Multi Layer Perceptron Mathematics

A) <u>Softmax activation backward pass :</u>

Equation of the Softmax activation function :

$$S_{i,j} = \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \quad \rightarrow \quad \frac{\partial S_{i,j}}{\partial z_{i,k}} = \frac{\partial \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}}}{\partial z_{i,k}}$$

Derivative of the division operation :

$$f(x) = \frac{g(x)}{h(x)} \quad \rightarrow \quad f'(x) = \frac{g'(x) \cdot h(x) - g(x) \cdot h'(x)}{[h(x)]^2}$$

Applying the derivative of the division operation :

$$= \frac{\frac{\partial}{\partial z_{i,k}} e^{z_{i,j}} \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot \frac{\partial}{\partial z_{i,k}} \sum_{l=1}^{L} e^{z_{i,l}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2} =$$

Derivative of e :

$$\frac{d}{dn} e^n = e^n \cdot \frac{d}{dn} n = e^n \cdot 1 = e^n$$

Solving last term if the equation :

$$\frac{\partial}{\partial z_{i,k}} \sum_{l=1}^{L} e^{z_{i,l}} = \frac{\partial}{\partial z_{i,k}} e^{z_{i,1}} + \frac{\partial}{\partial z_{i,k}} e^{z_{i,2}} + \ldots + \frac{\partial}{\partial z_{i,k}} e^{z_{i,k}} + \ldots + \frac{\partial}{\partial z_{i,k}} e^{z_{i,L-1}} + \frac{\partial}{\partial z_{i,k}} e^{z_{i,L}}$$

$$= 0 + 0 + \ldots + e^{z_{i,k}} + \ldots + 0 + 0 = e^{z_{i,k}}$$

Now we need to solve the partial derivative of $\frac{\partial}{\partial z_{i,k}} e^{z_{i,j}}$:

If j != k → 0
if j=k → $e^{z_{i,j}}$

We need to calculate the derivatives separately for both cases :

1) For j = k :

$$= \frac{e^{z_{i,j}} \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot e^{z_{i,k}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2}$$

$$= \frac{e^{z_{i,j}} \cdot (\sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,k}})}{\sum_{l=1}^{L} e^{z_{i,l}} \cdot \sum_{l=1}^{L} e^{z_{i,l}}}$$

$$= \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \cdot \frac{\sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}}}$$

$$= \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \cdot \left(\frac{\sum_{l=1}^{L} e^{z_{i,l}}}{\sum_{l=1}^{L} e^{z_{i,l}}} - \frac{e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}}}\right)$$

$$= S_{i,j} \cdot (1 - S_{i,k})$$

2) For j != k :

$$= \frac{0 \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot e^{z_{i,k}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2}$$

$$= \frac{-e^{z_{i,j}} \cdot e^{z_{i,k}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2}$$

$$= \frac{-e^{z_{i,j}} \cdot e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}} \cdot \sum_{l=1}^{L} e^{z_{i,l}}}$$

$$= -\frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \cdot \frac{e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}}}$$

$$= -S_{i,j} \cdot S_{i,k}$$

After resolving those 2 cases we have the solution of the derivative of the Softmax function :

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \begin{cases} S_{i,j} \cdot (1 - S_{i,k}) & j = k \\ -S_{i,j} \cdot S_{i,k} & j \neq k \end{cases}$$

We don’t want 2 different equations to code so we will morph the result of the second case of the derivative :

$$-S_{i,j} \cdot S_{i,k} = S_{i,j} \cdot (-S_{i,k}) = S_{i,j} \cdot (0 - S_{i,k})$$

Now we have :

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \begin{cases} S_{i,j} \cdot (1 - S_{i,k}) & j = k \\ S_{i,j} \cdot (0 - S_{i,k}) & j \neq k \end{cases}$$

We can now use the **Kronecker delta** function which is :

$$\delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

We now have :

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = S_{i,j} \cdot (\delta_{j,k} - S_{i,k})$$

We now multiply by $S_{i,j}$:

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = S_{i,j} \cdot (\delta_{j,k} - S_{i,k}) = S_{i,j}\delta_{j,k} - S_{i,j}S_{i,k}$$

