Math of NN

1. Consider a single layer NN (matrix multiplication) without nonlinearity:

$$\boldsymbol{z} = \boldsymbol{w}\boldsymbol{x} + \boldsymbol{b}$$

Or in matrix form

$$\begin{vmatrix} z_1 \\ z_2 \end{vmatrix} = \begin{vmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \end{vmatrix} + \begin{vmatrix} b_1 \\ b_2 \end{vmatrix}$$

With loss function

$$L = l\left(\begin{vmatrix} z_1 \\ z_2 \end{vmatrix}\right)$$

We are looking for $\frac{\partial L}{\partial \boldsymbol{w}}$ in order to minimize the loss function using gradient decent

$$\frac{\partial L}{\partial \boldsymbol{w}} = \begin{vmatrix} \frac{\partial L}{\partial w_{11}} & \frac{\partial L}{\partial w_{12}} \\ \frac{\partial L}{\partial w_{21}} & \frac{\partial L}{\partial w_{22}} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1}\frac{\partial z_1}{\partial w_{11}} & \frac{\partial L}{\partial z_1}\frac{\partial z_1}{\partial w_{12}} \\ \frac{\partial L}{\partial z_2}\frac{\partial z_2}{\partial w_{21}} & \frac{\partial L}{\partial z_2}\frac{\partial z_2}{\partial w_{22}} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1}x_1 & \frac{\partial L}{\partial z_1}x_2 \\ \frac{\partial L}{\partial z_2}x_1 & \frac{\partial L}{\partial z_2}x_2 \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1} \\ \frac{\partial L}{\partial z_2} \end{vmatrix} \begin{vmatrix} x_1 & x_2 \end{vmatrix}$$

Similarly, we have

$$\frac{\partial L}{\partial \boldsymbol{x}} = \begin{vmatrix} \frac{\partial L}{\partial x_1} \\ \frac{\partial L}{\partial x_2} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1}\frac{\partial z_1}{\partial x_1} + \frac{\partial L}{\partial z_2}\frac{\partial z_2}{\partial x_1} \\ \frac{\partial L}{\partial z_1}\frac{\partial z_1}{\partial x_2} + \frac{\partial L}{\partial z_2}\frac{\partial z_2}{\partial x_2} \end{vmatrix} = \begin{vmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{vmatrix} \begin{vmatrix} \frac{\partial L}{\partial z_1} \\ \frac{\partial L}{\partial z_2} \end{vmatrix}$$

and

$$\frac{\partial L}{\partial \boldsymbol{b}} = \begin{vmatrix} \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial b_2} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1}\frac{\partial z_1}{\partial b_1} \\ \frac{\partial L}{\partial z_2}\frac{\partial z_2}{\partial b_2} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1} \\ \frac{\partial L}{\partial z_2} \end{vmatrix}$$

Denote $\begin{vmatrix} \frac{\partial L}{\partial z_1} \\ \frac{\partial L}{\partial z_2} \end{vmatrix}$ as $\boldsymbol{\delta}$ (the backpropagated/remain error), then we have

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{\delta}\boldsymbol{x}^T$$

$$\frac{\partial L}{\partial \boldsymbol{x}} = \boldsymbol{w}^T\boldsymbol{\delta}$$

$$\frac{\partial L}{\partial \boldsymbol{b}} = \boldsymbol{\delta}$$

$\boldsymbol{\delta}$ can be calculated from nest layer/operation of the current layer. For example, if this is what happened in the loss function

$$\begin{vmatrix} c_1 \\ c_2 \end{vmatrix} = \begin{vmatrix} z_1 \\ z_2 \end{vmatrix} - \begin{vmatrix} y_1 \\ y_2 \end{vmatrix}$$

$$L = \frac{1}{2}\sum c^2$$

Then we can have

$$\boldsymbol{\delta} = \begin{vmatrix} \frac{\partial L}{\partial c_1} \frac{\partial c_1}{\partial z_1} \\ \frac{\partial L}{\partial c_2} \frac{\partial c_2}{\partial z_2} \end{vmatrix} = \begin{vmatrix} 1 \cdot c_1 \\ 1 \cdot c_2 \end{vmatrix} = \begin{vmatrix} z_1 \\ z_2 \end{vmatrix} - \begin{vmatrix} y_1 \\ y_2 \end{vmatrix}$$

In other word, the $\boldsymbol{\delta}$ of a layer is the partial derivative of its output (which is used as the input of the next layer) regarding the output of the next layer/operation

If we have nonlinearity

$$\begin{vmatrix} a_1 \\ a_2 \end{vmatrix} = f\left(\begin{vmatrix} z_1 \\ z_2 \end{vmatrix}\right)$$

