

## Lecture #4 Content: ANN Modeling

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### 5. Summary

## Lecture 4 How Artificial Neural Network (ANN) works?

### 1.0 Introduction

In the Previous chapter, we learned how the Linear regression (Simple linear, Polynomial, Multivariable) and the Non-Linear regression (Exponential, Logarithmic, Power, --) work. For these type of regression we need to first display data to estimate the best mapping function

On the other hand, when the dataset, for instance, behaves as the following, we can not map the dataset by the above regression functions



- For datasets such as these and even for linear/non linear trend dataset, ANN based modeling perform the job.

In this chapter, we will learn the basic concept of how ANN modeling works.

The issues to be discussed are.

- ⇒ ANN - building block / Perceptron
- ⇒ How - Perceptron perform computation
- ⇒ How ANN perform computation?
  - Forward feed / loss computation
  - Backward propagation / optimization
- ⇒ Finally, do practical ANN modeling with
  - (a) Synthetic data
  - (b) Field data



## Lecture How ANN works?

### Artificial neural network (ANN)

(2.0)  $\Rightarrow$  • ANN vs Biological neuron network  
ANN is a mathematical model of a system that simulates similar to a biological neural network in human brain capable of learning, prediction, and recognition

### 2.1 $\Rightarrow$ • Nodes vs Neurons

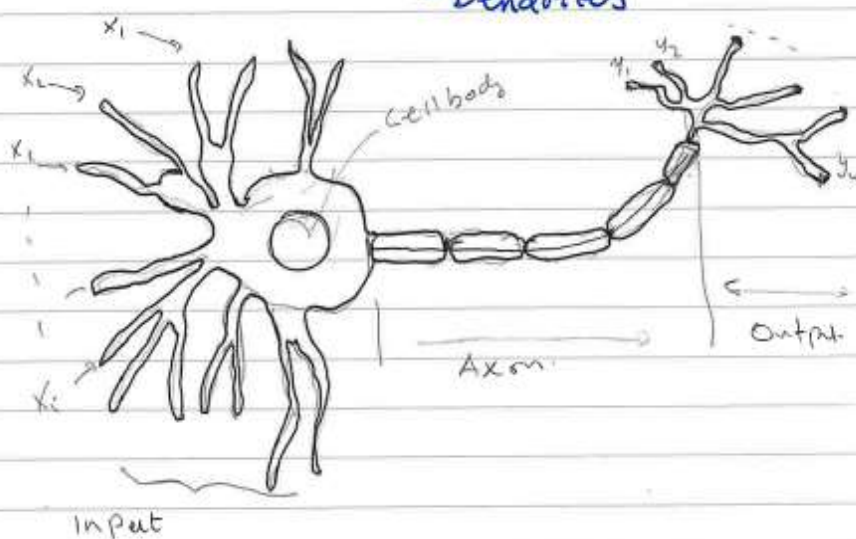
- ANN uses Nodes, which are similar to Neurons (<sup>cellular</sup> building block of brain)

- Cellular Neurons are interconnected, so does ANN nodes

$\Rightarrow$  Description of biological neurons:

Neurons includes (Fig below)

- $\rightarrow$  Cell
- $\rightarrow$  Axon
- $\rightarrow$  Dendrites



In 1943, Warren McCulloch and Walter Pitts created the first Mathematical model of a neural network to model/describe how brain works.

→ The model is a simple linear model that results in a positive or negative output given a set of inputs and weights.

The function reads

$$f(x, w) = x_1 w_1 + x_2 w_2 + \dots + x_n w_n$$

Where,  $f(x, w)$  = output

•  $x_i$  = input

•  $w_i$  = weight

→ This model of computation was called Neuron. Since it tried to simulate how the building block of the brain work

→ Their model doesn't learn to find weights

## 2.2 Perceptron

Being inspired from the biological neuron and its ability to learn, in 1957, Frank Rosenblatt introduced the concept of PERCEPTRON. He developed an algorithm that could learn the weight to produce output

— Perceptron is the basic

building block of a neural network

→ It is simple model of Neurons



→ The perceptron model is used for binary classifiers.

→ Perceptron consists of four parts.

- Input values
- Weights and a bias
- Weighted Sum
- Activation function

⇒ How perceptron works?

→ Perceptron works by receiving numerical input values along with weights and bias

Input ( $x_1, x_2, x_3$ ), weight ( $w_1, w_2, w_3$ ), bias

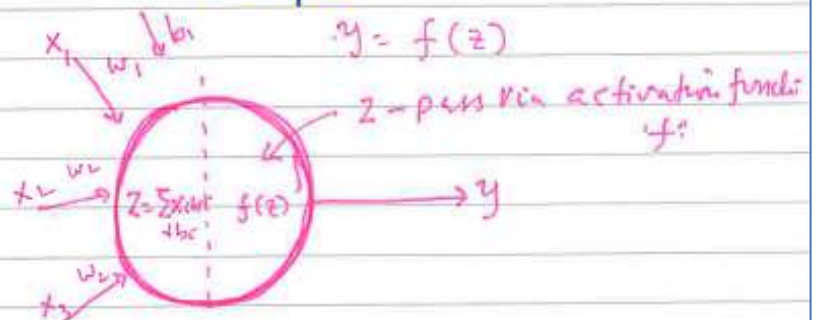
→ It then dot product the inputs and with the respective weights

