1 Foreword

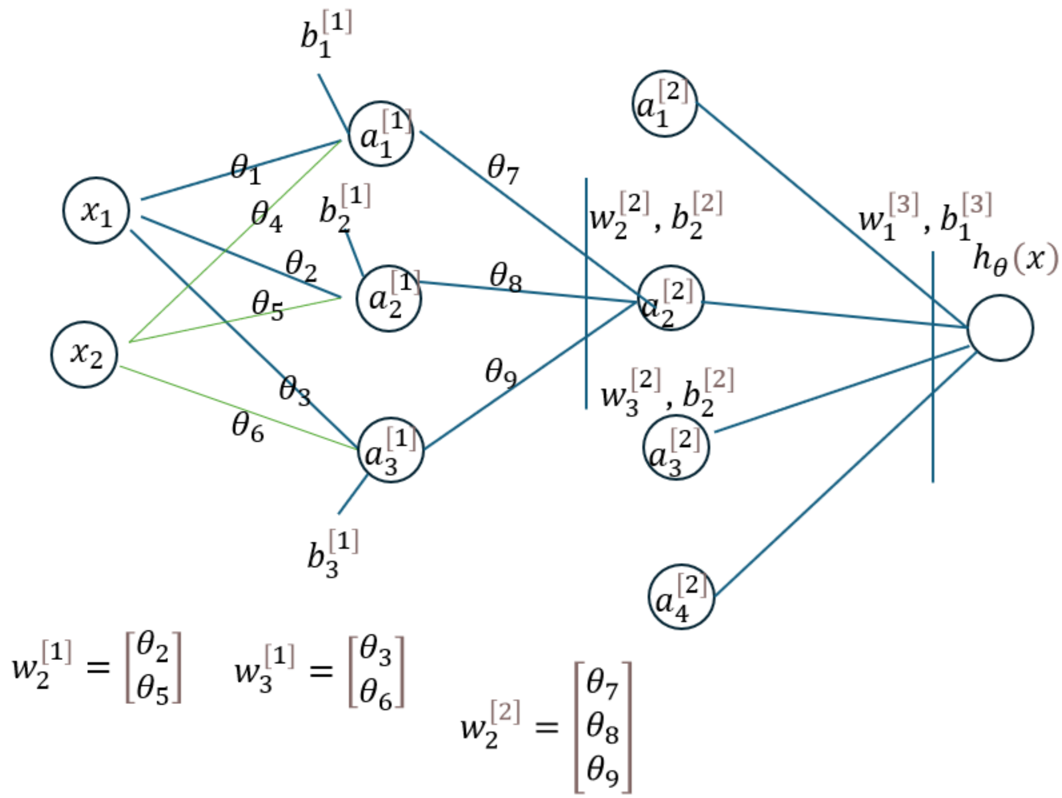
Author : Anderson Chau

Disclaimer : The notes are written only for my understanding and memorization purpose after I have self-studied those online lecture notes.

2 Main Idea

The old trick : (i) Forward feed (ii) Compute Loss (NN output vs training data) (iii) Backpropagation with Gradient Descent to tune parameters
2. Use activation functions to avoid the model to be a pure linear model, which is useless (just ax+b)
3. Examples of activation functions : Signmoid , (Leaky) ReLU, tanh etc.

3 ANN Structure



w's and b's are parameters : Totally ther are Hidden Layer 1 (layer 1) (2x3 + 3) + Hidden Layer 1 (layer 2) (3x4 + 4) + Output Layer (layer 3)(4x1 +1) number of parameters

4 Forward Feed (see above NN diagram)

$$a_1 = \text{ReLU}(\theta_1 x_1 + \theta_4 x_2 + b_1^{[1]})$$

$$a_2 = \text{ReLU}(\theta_2 x_1 + \theta_5 x_2 + b_2^{[1]})$$

Let i be i^{th} layer and j be j^{th} neuron (count vertifically) this layer of NN
Rewriting the notation : $w_j^{[i]}$ as **VECTOR** of input θ's for layer i and j^{th} neuron.
With the above, Layer 1 of NN can be expressed as:

For all $j \in [1, \ldots, m]$: (m=3, count vertically, is the number of number of neuron layer 1)

$$z_j = \mathbf{w}_j^{[1]\top}\mathbf{x} + b_j^{[1]} \quad \text{where} \quad \mathbf{w}_j^{[1]} \in R^d,\ b_j^{[1]} \in R$$