In which f is the sigmoid function

$$f(x) = \frac{1}{1 + e^{-x}}$$

$$f'(x) = f(x)f(-x) = f(x)\big(1 - f(x)\big)$$

Then the loss value is calculated by

$$L = l\left(\begin{vmatrix} a_1 \\ a_2 \end{vmatrix}\right)$$

In this case,

$$\boldsymbol{\delta} = \begin{vmatrix} \frac{\partial L}{\partial a_1} \frac{\partial a_1}{\partial z_1} \\ \frac{\partial L}{\partial a_2} \frac{\partial a_2}{\partial z_2} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial a_1} \\ \frac{\partial L}{\partial a_2} \end{vmatrix} \times \begin{vmatrix} \frac{\partial a_1}{\partial z_1} \\ \frac{\partial a_2}{\partial z_2} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial a_1} \\ \frac{\partial L}{\partial a_2} \end{vmatrix} \times \begin{vmatrix} a_1(1 - a_1) \\ a_2(1 - a_2) \end{vmatrix}$$

Where $\times$ denotes element-wise multiplication. Means that the gradients of element wise operations are multiplied to the backpropagated error

2. Consider a two-layer NN

$$\begin{vmatrix} z_1^{(l1)} \\ z_2^{(l1)} \end{vmatrix} = \begin{vmatrix} w_{11}^{(l1)} & w_{12}^{(l1)} \\ w_{21}^{(l1)} & w_{22}^{(l1)} \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \end{vmatrix} + \begin{vmatrix} b_1^{(l1)} \\ b_2^{(l1)} \end{vmatrix}$$

$$\begin{vmatrix} z_1^{(l2)} \\ z_2^{(l2)} \end{vmatrix} = \begin{vmatrix} w_{11}^{(l2)} & w_{12}^{(l2)} \\ w_{21}^{(l2)} & w_{22}^{(l2)} \end{vmatrix} \begin{vmatrix} z_1^{(l1)} \\ z_2^{(l1)} \end{vmatrix} + \begin{vmatrix} b_1^{(l2)} \\ b_2^{(l2)} \end{vmatrix}$$

With loss function

$$L = l\left(\begin{vmatrix} z_1^{(l2)} \\ z_2^{(l2)} \end{vmatrix}\right)$$

To get the gradient of layer 1 we need the backpropagated error

$$\boldsymbol{\delta}^{(l1)} = \frac{\partial L}{\partial \boldsymbol{z}^{(l1)}} = \begin{vmatrix} \frac{\partial L}{\partial z_1^{(l1)}} \\ \frac{\partial L}{\partial z_1^{(l1)}} \end{vmatrix}$$

Actually, this is the $\frac{\partial L}{\partial \boldsymbol{x}}$ shown in the 1-layer case as $\boldsymbol{z}^{(l1)}$ is at the position of $\boldsymbol{x}$ of the 2nd layer. Therefore,

$$\boldsymbol{\delta}^{(l1)} = \boldsymbol{w}^{(l2)T}\boldsymbol{\delta}^{(l2)}$$

This conclusion can be extended to multi-layer NNs

$$\boldsymbol{\delta}^{(l_n)} = \boldsymbol{w}^{(l_{n+1})T}\boldsymbol{\delta}^{(l_{n+1})}$$

3. Consider a nested NN in which *w* and *b* are reused

$$\begin{vmatrix} z_1^{(l1)} \\ z_2^{(l1)} \end{vmatrix} = \begin{vmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \end{vmatrix} + \begin{vmatrix} b_1 \\ b_2 \end{vmatrix}$$

$$\begin{vmatrix} z_1^{(l2)} \\ z_2^{(l2)} \end{vmatrix} = \begin{vmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{vmatrix} \begin{vmatrix} z_1^{(l1)} \\ z_2^{(l1)} \end{vmatrix} + \begin{vmatrix} b_1 \\ b_2 \end{vmatrix}$$

With loss function

$$L = l\left(\begin{vmatrix} z_1^{(l2)} \\ z_2^{(l2)} \end{vmatrix}\right)$$

We are interested in $\frac{\partial L}{\partial \boldsymbol{w}}$ and $\frac{\partial L}{\partial \boldsymbol{b}}$

$$\frac{\partial L}{\partial \boldsymbol{w}} = \begin{vmatrix} \frac{\partial L}{\partial w_{11}} & \frac{\partial L}{\partial w_{12}} \\ \frac{\partial L}{\partial w_{21}} & \frac{\partial L}{\partial w_{22}} \end{vmatrix}$$