$x_i w_i$

→ The individual weighted inputs are added and then added together along with the bias

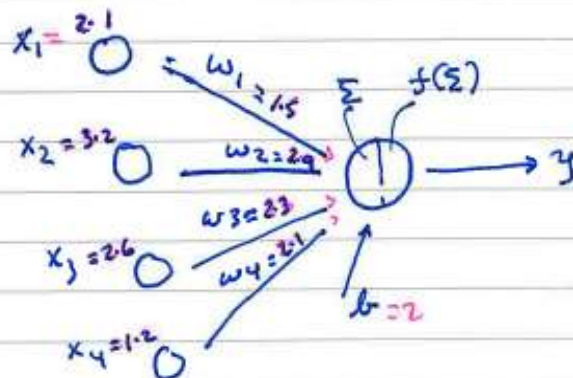
$$Z = \sum_{i=1}^n x_i w_i + b_i$$

→ The sum result will then pass through the activation function and return a final output



## Example 1: How a single perceptron computation performed in python?

Example 1: By implementing Perceptron Model



Input = [2.1, 3.2, 2.6, 1.2]

Weight = [1.5, 2.9, 2.3, 2.1]

bias = 2

Step 1: Compute Sum.

$$Z = \sum x_i w_i + b_i$$

$$= \text{Input}[0] * \text{Weight}[0] + \text{Input}[1] * \text{Weight}[1] + \text{Input}[2] * \text{Weight}[2] + \text{Input}[3] * \text{Weight}[3] + \text{bias}$$

Step 2: Pass the computed Sum through activation function.

Define activation functions

(1) Sigmoid function

```
def sigmoid(x):
```

```
    return 1 / (1 + np.exp(-x))
```

```
print('Sigmoid:', sigmoid(2))
```

## 2.3 ACTIVATION FUNCTIONS

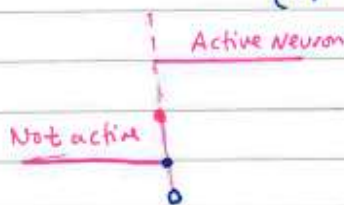
What are ACTIVATION Functions?

- > The activation function / transfer function CONVERT the input signal to the output signal.
- > There are various kind of activation function. These are

- (1) Binary step function
- (2) Linear function
- (3) Non-linear function

### > Description of activation functions

#### (1) Binary step function



⇒ The function decides whether a neuron should be ACTIVATED or Not based on the threshold value

Binary step

$$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$$

→ used for binary classifier.

Issue with binary step function:

- It is used for binary target value. If the targets are more than two, it is not useful.
- Derivative of step function = 0. This does not allow BACK PROPAGATION.



## (2) Relu activation function

```
def Relu(x):  
    return max(0, x)  
  
Print('Relu:', Relu(z))
```

## (3) Leaky Relu activation function

```
def LeakyRelu(x):  
    if x > 0:  
        return x  
    else:  
        return 0.01 * x  
  
Print('LeakyRelu:', LeakyRelu(z))
```

## (4) Tanh activation function

```
def Tanh(x)  
    return (np.exp(x) - np.exp(-x)) /  
           (np.exp(x) + np.exp(-x))  
  
Print('Tanh:', Tanh(z))
```

## (5) Swish activation function

```
def swish(x)  
    beta = 1.0  
    return x / (1 + np.exp(-beta * x))  
  
Print('Swish:', swish(z))
```



Example 2: By using numpy to compute perceptron model [perceptron computation]

Import library

import numpy as np

Input / Weight List + bias

input = [2.1, 3.2, 2.6, 1.2]

weight [1.5, 2.9, 2.3, 2.1] ← Single neuron

bias = 2

dot product ( $x_i \cdot w_i$ ) + bias

$z = \text{np.dot}(\text{input}, \text{weight}) + \text{bias}$

Print(z)

Pass the sum via activation function

Here define functions

(1) Sigmoid function

def sigmoid(x):

return  $1/(1 + \text{np.exp}(-x))$

Print('Sigmoid:', sigmoid(z))

(2) Relu function

def Relu(x):

return max(0, x)

Print('Relu:', Relu(z))

(3) Leaky Relu function

def LeakyRelu(x):

if  $x > 0$

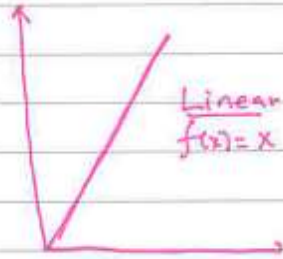
return x

else:

return 0.01x

Print('LeakyRelu:', LeakyRelu(z))

## (2) Linear Activation function



→ The activation function is proportional to the input  
 $f(x) = x$

→ Properties of the activation function

⇒ The gradient is non-zero, constant value

⇒ It allows backpropagation. But the updating factor is the same. Therefore, the network improves the error since the gradient is the same for every iteration.

