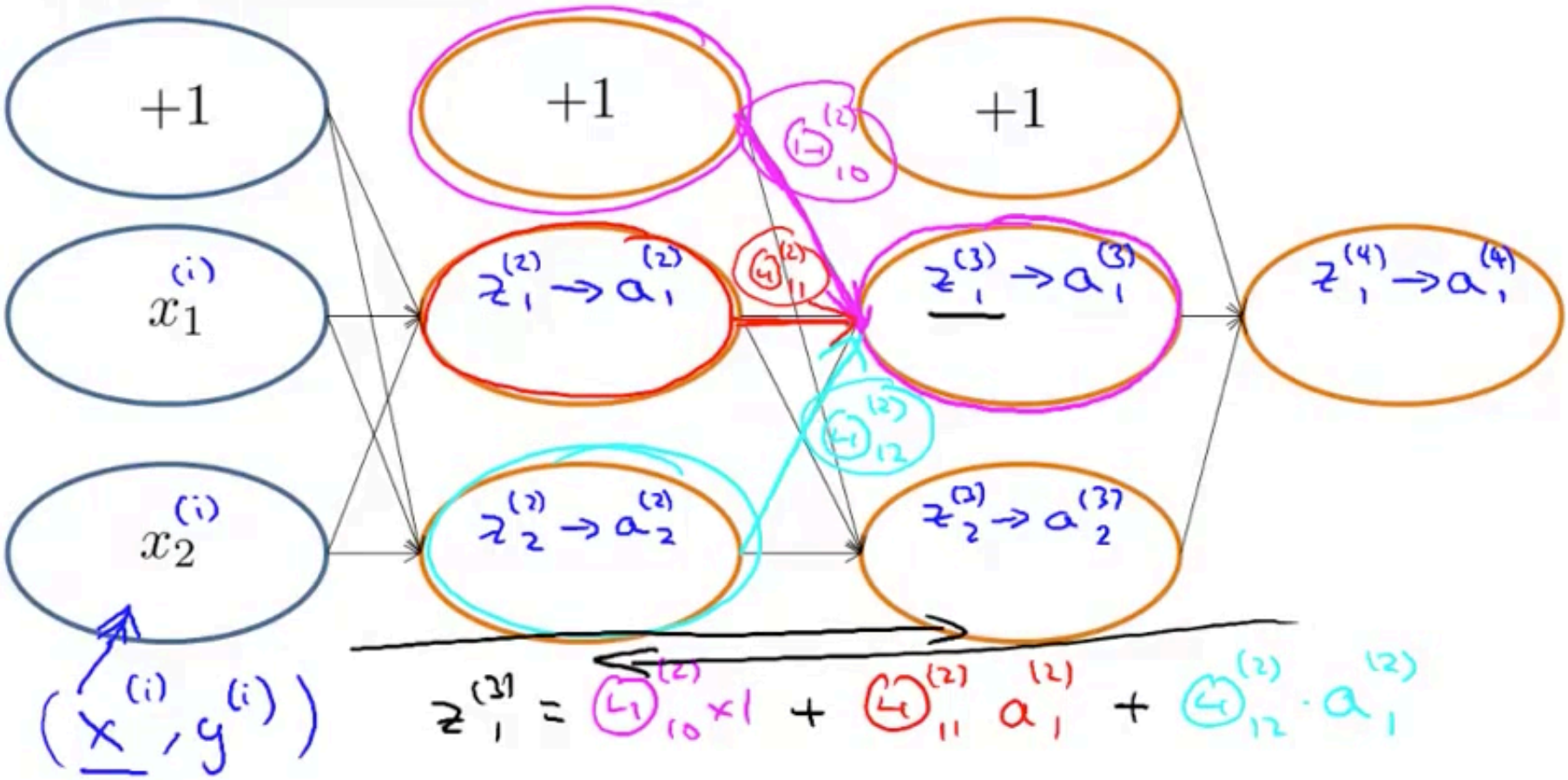
$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$.

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

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

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

Forward Propagation



What is backpropagation doing?