(d = 2 , count vertically, is the number of number of previous layer , layer 0)

$$a_j = \mathrm{ReLU}(z_j),$$

$$\mathbf{a} = [a_1, \dots, a_m]^\top \in R^m$$

For Layer 3 :

$$\bar{h}_\theta(\mathbf{x}) = \mathbf{w}^{[3]\top}\mathbf{a} + b^{[3]} \quad \text{where} \quad \mathbf{w}^{[3]} \in R^n,\ b^{[3]} \in R$$

(n = 4, count vertically, is the number of number of neuron layer, layer 2)

5 Vectorization of Forward Feeding

Just by stacking the parameters . for layer 1 :

$$W^{[1]} = \begin{bmatrix} -w_1^{[1]T}- \\ -w_2^{[1]T}- \\ \vdots \\ -w_m^{[1]T}- \end{bmatrix} \in R^{m\times d}$$

$$\mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{bmatrix} \in \mathbb{R}^{m\times 1} = \begin{bmatrix} -w_1^{[1]T}- \\ -w_2^{[1]T}- \\ \vdots \\ -w_m^{[1]T}- \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} + \begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ \vdots \\ b_m^{[1]} \end{bmatrix}$$

Hence we get:

$$\begin{aligned} z^{[1]} &= W^{[1]}x + b^{[1]} \\ a^{[1]} &= ReLU(z^{[1]}) \\ z^{[2]} &= W^{[2]}a^{[1]} + b^{[2]} \\ a^{[2]} &= ReLU(z^{[2]}) \\ h &= W^{[3]}a^{[2]} + b^{[3]} \end{aligned}$$

In General :

$$\begin{aligned} a^{[1]} &= \mathrm{ReLU}(W^{[1]}x + b^{[1]}) \\ a^{[2]} &= \mathrm{ReLU}(W^{[2]}a^{[1]} + b^{[2]}) \\ &\vdots \\ a^{[r-1]} &= \mathrm{ReLU}(W^{[r-1]}a^{[r-2]} + b^{[r-1]}) \\ h(x) &= W^{[r]}a^{[r-1]} + b^{[r]} \end{aligned}$$

Also, for loss function J

$$J = (1/2)(h - o)^2$$

Some common loss function for J : Common : (1) Mean Sequared Error (2) Cross Entropy Loss

6 Vector/Matrix Calculus: Some important equations

1. Gradient, where f is $R^n to R$:

$$\nabla f(x_1, x_2, \ldots, x_n) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x_1, x_2, \ldots, x_n) \\ \frac{\partial f}{\partial x_2}(x_1, x_2, \ldots, x_n) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x_1, x_2, \ldots, x_n) \end{bmatrix}$$

Example : $f(x_1, x_2) = 3x_1^2 x_2$, then $\nabla f(x_1, x_2) = [6x_1x_2, 3x_1]^T$

2. Jacobian of f, Note that there are m DIFFERENT functions

$$\begin{aligned} \mathbf{f}(\mathbf{x}) &= \mathbf{f}(x_1, x_2, \ldots, x_n) \\ &= (f_1(x_1, x_2, \ldots, x_n), , \ldots, f_m(x_1, x_2, \ldots, x_n)) \\ &= (f_1(\mathbf{x}), , \ldots, f_m(\mathbf{x})) \end{aligned}$$

$$\mathbb{J} = \begin{bmatrix} \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla^T f_1(\mathbf{x}) \\ \vdots \\ \nabla^T f_m(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(x_1, x_2 ...., x_n)}{\partial x_1} & \cdots & \frac{\partial f_1(x_1, x_2 ...., x_n)}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m((x_1, x_2 ...., x_n)}{\partial x_1} & \cdots & \frac{\partial f_m((x_1, x_2 ...., x_n)}{\partial x_n} \end{bmatrix}$$

3. (Law of total derivatives) for $f(g_1, g_2 ...., g_k)$, if **EACH** of $g_1, g_2 ...., g_k$ actually depends on $x_1, x_2 .... x_n$, then

$$\frac{\partial f_m((g_1, g_2 ...., g_n)}{\partial x_1} = \frac{\partial f}{\partial g_1}\frac{\partial g_1}{\partial x_1} + \frac{\partial f}{\partial g_2}\frac{\partial g_2}{\partial x_1} + ... + \frac{\partial f}{\partial u_n}\frac{\partial g_n}{\partial x_1}$$

$$\frac{\partial f_m((g_1, g_2 ...., g_n)}{\partial x_2} = \frac{\partial f}{\partial g_1}\frac{\partial g_1}{\partial x_2} + \frac{\partial f}{\partial g_2}\frac{\partial g_2}{\partial x_2} + ... + \frac{\partial f}{\partial u_n}\frac{\partial g_n}{\partial x_2}$$