## (3) Non-linear activation function

→ The linear activation does not allow the model to create complex mapping between the network's input/output.

→ Therefore, non-linear activation functions solve the limitations of linear activation functions such as:

→ The existence of gradient that allows backpropagation to update weights/biases.

### (a) Sigmoid activation function

→ Sigmoid is an S-shaped non-linear function.

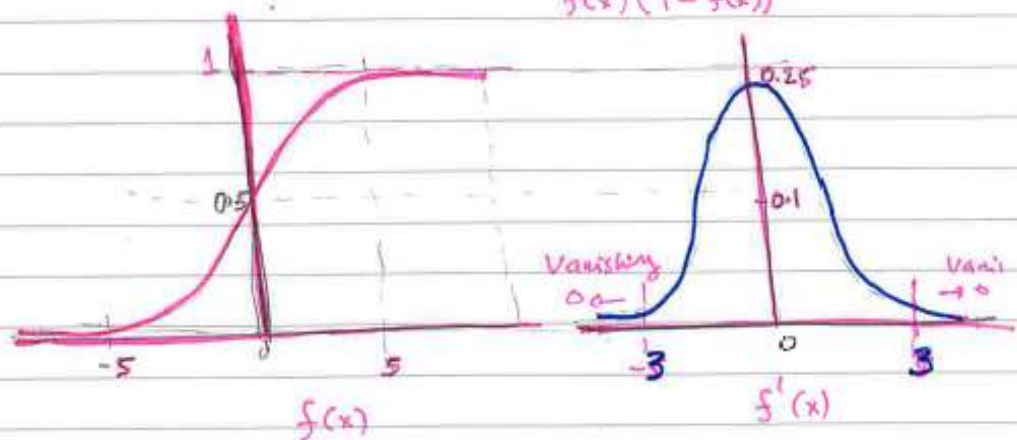
> Sigmoid function,  $f(x)$

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

> Derivative function  $\frac{df}{dx}$

$$f'(x) = \text{Sigmoid}(x) (1 - \text{Sigmoid}(x))$$

$f(x)(1 - f(x))$



→ For any input real value for the function, the output value will be in the range of 0 to 1

→ The decision for the outcome 0/1 is based on the threshold value 0.5

→ The gradient values are significant for the range -3 to 3

⇒ the values outside  $[-3, 3]$ , the function will have small gradient

⇒ Network stops LEARNING as the gradient approach zero

→ Sigmoid will return to zero/closer when the value  $< -5$  and closer to 1 when the value  $> 5$



## (b) Tanh Function (Hyperbolic Tangent)

→ The hyperbolic tangent is S-shaped like Sigmoid activation func

→ The difference is that the output is range of -1 to 1

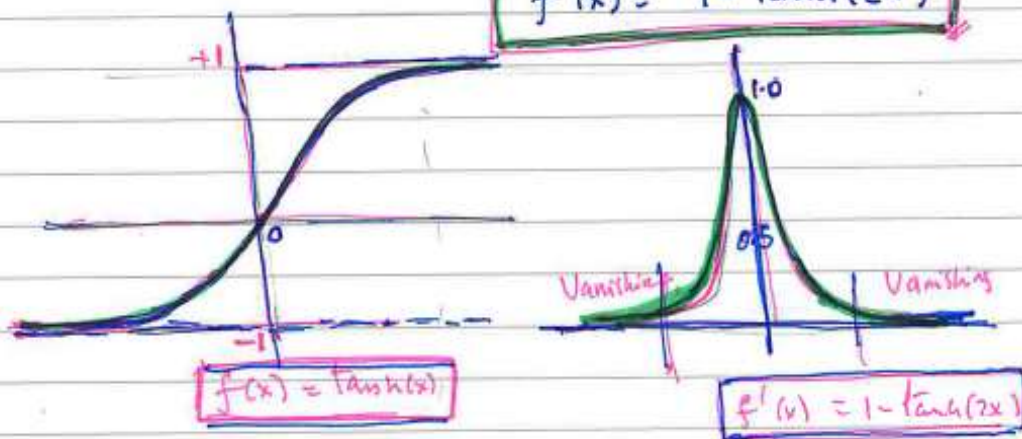
$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

→ at center, the output of the tanh function is zero

→ It is used as hidden layer in Neural network

Gradient function:  $\frac{df}{dx}$

$$f'(x) = 1 - \tanh^2(x)$$



→

→ The gradient is steeper as compared to the Sigmoid function

→ like Sigmoid, tanh also has the issue of vanishing gradient

→ Tanh is preferred to Sigmoid

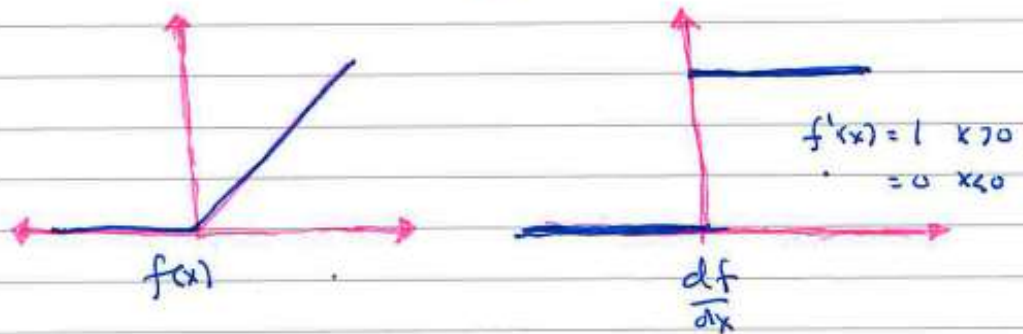
### (c) Relu Function (Rectified Linear Unit)