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

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

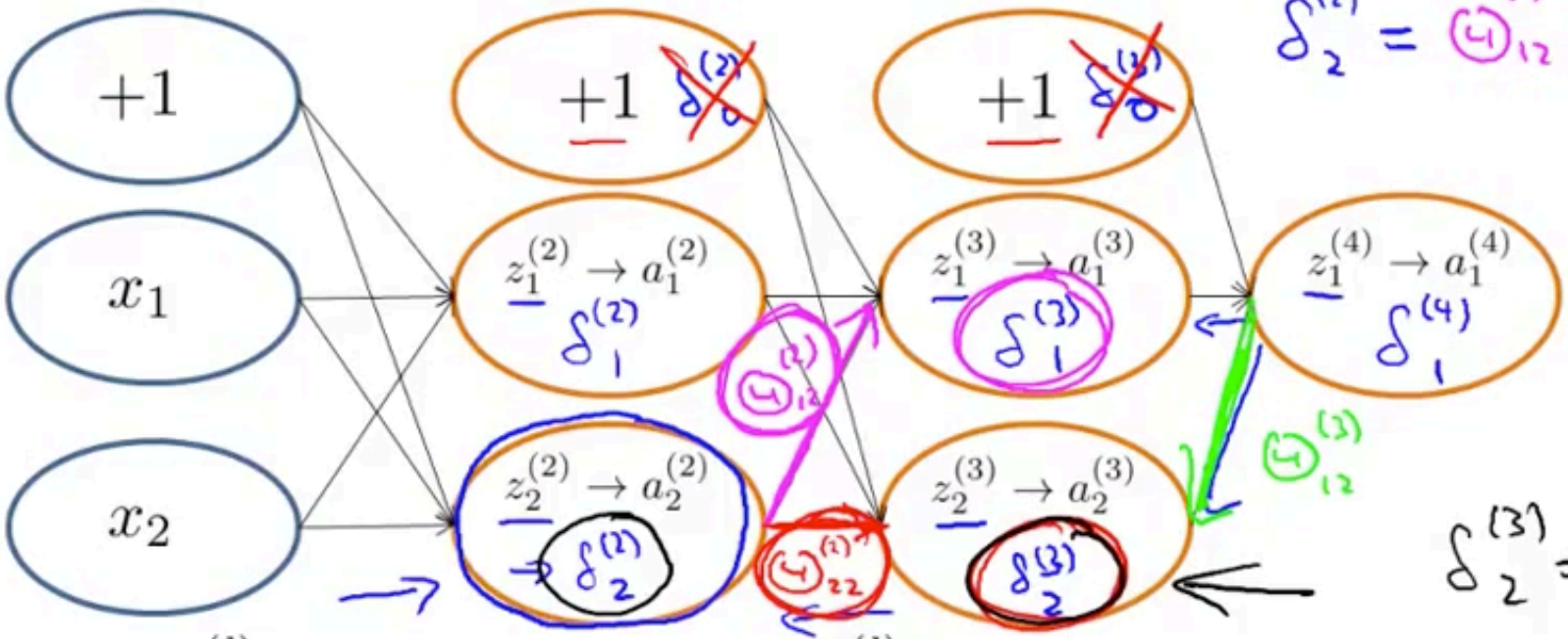
Focusing on a single example $x^{(i)}$, $y^{(i)}$, the case of 1 output unit, and ignoring regularization ($\lambda = 0$),

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

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

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

Forward Propagation



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

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

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

$\delta_j^{(l)}$ = "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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Advanced optimization

```
function [jVal, gradient] = costFunction(theta)
  ...
```

