Feedforward Neural Networks in Depth, Part 3: Cost Functions

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This post is the last of a three-part series in which we set out to derive the mathematics behind feedforward neural networks. In short, we covered forward and backward propagations in the first post, and we worked on activation functions in the second post. Moreover, we have not yet addressed cost functions and the backpropagation seed $\partial J/\partial \mathbf{A}^{[L]} = \partial J/\partial \hat{\mathbf{Y}}$. It is time we do that.

Binary Classification

In binary classification, the cost function is given by

$$\begin{aligned} J &= f(\hat{\mathbf{Y}}, \mathbf{Y}) = f(\mathbf{A}^{[L]}, \mathbf{Y}) \\ &= -\frac{1}{m} \sum_i (y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)) \\ &= -\frac{1}{m} \sum_i (y_i \log(a_i^{[L]}) + (1 - y_i) \log(1 - a_i^{[L]})), \end{aligned}$$

which we can write as

$$J = -\frac{1}{m} \underbrace{\sum_{\text{axis}=1} (\mathbf{Y} \odot \log(\mathbf{A}^{[L]}) + (1 - \mathbf{Y}) \odot \log(1 - \mathbf{A}^{[L]}))}_{\text{scalar}}. \tag{1}$$

Next, we construct a computation graph:

$$\begin{aligned} u_{0,i} &= a_i^{[L]}, \\ u_{1,i} &= 1 - u_{0,i}, \\ u_{2,i} &= \log(u_{0,i}), \\ u_{3,i} &= \log(u_{1,i}), \\ u_{4,i} &= y_i u_{2,i} + (1 - y_i) u_{3,i}, \\ u_5 &= -\frac{1}{m} \sum_i u_{4,i} = J. \end{aligned}$$

Derivative computations are now as simple as they get:

$$\begin{aligned} \frac{\partial J}{\partial u_5} &= 1, \\ \frac{\partial J}{\partial u_{4,i}} &= \frac{\partial J}{\partial u_5} \frac{\partial u_5}{\partial u_{4,i}} = -\frac{1}{m}, \\ \frac{\partial J}{\partial u_{3,i}} &= \frac{\partial J}{\partial u_{4,i}} \frac{\partial u_{4,i}}{\partial u_{3,i}} = -\frac{1}{m}(1 - y_i), \\ \frac{\partial J}{\partial u_{2,i}} &= \frac{\partial J}{\partial u_{4,i}} \frac{\partial u_{4,i}}{\partial u_{2,i}} = -\frac{1}{m} y_i, \\ \frac{\partial J}{\partial u_{1,i}} &= \frac{\partial J}{\partial u_{3,i}} \frac{\partial u_{3,i}}{\partial u_{1,i}} = -\frac{1}{m}(1 - y_i) \frac{1}{u_{1,i}} = -\frac{1}{m} \frac{1 - y_i}{1 - a_i^{[L]}}, \\ \frac{\partial J}{\partial u_{0,i}} &= \frac{\partial J}{\partial u_{1,i}} \frac{\partial u_{1,i}}{\partial u_{0,i}} + \frac{\partial J}{\partial u_{2,i}} \frac{\partial u_{2,i}}{\partial u_{0,i}} \\ &= \frac{1}{m}(1 - y_i) \frac{1}{u_{1,i}} - \frac{1}{m} y_i \frac{1}{u_{0,i}} \\ &= \frac{1}{m} \Big(\frac{1 - y_i}{1 - a_i^{[L]}} - \frac{y_i}{a_i^{[L]}} \Big). \end{aligned}$$

Thus,

$$\frac{\partial J}{\partial a_i^{[L]}} = \frac{1}{m} \Big(\frac{1 - y_i}{1 - a_i^{[L]}} - \frac{y_i}{a_i^{[L]}} \Big),$$

which implies that

$$\frac{\partial J}{\partial \mathbf{A}^{[L]}} = \frac{1}{m} \Big(\frac{1}{1 - \mathbf{A}^{[L]}} \odot (1 - \mathbf{Y}) - \frac{1}{\mathbf{A}^{[L]}} \odot \mathbf{Y} \Big). \tag{2}$$

In addition, since the sigmoid activation function is used in the output layer, we get

$$\begin{aligned} \frac{\partial J}{\partial z_i^{[L]}} &= \frac{\partial J}{\partial a_i^{[L]}} a_i^{[L]} (1 - a_i^{[L]}) \\ &= \frac{1}{m} \Big(\frac{1 - y_i}{1 - a_i^{[L]}} - \frac{y_i}{a_i^{[L]}} \Big) a_i^{[L]} (1 - a_i^{[L]}) \\ &= \frac{1}{m} ((1 - y_i) a_i^{[L]} - y_i (1 - a_i^{[L]})) \\ &= \frac{1}{m} (a_i^{[L]} - y_i). \end{aligned}$$

In other words,

$$\frac{\partial J}{\partial \mathbf{Z}^{[L]}} = \frac{1}{m} (\mathbf{A}^{[L]} - \mathbf{Y}). \tag{3}$$

Note that both $\partial J/\partial \mathbf{Z}^{[L]} \in \mathbb{R}^{1 \times m}$ and $\partial J/\partial \mathbf{A}^{[L]} \in \mathbb{R}^{1 \times m}$, because $n^{[L]} = 1$ in this case.