Unlike the case of 1-layer NN, here $\frac{\partial z_2^{(l2)}}{\partial w_{11}}$, $\frac{\partial z_2^{(l2)}}{\partial w_{12}}$, $\frac{\partial z_1^{(l2)}}{\partial w_{21}}$ and $\frac{\partial z_1^{(l2)}}{\partial w_{22}}$ are not zeros due $\boldsymbol{z}^{l1}$. Therefore

$$\begin{vmatrix} \frac{\partial L}{\partial w_{11}} & \frac{\partial L}{\partial w_{12}} \\ \frac{\partial L}{\partial w_{21}} & \frac{\partial L}{\partial w_{22}} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1^{(l2)}}\frac{\partial z_1^{(l2)}}{\partial w_{11}} + \frac{\partial L}{\partial z_2^{(l2)}}\frac{\partial z_2^{(l2)}}{\partial w_{11}} & \frac{\partial L}{\partial z_1^{(l2)}}\frac{\partial z_1^{(l2)}}{\partial w_{12}} + \frac{\partial L}{\partial z_2^{(l2)}}\frac{\partial z_2^{(l2)}}{\partial w_{12}} \\ \frac{\partial L}{\partial z_2^{(l2)}}\frac{\partial z_2^{(l2)}}{\partial w_{21}} + \frac{\partial L}{\partial z_1^{(l2)}}\frac{\partial z_1^{(l2)}}{\partial w_{21}} & \frac{\partial L}{\partial z_2^{(l2)}}\frac{\partial z_2^{(l2)}}{\partial w_{22}} + \frac{\partial L}{\partial z_1^{(l2)}}\frac{\partial z_1^{(l2)}}{\partial w_{22}} \end{vmatrix}$$

Which equals to

$$\begin{vmatrix} \frac{\partial L}{\partial z_1^{(l2)}}\left(z_1^{(l1)} + w_{11}\frac{\partial z_1^{(l1)}}{\partial w_{11}}\right) + \frac{\partial L}{\partial z_2^{(l2)}}\frac{\partial z_2^{(l2)}}{\partial z_1^{(l1)}}\frac{\partial z_1^{(l1)}}{\partial w_{11}} & \frac{\partial L}{\partial z_1^{(l2)}}\left(z_2^{(l1)} + w_{11}\frac{\partial z_1^{(l1)}}{\partial w_{12}}\right) + \frac{\partial L}{\partial z_2^{(l2)}}\frac{\partial z_2^{(l2)}}{\partial z_1^{(l1)}}\frac{\partial z_{21}^{(l1)}}{\partial w_{12}} \\ \frac{\partial L}{\partial z_2^{(l2)}}\left(z_1^{(l1)} + w_{22}\frac{\partial z_2^{(l1)}}{\partial w_{21}}\right) + \frac{\partial L}{\partial z_1^{(l2)}}\frac{\partial z_1^{(l2)}}{\partial z_2^{(l1)}}\frac{\partial z_2^{(l1)}}{\partial w_{21}} & \frac{\partial L}{\partial z_2^{(l2)}}\left(z_2^{(l1)} + w_{22}\frac{\partial z_2^{(l1)}}{\partial w_{22}}\right) + \frac{\partial L}{\partial z_1^{(l2)}}\frac{\partial z_1^{(l2)}}{\partial z_2^{(l1)}}\frac{\partial z_2^{(l1)}}{\partial w_{22}} \end{vmatrix}$$

The above matrix may seem very complicated, but here is the trick:

Rule1. w_{11} and w_{12} have "direct" connect to $z_1^{(l2)}$ due to the matrix multiplication, the same as w_{21} and w_{22} to $z_2^{(l2)}$. Therefore we can get:

$$\frac{\partial z_1^{(l2)}}{\partial w_{11}} = \left(z_1^{(l1)} + w_{11}\frac{\partial z_1^{(l1)}}{\partial w_{11}}\right)$$

$$\frac{\partial z_1^{(l2)}}{\partial w_{12}} = \left(z_2^{(l1)} + w_{11}\frac{\partial z_1^{(l1)}}{\partial w_{12}}\right)$$

$$\frac{\partial z_2^{(l2)}}{\partial w_{21}} = \left(z_1^{(l1)} + w_{22}\frac{\partial z_2^{(l1)}}{\partial w_{21}}\right)$$

$$\frac{\partial z_2^{(l2)}}{\partial w_{22}} = \left(z_2^{(l1)} + w_{22}\frac{\partial z_2^{(l1)}}{\partial w_{22}}\right)$$