Relu has a linear function

$$f(x) = \max(0, x)$$

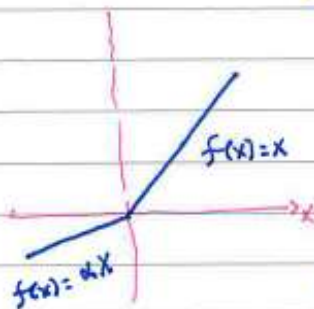
#### Gradient of Relu function

— has zero at negative slope.  
During backpropagation, it can create dead neurons which never get activated.



### (d) LeakyRelu Function (LeakyRelu)

→ LeakyRelu is a modified version of Relu. The difference is that it has a small slope for the negative ~~slope~~ values instead of a flat (0) slope.



→ The slope is determined before training. It means that slope is not learnt during training.

→

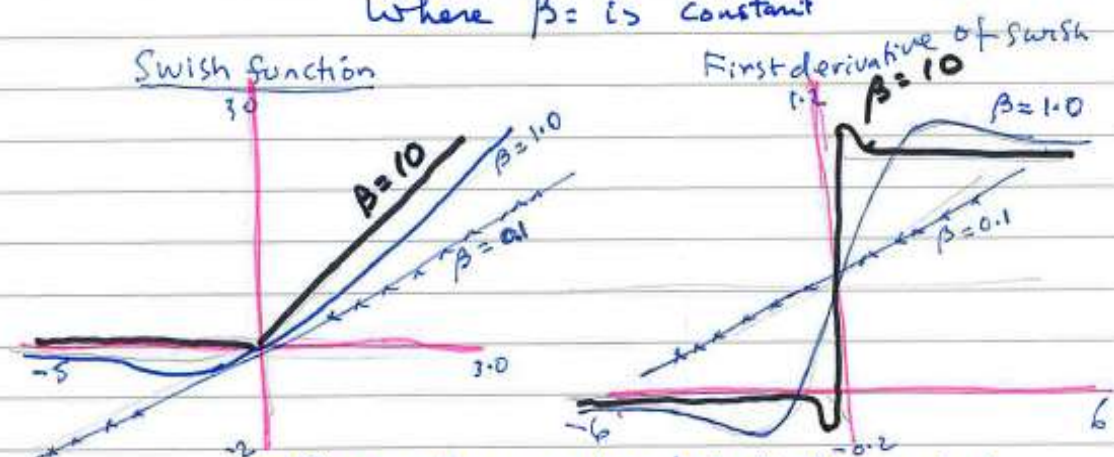


### (e) Swish Function

Swish is a modified Sigmoid function

$$f(x) = x \cdot \text{Sigmoid}(\beta x)$$

Where  $\beta$  is constant



- Researches indicated that using Swish function improves performance compared to Relu and Sigmoid

- Reason:

```
def swish(x):  
    beta = 1.0  
    return x / (1 + np.exp(-beta * x))  
output = 2  
print(swish(output))
```

The reason for the improvement is that the Swish function helps reduce the vanishing gradient problem during Backpropagation.

### (f) Softmax function

- The Softmax function is the combination of MULTIPLE SIGMOIDS

- Sigmoid is used for BINARY classification

- Softmax is used for multiclass classification



## Softmax function

$$f(z_i) = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

n Elements

⇒ Sigmoid function returns values between 0 and 1

⇒ Softmax function gives the probabilities of the data points belonging to the particular class.

Softmax is used for multiclass problem.

Eg. For the three classes, three neurons in the output layer are required

Example. For the output layer as [1.2, 0.9, 0.75] applying Softmax weights

List

$\begin{bmatrix} 1.2 \\ 0.9 \\ 0.75 \end{bmatrix}$

→

$\frac{\exp(z_i)}{\sum \exp(z_j)}$

→

$\begin{bmatrix} 0.42 \\ 0.32 \\ 0.26 \end{bmatrix}$

List

Example. For the output layer as [1.2, 0.9, 0.75] applying Softmax weights

$n=3 \quad i=1 \dots n$

```
def Softmax(x):
    return np.exp(x) / np.sum(np.exp(x))
```

output = [1.2, 0.9, 0.75]

print(Softmax(output))

$$f(1.2) = \frac{1.2}{1.2 + 0.9 + 0.75} = 0.42$$

$$f(0.9) = \frac{0.9}{1.2 + 0.9 + 0.75} = 0.32$$

$$f(0.75) = \frac{0.75}{1.2 + 0.9 + 0.75} = 0.26$$

The sum of all values = 1

Softmax is often used as the last activation function of neural network to normalize the output of neural network to a probability distribution over predicted output

## Choosing the Right Activation Functions

For hidden layer

— As a rule of thumb, begin with Relu, then try with other provided that Relu doesn't give optimum result.