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

```
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`)

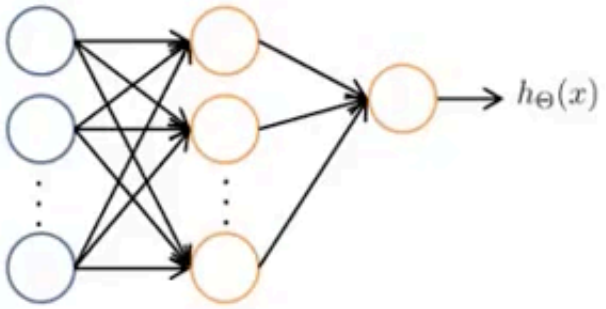
"Unroll" into vectors

Example

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

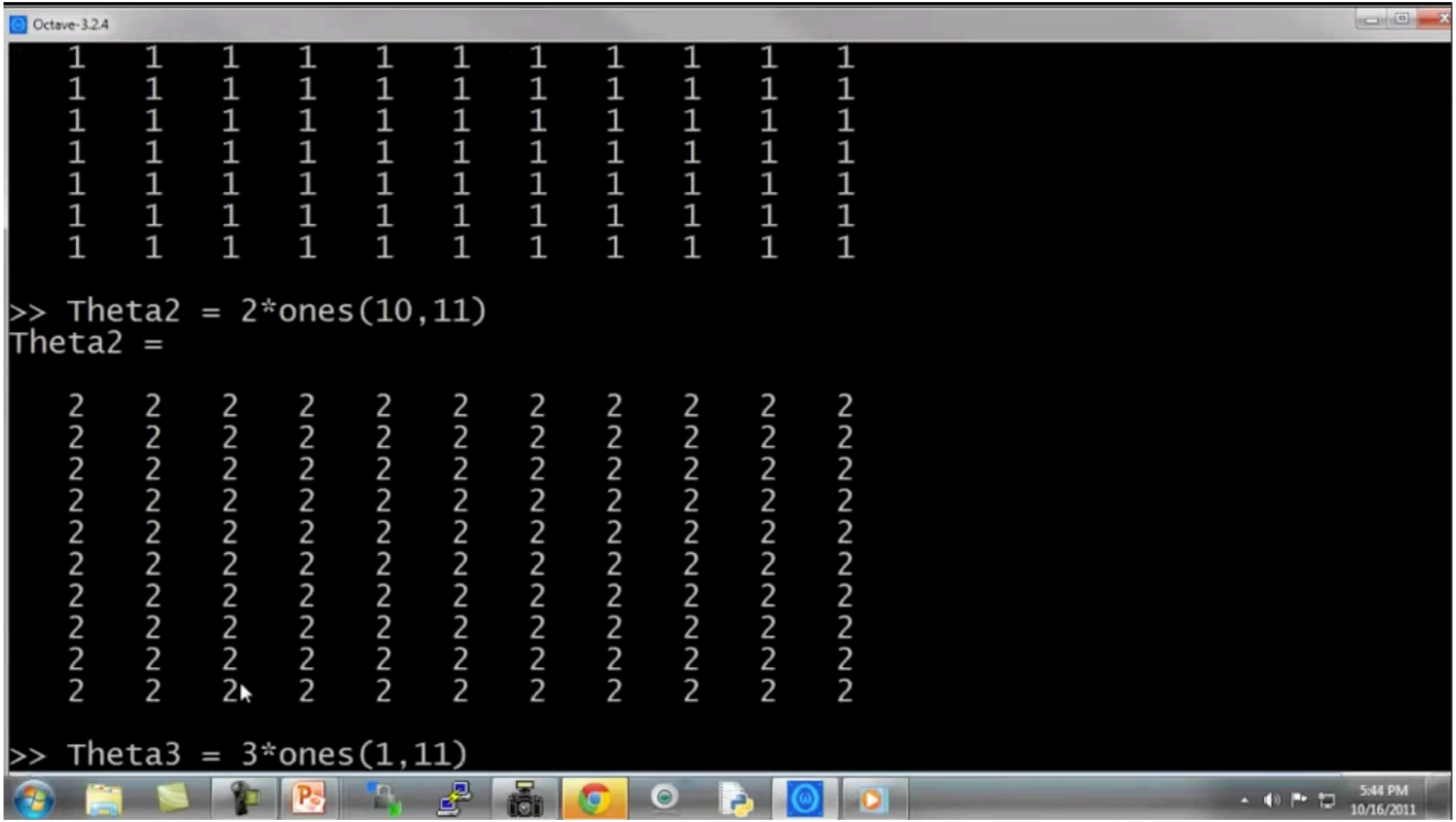
$\Theta^{(1)} \in \mathbb{R}^{10\times 11}, \Theta^{(2)} \in \mathbb{R}^{10\times 11}, \Theta^{(3)} \in \mathbb{R}^{1\times 11}$

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




