Coursera Machine Learning Notes

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Chapter 1

Neural Networks

1.1 Notations

- $a_k^{(i)}$: activation energy at layer i of element k.
- $a^{(L)}$: the activation energy of the last layer, i.e. the values in the output layer.
- $\Theta_{ij}^{(l)}$: the weight between the element i in layer l+1 and the element j in layer l.
- y (or Y): target output(s).
- \hat{y} (or \hat{Y}): derived output(s), equivalent to $a^{(L)}$.

1.2 Backward Propagation Derivation/Proof

As seen in the previous chapters, after deriving $J(\Theta)$, i.e.

$$J(\Theta) = \frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} \left[-y_k^{(i)} \log \left((h_{\theta}(x^{(i)}))_k \right) - (1 - y_k^{(i)}) \log \left(1 - (h_{\theta}(x^{(i)}))_k \right) \right],$$

or

$$J(\Theta) = \frac{1}{m} * \mathcal{S}(-Y . * \log(\hat{Y}) - (1 - Y) . * \log(1 - \hat{Y})),$$

where \mathscr{S} refers to the sum of all the elements in the matrix, and .* refers to element-wise multiplication. The next challenge is, as with previous chapters, to find out what represents

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

For the sake of illustration, we are ignoring the regularization terms and dimension incompatibility.

Now the following is where the magic begins. It turns out that

$$\begin{split} \Delta^{(l)} := \frac{\partial J}{\partial \Theta^{(l)}} &= \frac{\partial z^{(l)}}{\partial \Theta^{(l)}} \frac{\partial J}{\partial z^{(l)}} \\ &= \frac{\partial \left(\Theta^{(l)} * a^{(l-1)}\right)}{\partial \Theta^{(l)}} \delta^{(l)} \\ &= a^{(l-1)} \delta^{(l)}, \end{split}$$

where

$$\begin{split} \delta^{(l)} &:= \frac{\partial J}{\partial z^{(l)}} = \frac{\partial z^{(l+1)}}{\partial z^{(l)}} \frac{\partial J}{\partial z^{(l+1)}} \\ &= \frac{\partial \left(\Theta^{(l+1)} * g(z^{(l)})\right)}{\partial z^{(l)}} \delta^{(l+1)} \\ &= \delta^{(l+1)} \Theta^{(l+1)} g'(z^{(l)}) \end{split}$$

and

$$\delta^{(L)} = \frac{\partial J}{\partial z^{(L)}}$$
$$= \frac{\partial \hat{y}}{\partial z^{(L)}} \frac{\partial J}{\partial \hat{y}},$$

so we need to figure out the value of the two fractions to obtain the "terminating value" of the δs . On the other hand, we can also derive this by figuring out

$$\delta_k^{(L)} = \frac{\partial \hat{y}_k}{\partial z_k^{(L)}} \frac{\partial J}{\partial \hat{y}_k} \tag{1.1}$$

and line them up to return to vector form, $\delta^{(L)}$. For the sake of clarity of proof, we will use equation (1.1).

Let's tackle the first fraction. Since $\hat{y}_k = \sigma(z_k^{(L)})$, and

$$\sigma'(z) = (-1)(1 + e^{-z})^{-2} \frac{\partial (1 + e^{-z})}{\partial z}$$

$$= \frac{1}{1 + e^{-z}} \cdot \frac{1 + e^{-z} - 1}{1 + e^{-z}}$$

$$= \sigma(z)(1 - \sigma(z)),$$

we can derive that

$$\frac{\partial \hat{y}_k}{\partial z_k^{(L)}} = \hat{y}_k (1 - \hat{y}_k). \tag{1.2}$$

Now let's tackle the second fraction. From the provided $J(\Theta)$, we look at the k-th output, and calculate the derivative of the loss with respect to its activation energy: (In the following equation, y_k is abbreviated to \hat{y} for clarity)

$$\begin{split} \frac{\partial J}{\partial \hat{y}} &= -\frac{y}{\hat{y}} + \frac{1-y}{1-\hat{y}} \\ &= \frac{\hat{y}(1-y) - (1-\hat{y})y}{\hat{y}(1-\hat{y})} \\ &= \frac{\hat{y} - y}{\hat{y}(1-\hat{y})}. \end{split}$$

i.e.

$$\frac{\partial J}{\partial \hat{y}_k} = \frac{\hat{y}_k - y_k}{\hat{y}_k (1 - \hat{y}_k)} \tag{1.3}$$

Substituting equations (1.2) and (1.3) into (1.1), and convert into vectorized form, we can get that

$$\delta^{(L)} = \hat{y} - y.$$