4. By 3 , Jacobian again, but this time :

$$y_1 = f_1(g_1(x_1, ..., x_n), g_2(x_1, ..., x_n), ..., g_k(x_1, ..., x_n))$$
$$y_2 = f_1(g_1(x_1, ..., x_n), g_2(x_1, ..., x_n), ..., g_k(x_1, ..., x_n))$$

$$....$$

$$y_m = f_m(g_1(x_1,...,x_n), g_2(x_1,...,x_n), ..., g_k(x_1,...,x_n))$$

$$\mathbf{y} = (y_1, y_2..., y_m), \mathbf{x} = (x_1,...,x_n)$$

$$J = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \nabla^T f_1(\mathbf{x}) \\ \nabla^T f_2(\mathbf{x}) \\ \vdots \\ \nabla^T f_m(\mathbf{x}) \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{i=1}^k \frac{\partial f_1}{\partial g_i}\frac{\partial g_i}{\partial x_1} & \sum_{i=1}^k \frac{\partial f_1}{\partial g_i}\frac{\partial g_i}{\partial x_2} & \cdots & \sum_{i=1}^k \frac{\partial f_1}{\partial g_i}\frac{\partial g_i}{\partial x_2} \\ \sum_{i=1}^k \frac{\partial f_2}{\partial g_i}\frac{\partial g_i}{\partial x_1} & \sum_{i=1}^k \frac{\partial f_2}{\partial g_i}\frac{\partial g_i}{\partial x_2} & \cdots & \sum_{i=1}^k \frac{\partial f_2}{\partial g_i}\frac{\partial g_i}{\partial x_2} \\ \cdots & \cdots & \cdots & \cdots \\ \sum_{i=1}^k \frac{\partial f_m}{\partial g_i}\frac{\partial g_i}{\partial x_1} & \sum_{i=1}^k \frac{\partial f_m}{\partial g_i}\frac{\partial g_i}{\partial x_2} & \cdots & \sum_{i=1}^k \frac{\partial f_m}{\partial g_i}\frac{\partial g_i}{\partial x_2} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial f_1}{\partial g_1} & \frac{\partial f_1}{\partial g_2} & \cdots & \frac{\partial f_1}{\partial g_k} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial f_m}{\partial g_1} & \frac{\partial f_m}{\partial g_2} & \cdots & \frac{\partial f_m}{\partial g_k} \end{bmatrix} \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial g_k}{\partial x_1} & \frac{\partial g_k}{\partial x_2} & \cdots & \frac{\partial g_k}{\partial x_n} \end{bmatrix}$$

5. Jacobian of elementwise operation fuunction are diagonal. Therefore $\frac{\partial a^{[i]}}{\partial z^{[i]}}$ is a diagonal matrix

7 Vectorized Backpropagation

Our objective is to make use of matrix calculus, gradient descent to tune W and b to minimize J by SGD or mini-batch GD

Algo 1 SGD : 1: Hyperparameter: learning rate α, number of total iteration n_{iter}.
2: Initialize θ randomly.
3: for i = 1 to niter do
4: Sample j uniformly from 1,...,n, and update θ by

$$\theta := \theta - \alpha \nabla_\theta J^{(j)}(\theta)$$

By Chain Rule of matrix calculus

$$\frac{\partial L}{\partial W_{ij}^{[2]}} = (\frac{\partial L}{\partial a^{[3]}}\frac{\partial a^{[3]}}{\partial z^{[3]}})(\frac{\partial z^{[3]}}{\partial a^{[2]}})(\frac{\partial a^{[2]}}{\partial z^{[2]}})(\frac{\partial z^{[2]}}{\partial W_{ij}^{[2]}})$$

$$= [(a^{[3]} - y)W[3] \bigodot g(z^{[2]})]_i a_j^{[1]T}$$

stacking up again :

$$\frac{\partial L}{\partial W^{[2]}} = [(a^{[3]} - y)W[3] \bigodot g(z^{[2]})]a^{[1]T}$$

We see here the step of GD is based on next layer's value, therefore we have update back propagated to previous layer.

8 Testing

$$\sum_{i=1}^{k} \frac{\partial f_i}{\partial x_i} dx_i$$