```
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);
```


Octave-3.2.4
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1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
>> Theta2 = 2*ones(10,11)
Theta2 =
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
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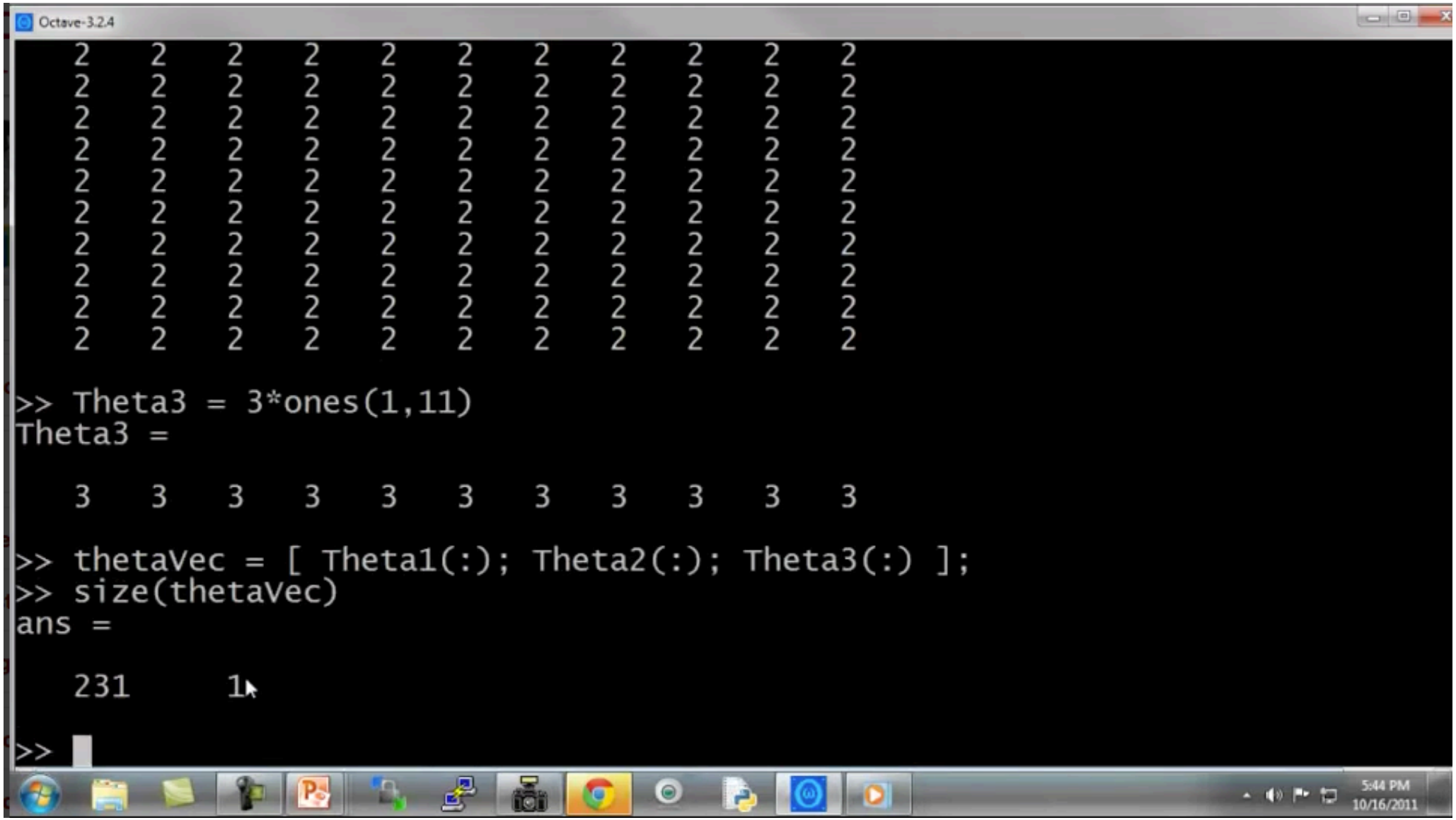
2 2 2 2 2 2 2 2 2 2 2
>> Theta3 = 3*ones(1,11)
5:44 PM
10/16/2011


Octave-3.2.4
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2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
>> Theta3 = 3*ones(1,11)
Theta3 =
3 3 3 3 3 3 3 3 3 3 3
>> thetaVec = [Theta1(:); Theta2(:); Theta3(:)];
>> size(thetaVec)
ans =
231 1
>>
5:44 PM