Our final equation is :

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = S_{i,j} \cdot (\delta_{j,k} - S_{i,k}) = S_{i,j}\delta_{j,k} - S_{i,j}S_{i,k}$$

B) <u>Softmax + Categorical Cross-Entropy backward pass :</u>

$$\frac{\partial L_i}{\partial z_{i,k}} = \frac{\partial L_i}{\partial \hat{y}_{i,j}} \cdot \frac{\partial S_{i,j}}{\partial z_{i,k}} =$$

We know that the input to the loss function $y\text{-}hat_{i,j}$ (categorical cross-entropy) are the output of the activation function $S_{i,j}$ (softmax) :

$$\hat{y}_{i,j} = S_{i,j}$$

Our equation is now :

$$= \frac{\partial L_i}{\partial \hat{y}_{i,j}} \cdot \frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}}$$

We have :

$$\frac{\partial L_i}{\partial \hat{y}_{i,j}} = -\sum_j \frac{y_{i,j}}{\hat{y}_{i,j}}$$

So we get our equation :

$$= -\sum_j \frac{y_{i,j}}{\hat{y}_{i,j}} \cdot \frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}} =$$

We previously got this system :

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \begin{cases} S_{i,j} \cdot (1 - S_{i,k}) & j = k \\ -S_{i,j} \cdot S_{i,k} & j \neq k \end{cases}$$

So we will do the same here for our equation :

$$\frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}} = \begin{cases} \hat{y}_{i,j} \cdot (1 - \hat{y}_{i,k}) & j = k \\ -\hat{y}_{i,j} \cdot \hat{y}_{i,k} & j \neq k \end{cases}$$

We now need to split for both cases j = k and j != k :

$$-\sum_j \frac{y_{i,j}}{\hat{y}_{i,j}} \cdot \frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}} = -\frac{y_{i,k}}{\hat{y}_{i,k}} \cdot \frac{\partial \hat{y}_{i,k}}{\partial z_{i,k}} - \sum_{j \neq k} \frac{y_{i,j}}{\hat{y}_{i,j}} \cdot \frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}}$$

For the j != k case we just updated the sum operator tu exclude k :

$$-\sum_{j \neq k} \frac{y_{i,j}}{\hat{y}_{i,j}} \cdot \frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}}$$

For the j = k case we do not need the sum element as it will sum only one element of index k :

$$-\frac{y_{i,k}}{\hat{y}_{i,k}} \cdot \frac{\partial \hat{y}_{i,k}}{\partial z_{i,k}}$$

We can get back to our equation :

$$= -\frac{y_{i,k}}{\hat{y}_{i,k}} \cdot \frac{\partial \hat{y}_{i,k}}{\partial z_{i,k}} - \sum_{j \neq k} \frac{y_{i,j}}{\hat{y}_{i,j}} \cdot \frac{\partial \hat{y}_{i,j}}{\partial z_{i,k}} =$$

Thanks to our previous work we know that :

$$= -\frac{y_{i,k}}{\hat{y}_{i,k}} \cdot \hat{y}_{i,k} \cdot (1 - \hat{y}_{i,k}) - \sum_{j \neq k} \frac{y_{i,j}}{\hat{y}_{i,j}} (-\hat{y}_{i,j} \hat{y}_{i,k}) =$$

We can simplify by $y\text{-}hat_{i,k}$:

$$= -y_{i,k} \cdot (1 - \hat{y}_{i,k}) + \sum_{j \neq k} y_{i,j} \hat{y}_{i,k} =$$

And now multiply by $-y_{i,k}$' :

$$= -y_{i,k} + y_{i,k} \hat{y}_{i,k} + \sum_{j \neq k} y_{i,j} \hat{y}_{i,k}$$

We can now join the 2 parts since we have the product excluding k on the right and the product with k on the left :

$$= -y_{i,k} + \sum_{j} y_{i,j}\hat{y}_{i,k}$$

We can now simplify since we know that $y_{i,j}$ for each i the the one-hot encoded vector of ground-truth values, the sum of all its element equals 1. Final equation :

$$= -y_{i,k} + \hat{y}_{i,k} = \hat{y}_{i,k} - y_{i,k}$$