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

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

Backpropagation algorithm

Gradient computation

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

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

Backpropagation algorithm

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

$\frac{\partial z_i^{l+1}}{\partial\Theta_{ij}^{(l)}} = w_i = a_j^l$

$\frac{\partial a_i^{l+1}}{\partial z_i^{l+1}} = \frac{\partial g(z_i^{l+1})}{\partial z_i^{l+1}} = g(z_i^{l+1})(1-g(z_i^{l+1})) = a_i^{l+1}(1-a_i^{l+1})$

$$\begin{aligned}\frac{\partial J(\Theta)}{\partial a_i^{l+1}} &= \sum_j \frac{\partial J(\Theta)}{\partial a_j^{l+2}} * \frac{\partial a_j^{l+2}}{\partial a_i^{l+1}} \\ &= \sum_j \frac{\partial J(\Theta)}{\partial a_j^{l+2}} * \frac{\partial a_j^{l+2}}{\partial z_j^{l+2}} * \frac{\partial z_j^{l+2}}{\partial a_i^{l+1}}\end{aligned}$$

$\frac{\partial z_j^{l+2}}{\partial a_i^{l+1}} = \Theta_{ji}^{(l+1)}$
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.

Pseudo code:

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

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

For $i = 1\ to\ m$

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

  Perform forward propagation to compare $a^{(l)}$ for $l = 2, 3, ..., L$

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

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

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

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

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

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

Backpropagation intuition

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

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

$\delta_j^{(l)}$ = "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.

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

$\delta_j^L = \frac{\partial J(\Theta)}{\partial a_j^L} * \frac{\partial a_j^L}{\partial z_j^L}$

$\frac{\partial J(\Theta)}{\partial a_j^L} = \frac{1-y_j}{1-a_j^L} - \frac{y_j}{a_j^L}$

So, $\delta_j^L = (\frac{1-y_j}{1-a_j^L} - \frac{y_j}{a_j^L}) * (a_j^L(1 - a_j^L)) = a_j^L - y_j$

For example,

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

Implementation note: Unrolling parameters

Advanced optimization

Example

$s_1 = 10, s_2 = 10, s_3 = 1$
$\Theta^{(1)} \in \mathbb{R}^{10 \cdot 11}, \Theta^{(2)} \in \mathbb{R}^{10 \cdot 11}, \Theta^{(3)} \in \mathbb{R}^{1 \cdot 11}$
$D^{(1)} \in \mathbb{R}^{10 \cdot 11}, D^{(2)} \in \mathbb{R}^{10 \cdot 11}, D^{(3)} \in \mathbb{R}^{1 \cdot 11}$

```
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

1. Have initial parameters $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$;
2. Unroll to get $initialTheta$ to pass to $fminunc(@costFunction,\ initialTheta,\ options)$;
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 $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$;

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