Rule 2. w_{11} and w_{12} are not "direct" connect to $z_2^{(l2)}$ in the 2nd layer, but due to $z_1{}^{(l1)}$, the term $\frac{\partial z_2^{(l2)}}{\partial w_{11}}$ and $\frac{\partial z_2^{(l2)}}{\partial w_{12}}$ are not zero, similarly as of w_{21} and w_{22} to $z_1^{(l2)}$ due to $z_2{}^{(l1)}$. Therefore we have

$$\frac{\partial z_2^{(l2)}}{\partial w_{11}} = \frac{\partial z_2^{(l2)}}{\partial z_1^{(l1)}}\frac{\partial z_1^{(l1)}}{\partial w_{11}}$$

$$\frac{\partial z_2^{(l2)}}{\partial w_{12}} = \frac{\partial z_2^{(l2)}}{\partial z_1^{(l1)}}\frac{\partial z_1^{(l1)}}{\partial w_{12}}$$

$$\frac{\partial z_1^{(l2)}}{\partial w_{21}} = \frac{\partial z_1^{(l2)}}{\partial z_2^{(l1)}}\frac{\partial z_2^{(l1)}}{\partial w_{21}}$$

$$\frac{\partial z_1^{(l2)}}{\partial w_{22}} = \frac{\partial z_1^{(l2)}}{\partial z_2^{(l1)}}\frac{\partial z_2^{(l1)}}{\partial w_{22}}$$

In other word, take w_{11} as an example, the connections are $w_{11} \to z_1^{(l2)}$ (Rule 1) and $w_{11} \to z_1^{(l1)} \to \left(z_1^{(l2)}, z_2^{(l2)}\right)$ (Rule 2)

Therefore, we have

$$\begin{vmatrix} \frac{\partial L}{\partial w_{11}} & \frac{\partial L}{\partial w_{12}} \\ \frac{\partial L}{\partial w_{21}} & \frac{\partial L}{\partial w_{22}} \end{vmatrix} = \begin{vmatrix} \frac{\partial L}{\partial z_1^{(l2)}}\left(z_1^{(l1)} + w_{11}x_1\right) + \frac{\partial L}{\partial z_2^{(l2)}}w_{21}x_1 & \frac{\partial L}{\partial z_1^{(l2)}}\left(z_2^{(l1)} + w_{11}x_2\right) + \frac{\partial L}{\partial z_2^{(l2)}}w_{21}x_2 \\ \frac{\partial L}{\partial z_2^{(l2)}}\left(z_1^{(l1)} + w_{22}x_1\right) + \frac{\partial L}{\partial z_1^{(l2)}}w_{12}x_1 & \frac{\partial L}{\partial z_2^{(l2)}}\left(z_2^{(l1)} + w_{22}x_2\right) + \frac{\partial L}{\partial z_1^{(l2)}}w_{12}x_2 \end{vmatrix}$$

Which equals to

$$\begin{vmatrix} \frac{\partial L}{\partial z_1^{(l2)}}z_1^{(l1)} + x_1\left(\frac{\partial L}{\partial z_1^{(l2)}}w_{11} + \frac{\partial L}{\partial z_2^{(l2)}}w_{21}\right) & \frac{\partial L}{\partial z_1^{(l2)}}z_2^{(l1)} + x_2\left(\frac{\partial L}{\partial z_1^{(l2)}}w_{11} + \frac{\partial L}{\partial z_2^{(l2)}}w_{21}\right) \\ \frac{\partial L}{\partial z_2^{(l2)}}z_1^{(l1)} + x_1\left(\frac{\partial L}{\partial z_1^{(l2)}}w_{12} + \frac{\partial L}{\partial z_2^{(l2)}}w_{22}\right) & \frac{\partial L}{\partial z_2^{(l2)}}z_2^{(l1)} + x_2\left(\frac{\partial L}{\partial z_1^{(l2)}}w_{12} + \frac{\partial L}{\partial z_2^{(l2)}}w_{22}\right) \end{vmatrix}$$

And

$$\begin{vmatrix} \frac{\partial L}{\partial z_1^{(l2)}} \\ \frac{\partial L}{\partial z_2^{(l2)}} \end{vmatrix} \begin{vmatrix} z_1^{(l1)} & z_2^{(l1)} \end{vmatrix} + \left(\begin{vmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{vmatrix} \begin{vmatrix} \frac{\partial L}{\partial z_1^{(l2)}} \\ \frac{\partial L}{\partial z_2^{(l2)}} \end{vmatrix} \right) \begin{vmatrix} x_1 & x_2 \end{vmatrix}$$

Therefore in the nested NN

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{\delta}^{(l2)} \boldsymbol{z}^{(l2)} + \left(\boldsymbol{w}^T \boldsymbol{\delta}^{(l2)} \right) \boldsymbol{x} = \boldsymbol{\delta}^{(l2)} \boldsymbol{z}^{(l2)} + \boldsymbol{\delta}^{(l1)} \boldsymbol{x}$$

Similarly

$$\frac{\partial L}{\partial \boldsymbol{b}} = \boldsymbol{\delta}^{(l2)} + \boldsymbol{w}^T \boldsymbol{\delta}^{(l2)} = \boldsymbol{\delta}^{(l2)} + \boldsymbol{\delta}^{(l1)}$$

This is a good news as the gradient of reused weights are the sum of gradients from the corresponding layers

4. Computational graph