→ Swish function is believed to reduce the vanishing gradient problem during back propagation

→ Tanh and Sigmoid has vanishing gradient issue.

→ For output layer →

— Regression → use linear activation function

→ Binary classification → use sigmoid/activation function

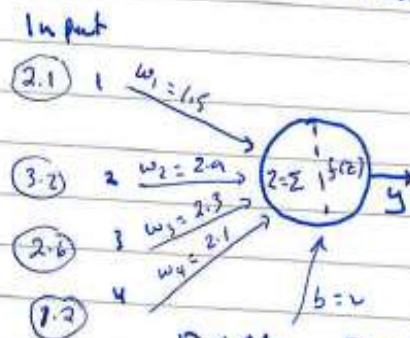
→ Multiclass classification → use softmax



# Lab# How Perceptron Computation perform (use 6 activation functions)

## Ex1a Single Perceptron Computation

→ Here, by app implimenting the perceptron model.



$$\text{Input} = [2.1, 3.2, 2.6, 1.2]$$

$$\text{weight} = [1.5, 2.9, 2.3, 2.1]$$

$$\text{bias} = 2$$

## Ex1b Single Perceptron Computation

Here we use numpy to perform the computation:

$$\text{Input} = [2.1, 3.2, 2.6, 1.2]$$

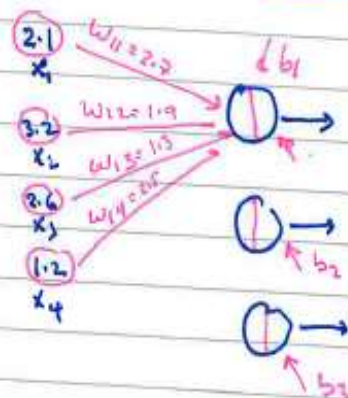
$$\text{weight} = [1.5, 2.9, 2.3, 2.1]$$

$$\text{bias} = 2$$

Compare the results of Ex1a and 1b. Which one is easy for the computation?

## Ex. 2a Multi-layer perceptron Computation in hidden layer

→ use: implimenting the perceptron model.



$$\text{Inputs} = [2.1, 3.2, 2.6, 1.2]$$

$$\text{weight 1} = [2.7, 1.9, 1.3, 2.5]$$

$$\text{weight 2} = [2.5, 3.9, 2.9, 2.5]$$

$$\text{weight 3} = [2.5, 3.9, 4.3, 5.1]$$

$$\text{bias 1} = 1, \text{bias 2} = 2, \text{bias 3} = 3$$

Ex. 2b: Using the inputs/weights/biases of Ex1a, applying numpy, perform perceptron computation.

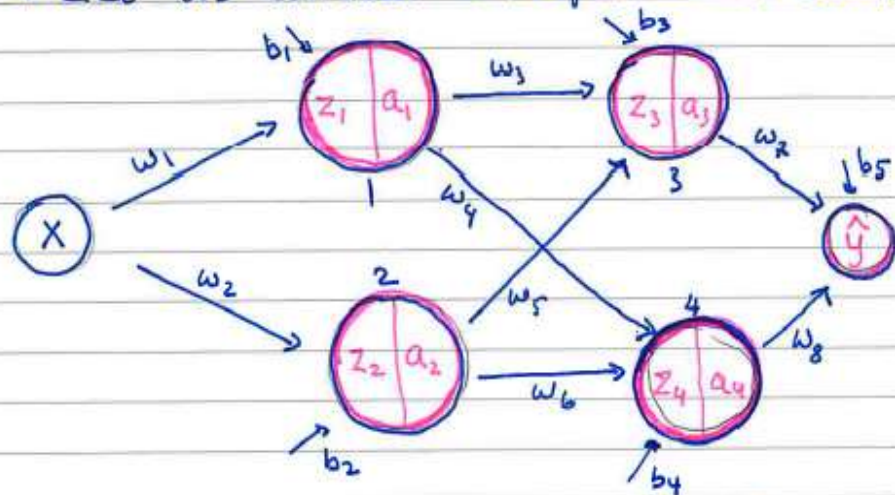
Finally → Compare the results of Ex2a and 2b. Which one is easy to perform the computation?



### 3.0 ANN - COMPUTATION

ANN → How Forward and Back propagation Performed to TRAIN the dataset?

→ Let us consider a simple neural network



- a<sub>1</sub>, a<sub>2</sub>, a<sub>3</sub>, a<sub>4</sub> are activation function
- for hidden layer, as a rule of thumb, we use Relu activation function
- z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub> and z<sub>4</sub> are linear sum of  $\sum w_i x_i + b$
- The input data (x) Pass through node 1 and node 2

→ The output from nodes 1 and 2 will feed nodes 3 and 4 respectively.

→ Finally, nodes 3 and 4 feed the output node.