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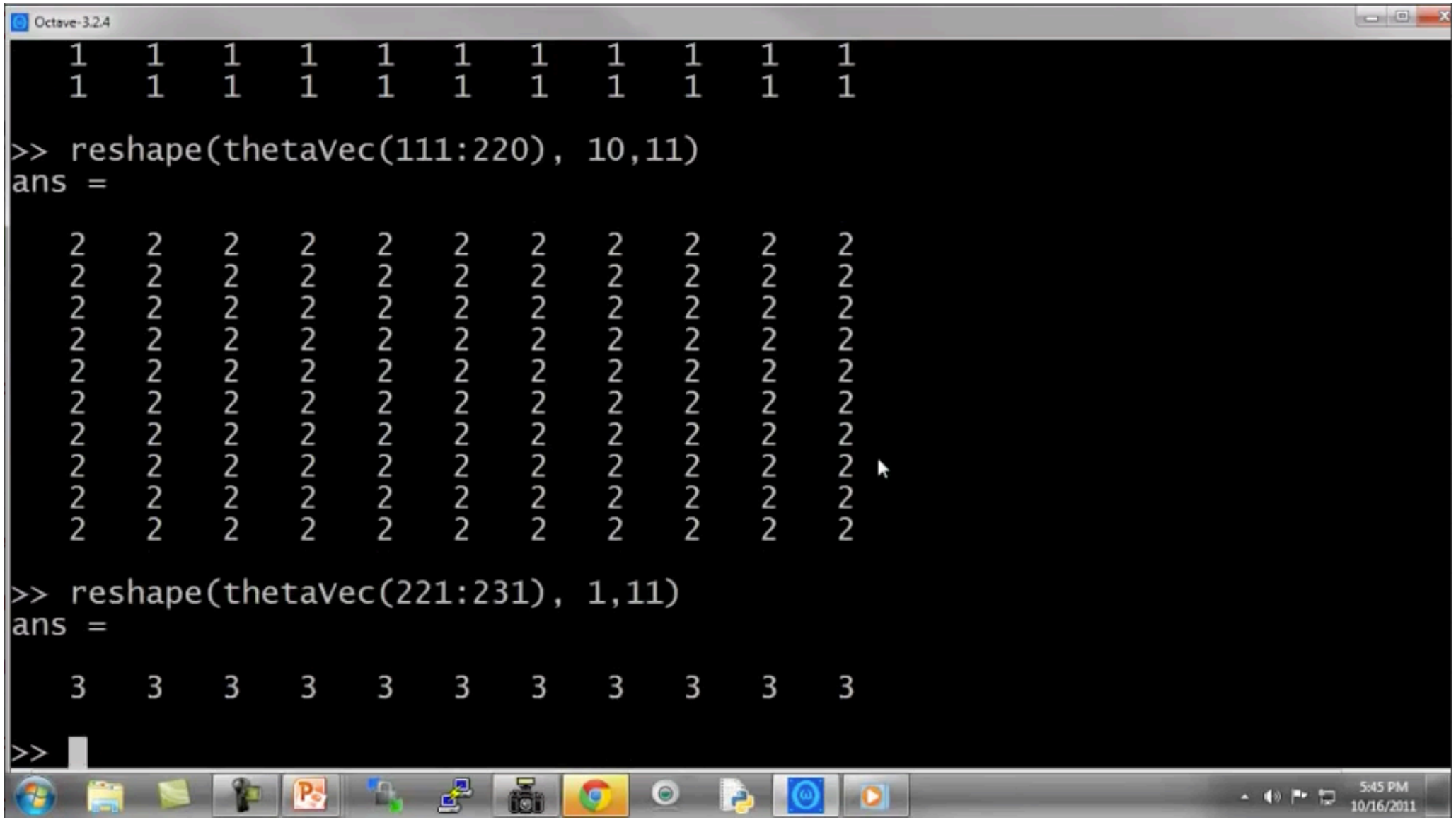
Octave-3.2.4
1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
>> reshape(thetaVec(111:220), 10,11)
ans =
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
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2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2
>> reshape(thetaVec(221:231), 1,11)
ans =
3 3 3 3 3 3 3 3 3 3 3
>>
5:45 PM
10/16/2011

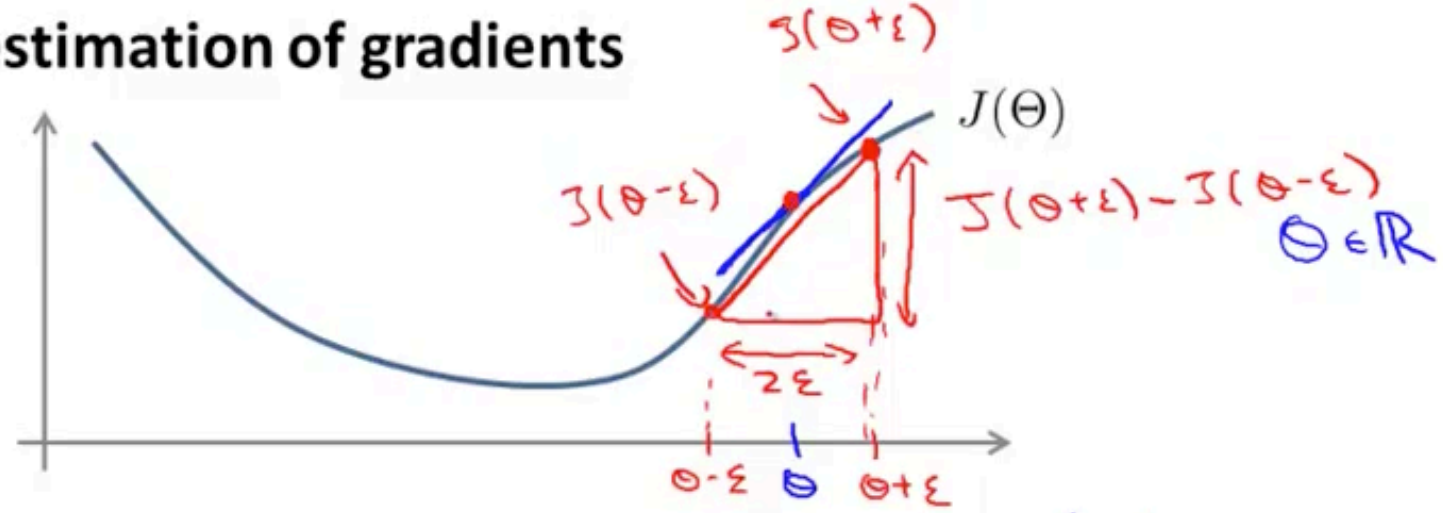
Learning Algorithm

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

Numerical estimation of gradients



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

$\varepsilon = 10^{-4}$

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

ε

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 $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$)
- $\theta = [\theta_1, \theta_2, \theta_3, \ldots, \theta_n]$
- $\frac{\partial}{\partial \theta_1} J(\theta) \approx \frac{J(\theta_1+\epsilon, \theta_2, \theta_3, \ldots, \theta_n) - J(\theta_1-\epsilon, \theta_2, \theta_3, \ldots, \theta_n)}{2\epsilon}$
- $\frac{\partial}{\partial \theta_2} J(\theta) \approx \frac{J(\theta_1, \theta_2+\epsilon, \theta_3, \ldots, \theta_n) - J(\theta_1, \theta_2-\epsilon, \theta_3, \ldots, \theta_n)}{2\epsilon}$

$\vdots$

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

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```
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;
```

