Neural Networks: Cost Function

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Classification

L = total no. of layers in network

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

Binary classification	Multi-class classification (K classes)
$y = 0 \ or \ 1$	$y \in \mathbb{R}^K$
1 output unit	K output units

Cost function

Logitic regression:

$$J(\Theta) = -rac{1}{m}[\sum_{i=1}^{m}(y^{(i)}log(h_{\Theta}(x^{(i)})) + (1-y^{(i)})log(1-h_{\Theta}(x^{(i)})))] + rac{\lambda}{2m}\sum_{j=1}^{n}\Theta_{j}^{2}$$

Neural network:

$$egin{aligned} h_{\Theta}(x) &\in \mathbb{R}^K \;, (h_{\Theta}(x))_i = i^{th}output \ J(\Theta) &= -rac{1}{m}[\sum_{i=1}^m \sum_{k=1}^K (y_k^{(i)}log(h_{\Theta}(x^{(i)}))_k + (1-y_k^{(i)})log(1-h_{\Theta}(x^{(i)})_k))] + rac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (\Theta_{ji}^{(l)})^2 \end{aligned}$$

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 to compute:

$$J(\Theta) \over rac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$$

Backpropagation algorithm

$$\begin{split} \frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = & \frac{\partial J(\Theta)}{\partial a_i^{l+1}} * \frac{\partial a_i^{l+1}}{\partial \Theta_{ij}^{(l)}} \\ = & \frac{\partial J(\Theta)}{\partial a_i^{l+1}} * \frac{\partial a_i^{l+1}}{\partial z_i^{l+1}} * \frac{\partial z_i^{l+1}}{\partial \Theta_{ij}^{(l)}} \end{split}$$

$$\begin{split} \frac{\partial z_i^{l+1}}{\partial \Theta_{ij}^{(l)}} &= w_i = a_j^l \\ \frac{\partial a_i^{l+1}}{\partial z_i^{l+1}} &= \frac{\partial g(z_i^{l+1})}{\partial z_i^{l+1}} = g(z_i^{l+1})(1 - g(z_i^{l+1})) = a_i^{l+1}(1 - a_i^{l+1}) \\ \frac{\partial J(\Theta)}{\partial a_i^{l+1}} &= \sum_j \frac{\partial J(\Theta)}{\partial a_j^{l+2}} * \frac{\partial a_j^{l+2}}{\partial a_i^{l+1}} \\ &= \sum_j \frac{\partial J(\Theta)}{\partial a_j^{l+2}} * \frac{\partial a_j^{l+2}}{\partial z_j^{l+2}} * \frac{\partial z_j^{l+2}}{\partial a_i^{l+1}} \end{split}$$

$$rac{\partial z_{j}^{l+2}}{\partial a_{i}^{l+1}}=\Theta_{ji}^{(l+1)}$$

If we have got $\frac{\partial J(\Theta)}{\partial a_j^{l+2}}$, we can calculate $\frac{\partial J(\Theta)}{\partial a_j^{l+1}}$, and next $\frac{\partial J(\Theta)}{\partial a_j^{l}}$, and so on.

Backpropagation intuition

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

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

$$cost(i) = y^{(i)}log(h_{\Theta}(x^{(i)})) + (1-y^{(i)})log(1-h_{\Theta}(x^{(i)}))$$
 or $cost(i) pprox (h_{\Theta}(x^{(i)}) - y^{(i)})^2$

 $\delta_j^{(l)}=$ "error" of cost for $a_j^{(l)}$ (unit j in layer l). However, **in my opinion**, it's "error" of cost $z_j^{(l)}$ from a view of calculus.

$$\begin{split} \delta_j^{(l)} &= \frac{\partial J(\Theta)}{\partial a_i^l} * \frac{\partial a_j^l}{\partial z_j^l} = \frac{\partial J(\Theta)}{\partial a_i^l} * a_i^l * (1 - a_i^l), \text{ so we have } \frac{\partial J(\Theta)}{\partial a_i^l} = \sum_j \frac{\partial J(\Theta)}{\partial a_j^{l+1}} * \frac{\partial a_j^{l+1}}{\partial z_j^{l+1}} * \frac{\partial z_j^{l+1}}{\partial a_i^l} = \sum_j \Theta_{ji}^{(l)} * \delta_j^{(l+1)} = \left[\Theta_{ji}^{(l)}\right]^T * \delta_j^{(l+1)} \end{split}$$

For example,

$$egin{aligned} \delta_1^{(4)} &= a_1^{(4)} - y^{(i)} \ \delta_2^{(3)} &= \Theta_{12}^{(3)} * \delta_1^{(4)} \ \delta_2^{(2)} &= \Theta_{12}^{(2)} * \delta_1^{(3)} + \Theta_{22}^{(2)} * \delta_2^{(3)} \end{aligned}$$

Implementation note: Unrolling parameters

Advanced optimization

Example

```
s_1=10, s_2=10, s_3=1 \Theta^{(1)}\in\mathbb{R}^{10\cdot11}, \Theta^{(2)}\in\mathbb{R}^{10\cdot11}, \Theta^{(3)}\in\mathbb{R}^{1\cdot11} D^{(1)}\in\mathbb{R}^{10\cdot11}, D^{(2)}\in\mathbb{R}^{10\cdot11}, D^{(3)}\in\mathbb{R}^{1\cdot11} 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

- 1. Have initial parameters $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$;
- 2. Unroll to get initial Theta to pass to $fminunc (@costFunction,\ initial Theta,\ options)$:
- 3. function [jval, gradientVec] = costFunction(thetaVec);
 - 3.1 From thetaVec, get $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$;
 - 3.2 Use forward prop/back prop to compute $D^{(1)}, D^{(2)}, D^{(3)}$ and $J(\Theta)$;
 - 3.3 Unroll $D^{(1)}, D^{(2)}, D^{(3)}$ to get gradientVec.

Gradient checking

```
Implement: gradApprox = \frac{J(\theta+\epsilon)-J(\theta-\epsilon)}{2\epsilon} Check that gradApprox \approx DVec
```

Implement Node:

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

Random initialization

Symmetry breaking

```
Initialize each \Theta_{ij}^{(l)} to a random value [-\epsilon,\ \epsilon]. Theta1 = rand(10, 11) * (2 * INIT_EPSILON) - EPSILON;
```

Putting it together

Training a neural network

Pick a network architecture.

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

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

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