→ The weights for each node labeled as w<sub>1</sub> to w<sub>8</sub> and bias b<sub>1</sub> to b<sub>5</sub>

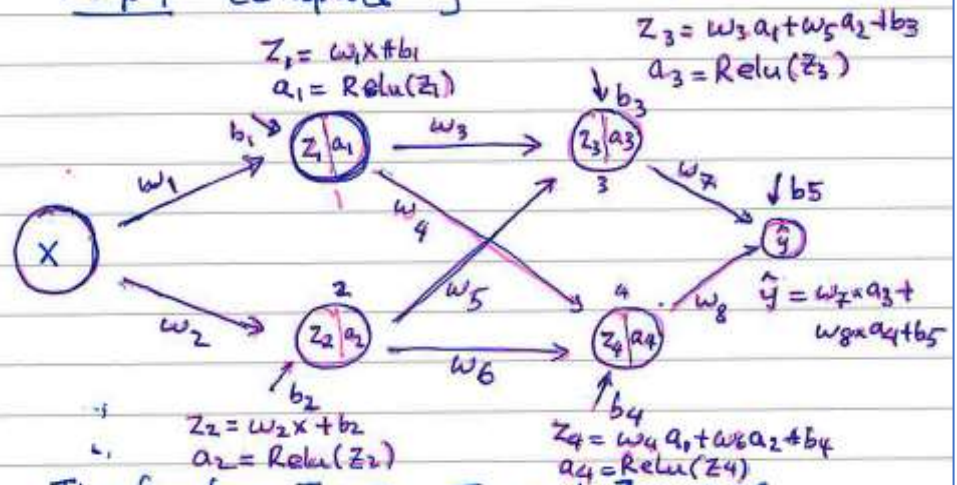
### 3.1 FORWARD Propagation / Pass.

- The two steps during forward Pass are (a) Computation of the output  $\hat{y}$
- (b) Then, compute the loss (MSE)

How to compute the output  $\hat{y}$  and loss?

For the better illustration, the following figure shows the details of forward pass calculation to get  $\hat{y}$  and loss?

Step 1 compute  $\hat{y}$



The functions  $Z_1$ ,  $Z_2$ ,  $Z_3$  and  $Z_4$  are obtained through matrix multiplication

$$\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = \begin{bmatrix} w_1 & b_1 \\ w_2 & b_2 \end{bmatrix} \begin{bmatrix} X \\ 1 \end{bmatrix} = \begin{bmatrix} w_1X + b_1 \\ w_2X + b_2 \end{bmatrix}$$

$$\begin{bmatrix} Z_3 \\ Z_4 \end{bmatrix} = \begin{bmatrix} w_3 & w_5 & b_3 \\ w_4 & w_6 & b_4 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} Z_3 \\ Z_4 \end{bmatrix} = \begin{bmatrix} w_3a_1 + w_5a_2 + b_3 \\ w_4a_1 + w_6a_2 + b_4 \end{bmatrix}$$

$$\hat{y} = \begin{bmatrix} w_7 & w_8 & b_5 \end{bmatrix} \begin{bmatrix} a_3 \\ a_4 \\ 1 \end{bmatrix}$$

$$\hat{y} = w_7a_3 + w_8a_4 + b_5$$

Step 2 Loss.



## 3.2 Backpropagation

→ The unknown parameters of the neural network are their weights and biases

⇒ The right values of weights and biases need to be determine, so that they allow the best fit for our datasets.

⇒ Best fit model means that the loss/error between the model and the dataset is Minimized.

How to find the optimized weights/bias?

→ we use the gradient decent algorithm to minimize the error between the Predicted ( $\hat{y}$ ) and the target ( $y$ )

### 3.2.1 Gradient descent

2

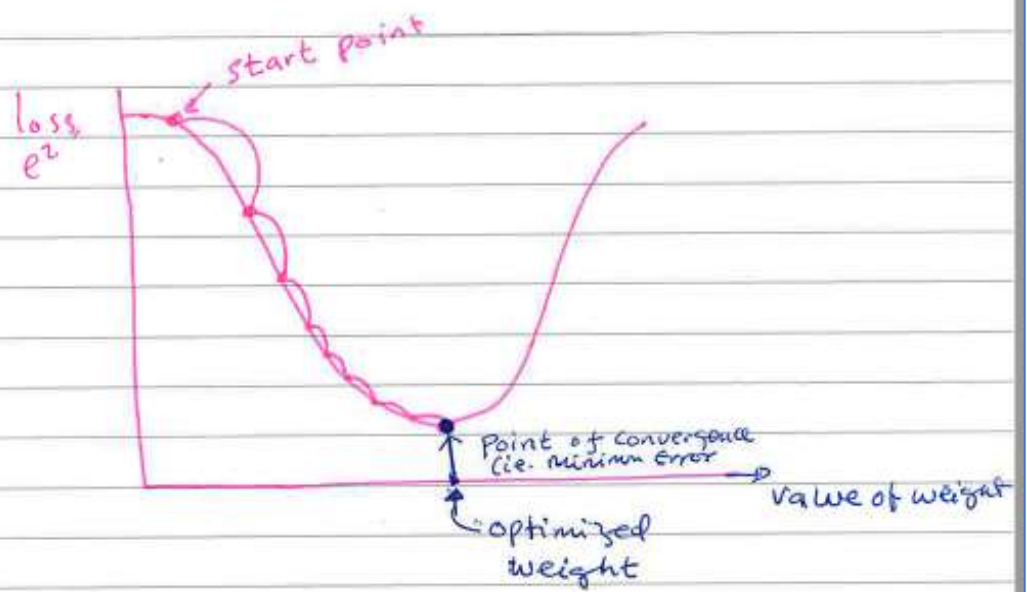
→ Gradient decent is an optimization algorithm that uses the gradient of the loss function to search for the minimum Error

» As the minimization process starts, the neural network uses random weight and biases. It means that we start at a random point on the loss surface.