Multiclass Classification

In multiclass classification, the cost function is instead given by

$$\begin{aligned} J &= f(\hat{\mathbf{Y}}, \mathbf{Y}) = f(\mathbf{A}^{[L]}, \mathbf{Y}) \\ &= -\frac{1}{m} \sum_i \sum_j y_{j,i} \log(\hat{y}_{j,i}) \\ &= -\frac{1}{m} \sum_i \sum_j y_{j,i} \log(a_{j,i}^{[L]}), \end{aligned}$$

where $j = 1, \dots, n^{[L]}$.

We can vectorize the cost expression:

$$J = -\frac{1}{m} \underbrace{\sum_{\substack{\text{axis}=0 \\ \text{axis}=1}} \mathbf{Y} \odot \log(\mathbf{A}^{[L]})}_{\text{scalar}}. \tag{4}$$

Next, let us introduce intermediate variables:

$$\begin{aligned} u_{0,j,i} &= a_{j,i}^{[L]}, \\ u_{1,j,i} &= \log(u_{0,j,i}), \\ u_{2,j,i} &= y_{j,i} u_{1,j,i}, \\ u_{3,i} &= \sum_j u_{2,j,i}, \\ u_4 &= -\frac{1}{m} \sum_i u_{3,i} = J. \end{aligned}$$

With the computation graph in place, we can perform backward propagation:

$$\begin{aligned} \frac{\partial J}{\partial u_4} &= 1, \\ \frac{\partial J}{\partial u_{3,i}} &= \frac{\partial J}{\partial u_4} \frac{\partial u_4}{\partial u_{3,i}} = -\frac{1}{m}, \\ \frac{\partial J}{\partial u_{2,j,i}} &= \frac{\partial J}{\partial u_{3,i}} \frac{\partial u_{3,i}}{\partial u_{2,j,i}} = -\frac{1}{m}, \\ \frac{\partial J}{\partial u_{1,j,i}} &= \frac{\partial J}{\partial u_{2,j,i}} \frac{\partial u_{2,j,i}}{\partial u_{1,j,i}} = -\frac{1}{m} y_{j,i}, \\ \frac{\partial J}{\partial u_{0,j,i}} &= \frac{\partial J}{\partial u_{1,j,i}} \frac{\partial u_{1,j,i}}{\partial u_{0,j,i}} = -\frac{1}{m} y_{j,i} \frac{1}{u_{0,j,i}} = -\frac{1}{m} \frac{y_{j,i}}{a_{j,i}^{[L]}}. \end{aligned}$$

Hence,

$$\frac{\partial J}{\partial a_{j,i}^{[L]}} = -\frac{1}{m} \frac{y_{j,i}}{a_{j,i}^{[L]}}.$$

Vectorization is trivial:

$$\frac{\partial J}{\partial \mathbf{A}^{[L]}} = -\frac{1}{m} \frac{1}{\mathbf{A}^{[L]}} \odot \mathbf{Y}. \tag{5}$$

Furthermore, since the output layer uses the softmax activation function, we get

$$\begin{aligned} \frac{\partial J}{\partial z_{j,i}^{[L]}} &= a_{j,i}^{[L]} \Big(\frac{\partial J}{\partial a_{j,i}^{[L]}} - \sum_p \frac{\partial J}{\partial a_{p,i}^{[L]}} a_{p,i}^{[L]} \Big) \\ &= a_{j,i}^{[L]} \Big(-\frac{1}{m} \frac{y_{j,i}}{a_{j,i}^{[L]}} + \sum_p \frac{1}{m} \frac{y_{p,i}}{a_{p,i}^{[L]}} a_{p,i}^{[L]} \Big) \\ &= \frac{1}{m} \Big(-y_{j,i} + a_{j,i}^{[L]} \underbrace{\sum_p y_{p,i}}_{\sum \text{probabilities}=1} \Big) \\ &= \frac{1}{m} (a_{j,i}^{[L]} - y_{j,i}). \end{aligned}$$

Note that $p = 1, \dots, n^{[L]}$.

To conclude,

$$\frac{\partial J}{\partial \mathbf{Z}^{[L]}} = \frac{1}{m} (\mathbf{A}^{[L]} - \mathbf{Y}). \tag{6}$$

Multi-Label Classification

We can view multi-label classification as j binary classification problems:

$$\begin{aligned} J &= f(\hat{\mathbf{Y}}, \mathbf{Y}) = f(\mathbf{A}^{[L]}, \mathbf{Y}) \\ &= \sum_j \Big(-\frac{1}{m} \sum_i (y_{j,i} \log(\hat{y}_{j,i}) + (1 - y_{j,i}) \log(1 - \hat{y}_{j,i})) \Big) \\ &= \sum_j \Big(-\frac{1}{m} \sum_i (y_{j,i} \log(a_{j,i}^{[L]}) + (1 - y_{j,i}) \log(1 - a_{j,i}^{[L]})) \Big), \end{aligned}$$

where once again $j = 1, \dots, n^{[L]}$.