$\theta = [\theta_1, \theta_2, \ldots, \theta_i + \varepsilon \rightarrow \theta_i - \varepsilon, \ldots, \theta_n]$

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

Check that `gradApprox` $\approx$ `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

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.

Initial value of Θ

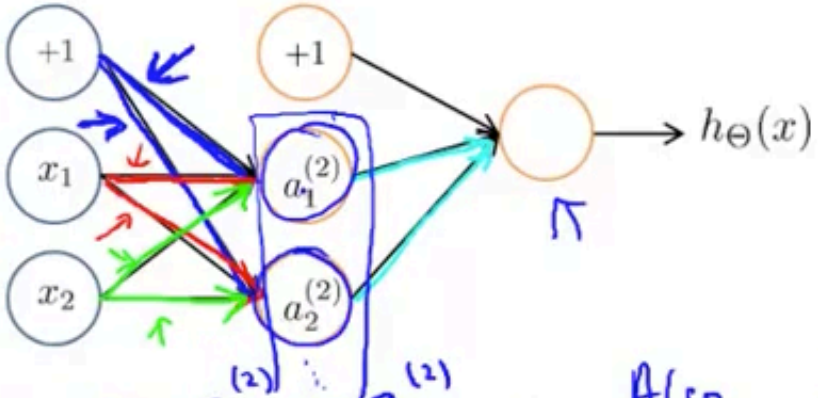
For gradient descent and advanced optimization method, need initial value for Θ.

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

Consider gradient descent

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

Zero initialization



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

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

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

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)

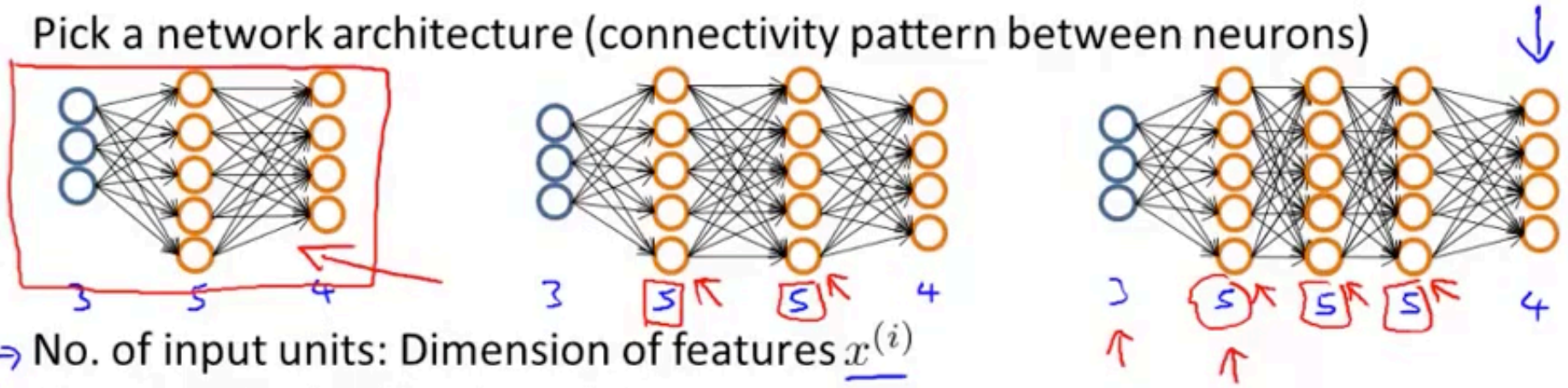
→
```
Theta1 = rand(10,11)*(2*INIT_EPSILON)
         - INIT_EPSILON;
```

$[-\epsilon, \epsilon]$

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

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)

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

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

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

```
for i = 1:m {
```

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

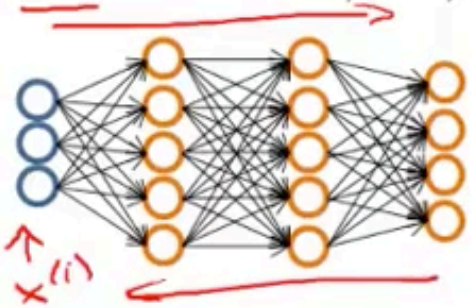
- Perform forward propagation and backpropagation using example $(x^{(i)}, y^{(i)})$
  (Get activations $a^{(l)}$ and delta terms $\delta^{(l)}$ for $l = 2, \ldots, L$).