» To reach the lowest point on the surface, we start taking steps along the direction of the steepest down

→ The name is therefore called GRADIENT DECENT <sup>steepest down</sup> <sub>slope</sub>





→ The gradient decent algorithm can achieve finding the point of minimum during each training epoch or iteration process.

→ For  $n^{\text{th}}$  iteration (epoch), the gradient decent back method will update the Weight and biases by the following method

$$W_i^{n+1} = W_i^n - \beta \nabla_w L \quad i=1 \dots m$$

where

$W_i^{n+1}$  = Newly updated weight/bias

$m$  = total # of weight/bias in the network

$\beta$  = Learning rate that determines the size of each steps

### Effect of Learning rate



Small Size Learning rate



Large Learning rate

→ Small size - gives good precision, but ~~take time~~ takes time

→ Large size → risk of overshooting the minimum

The partial derivative of the loss function with respect to each weight and bias is calculated during the backpropagation process as

$$\nabla_w L = \begin{bmatrix} \frac{\partial L}{\partial w_1} \\ \vdots \\ \frac{\partial L}{\partial w_n} \end{bmatrix}$$

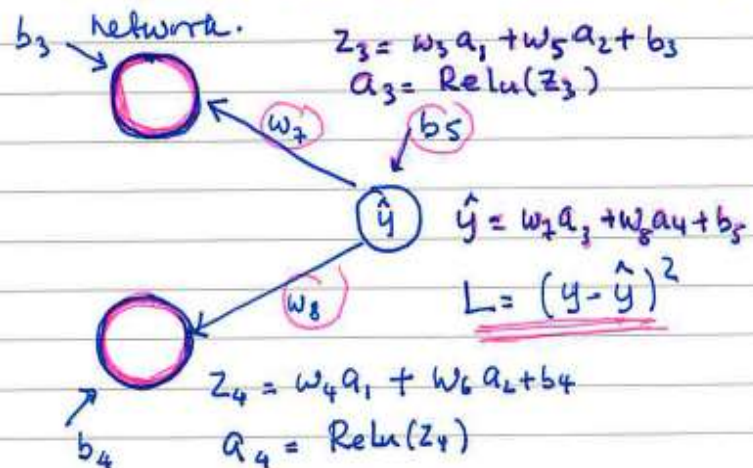
where  $L = \text{loss} = (\hat{y} - y_i)^2$

➤ Backward propagation computation process starts at the output node, it systematically progress through the layers until reaching the input layer

➤ Therefore the name backward propagation is derived from the computation process.

➤ During the computation process, the chain rule is applied for computing the derivations at each step.

**Example #1** Let us now compute the partial derivation for the Considered neural



For the above nodes, we will apply the Partial derivative with respect to  $w_7$ ,  $w_8$  and  $b_5$

⇒ We first start <sup>with</sup> the partial derivative of the loss,  $L$ , w.r.t the output  $\hat{y}$

$$L_y = \frac{\partial L}{\partial \hat{y}} = -2(y - \hat{y})$$

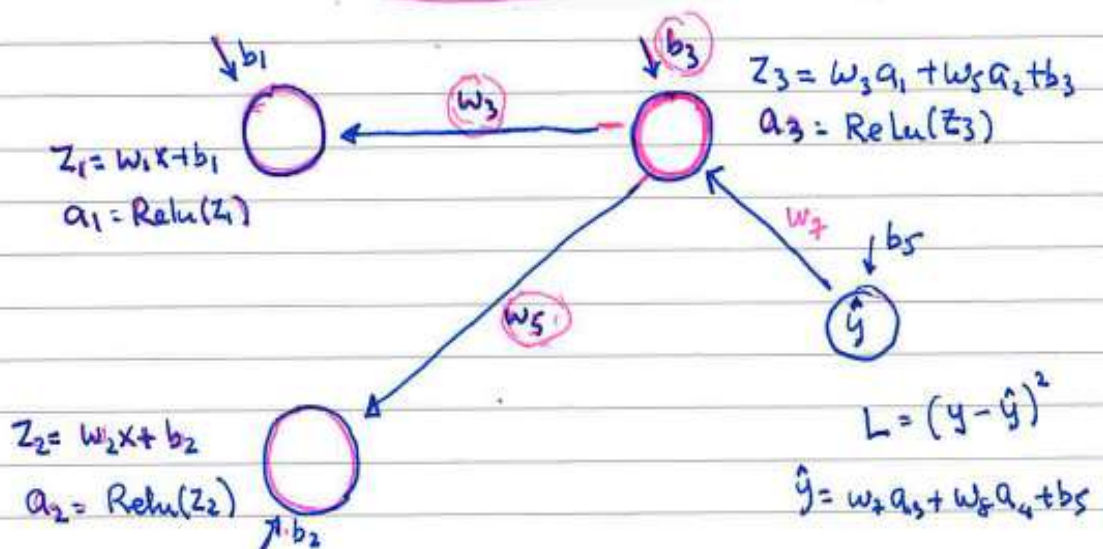
⇒ Applying the partial derivation of the loss w.r.t the weight,  $w_7$

$$\frac{\partial L}{\partial w_7} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_7} = L_y \cdot a_3$$