Vectorization gives

$$J = -\frac{1}{m} \underbrace{\sum_{\substack{\text{axis}=1 \\ \text{axis}=0}} (\mathbf{Y} \odot \log(\mathbf{A}^{[L]}) + (1 - \mathbf{Y}) \odot \log(1 - \mathbf{A}^{[L]}))}_{\text{scalar}}. \tag{7}$$

It is no coincidence that the following computation graph resembles the one we constructed for binary classification:

$$\begin{aligned} u_{0,j,i} &= a_{j,i}^{[L]}, \\ u_{1,j,i} &= 1 - u_{0,j,i}, \\ u_{2,j,i} &= \log(u_{0,j,i}), \\ u_{3,j,i} &= \log(u_{1,j,i}), \\ u_{4,j,i} &= y_{j,i} u_{2,j,i} + (1 - y_{j,i}) u_{3,j,i}, \\ u_{5,j} &= -\frac{1}{m} \sum_i u_{4,j,i}, \\ u_6 &= \sum_j u_{5,j} = J. \end{aligned}$$

Next, we compute the partial derivatives:

$$\begin{aligned} \frac{\partial J}{\partial u_6} &= 1, \\ \frac{\partial J}{\partial u_{5,j}} &= \frac{\partial J}{\partial u_6} \frac{\partial u_6}{\partial u_{5,j}} = 1, \\ \frac{\partial J}{\partial u_{4,j,i}} &= \frac{\partial J}{\partial u_{5,j}} \frac{\partial u_{5,j}}{\partial u_{4,j,i}} = -\frac{1}{m}, \\ \frac{\partial J}{\partial u_{3,j,i}} &= \frac{\partial J}{\partial u_{4,j,i}} \frac{\partial u_{4,j,i}}{\partial u_{3,j,i}} = -\frac{1}{m}(1 - y_{j,i}), \\ \frac{\partial J}{\partial u_{2,j,i}} &= \frac{\partial J}{\partial u_{4,j,i}} \frac{\partial u_{4,j,i}}{\partial u_{2,j,i}} = -\frac{1}{m} y_{j,i}, \\ \frac{\partial J}{\partial u_{1,j,i}} &= \frac{\partial J}{\partial u_{3,j,i}} \frac{\partial u_{3,j,i}}{\partial u_{1,j,i}} = -\frac{1}{m}(1 - y_{j,i}) \frac{1}{u_{1,j,i}} = -\frac{1}{m} \frac{1 - y_{j,i}}{1 - a_{j,i}^{[L]}}, \\ \frac{\partial J}{\partial u_{0,j,i}} &= \frac{\partial J}{\partial u_{1,j,i}} \frac{\partial u_{1,j,i}}{\partial u_{0,j,i}} + \frac{\partial J}{\partial u_{2,j,i}} \frac{\partial u_{2,j,i}}{\partial u_{0,j,i}} \\ &= \frac{1}{m}(1 - y_{j,i}) \frac{1}{u_{1,j,i}} - \frac{1}{m} y_{j,i} \frac{1}{u_{0,j,i}} \\ &= \frac{1}{m} \Big(\frac{1 - y_{j,i}}{1 - a_{j,i}^{[L]}} - \frac{y_{j,i}}{a_{j,i}^{[L]}} \Big). \end{aligned}$$

Simply put, we have

$$\frac{\partial J}{\partial a_{j,i}^{[L]}} = \frac{1}{m} \Big(\frac{1 - y_{j,i}}{1 - a_{j,i}^{[L]}} - \frac{y_{j,i}}{a_{j,i}^{[L]}} \Big),$$

and

$$\frac{\partial J}{\partial \mathbf{A}^{[L]}} = \frac{1}{m} \Big(\frac{1}{1 - \mathbf{A}^{[L]}} \odot (1 - \mathbf{Y}) - \frac{1}{\mathbf{A}^{[L]}} \odot \mathbf{Y} \Big). \tag{8}$$

Bearing in mind that we view multi-label classification as j binary classification problems, we also know that the output layer uses the sigmoid activation function. As a result,

$$\begin{aligned} \frac{\partial J}{\partial z_{j,i}^{[L]}} &= \frac{\partial J}{\partial a_{j,i}^{[L]}} a_{j,i}^{[L]} (1 - a_{j,i}^{[L]}) \\ &= \frac{1}{m} \Big(\frac{1 - y_{j,i}}{1 - a_{j,i}^{[L]}} - \frac{y_{j,i}}{a_{j,i}^{[L]}} \Big) a_{j,i}^{[L]} (1 - a_{j,i}^{[L]}) \\ &= \frac{1}{m} ((1 - y_{j,i}) a_{j,i}^{[L]} - y_{j,i} (1 - a_{j,i}^{[L]})) \\ &= \frac{1}{m} (a_{j,i}^{[L]} - y_{j,i}), \end{aligned}$$

which we can vectorize as

$$\frac{\partial J}{\partial \mathbf{Z}^{[L]}} = \frac{1}{m} (\mathbf{A}^{[L]} - \mathbf{Y}). \tag{9}$$