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

...

}

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



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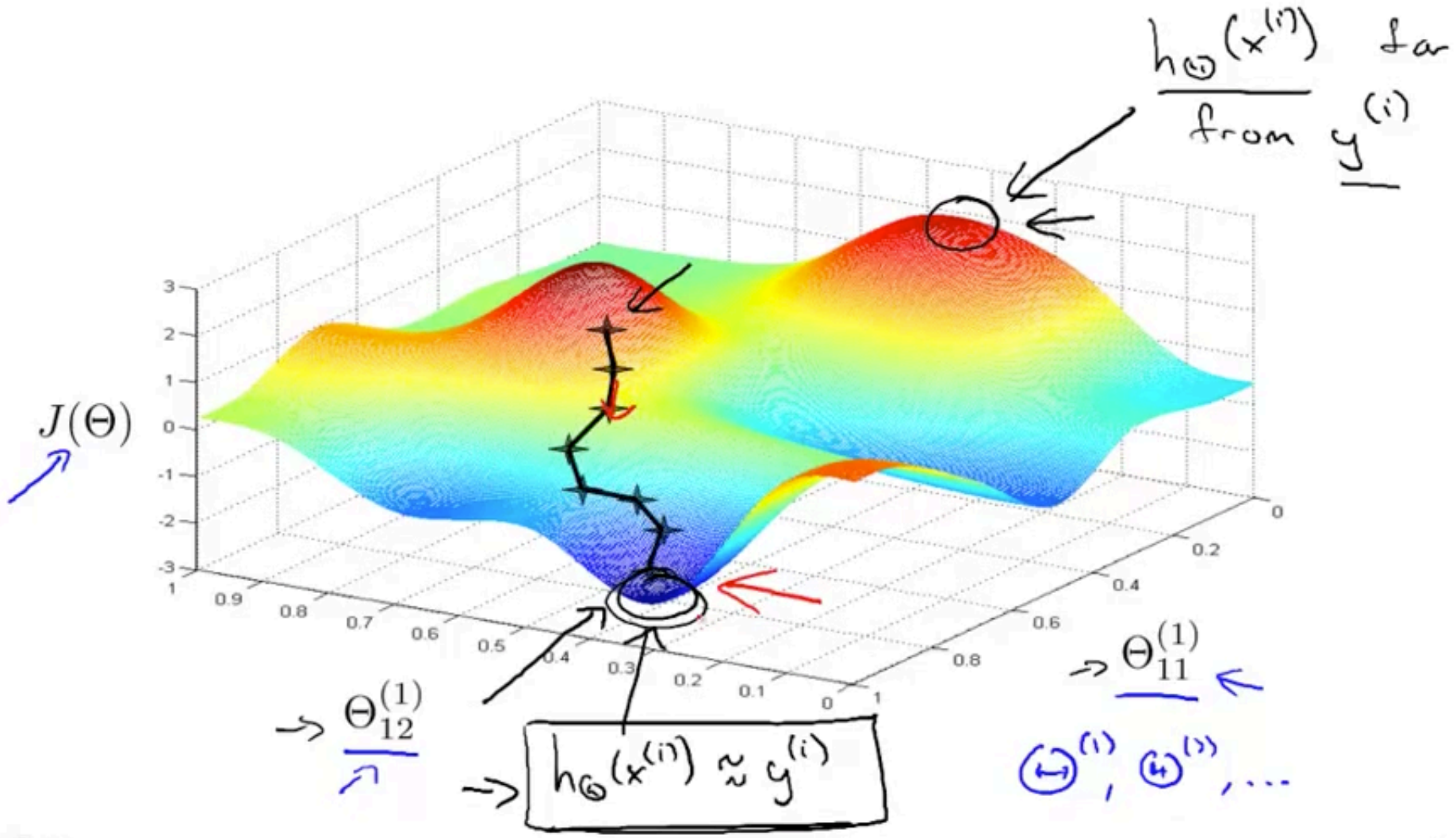
Training a neural network

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

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

$J(\Theta)$

$J(\Theta)$ — non-convex.


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