⇒ Apply Partial derivation w.r.t  $w_8$ , and  $b_5$

$$\frac{\partial L}{\partial w_8} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_8} = L_y \cdot a_4$$

$$\frac{\partial L}{\partial b_5} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial b_5} = L_y$$





For the above nodes, we will apply Partial derivation wrt  $w_3, w_5$  and  $b_3$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_3} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_3}$$

$$= L_y \cdot w_7 \cdot dRL(z_3) \cdot a_1$$

where  $dRL(z_3) = \frac{d \text{Relu}(z_3)}{dz_3}$

$$\frac{\partial L}{\partial w_5} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_5} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_5}$$

$$= L_y \cdot w_7 \cdot dRL(z_3) \cdot a_2$$

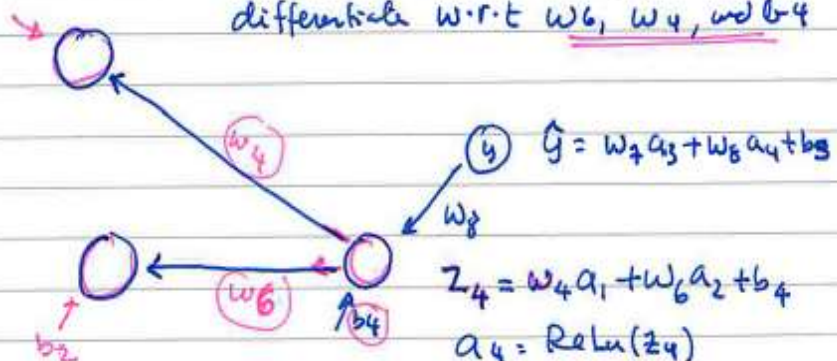
where  $dRL(z_3) = \frac{d \text{Relu}(z_3)}{dz_3}$

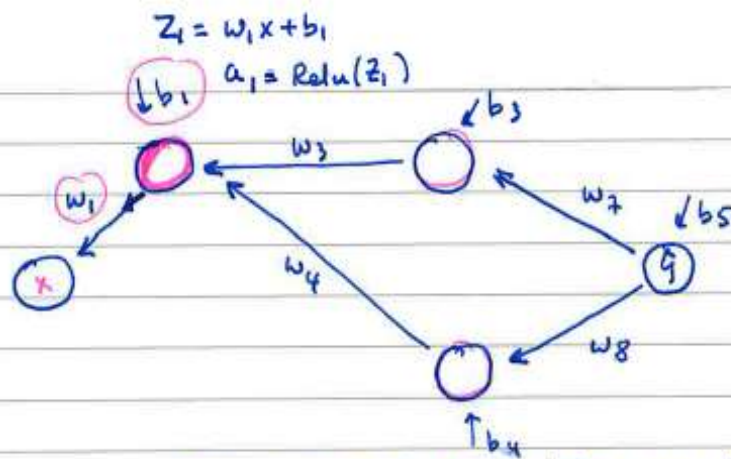
$$\frac{\partial L}{\partial b_3} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial b_3} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial b_3}$$

$$= L_y \cdot w_7 \cdot dRL(z_3)$$

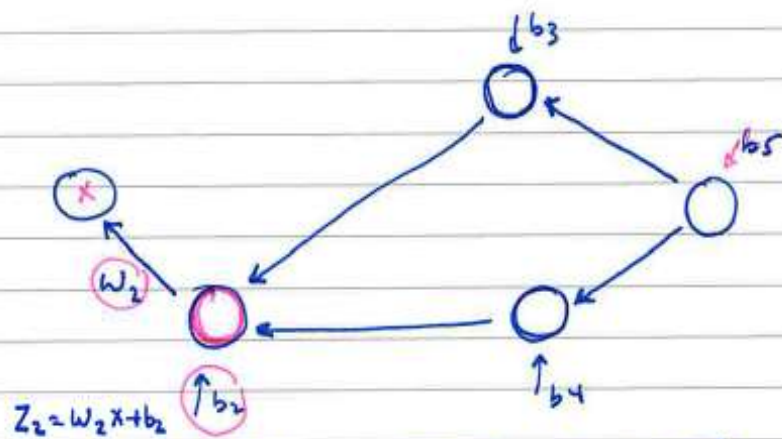
where  $dRL(z_3) = \frac{d \text{Relu}(z_3)}{dz_3}$

And we continue for the following,  
differentiate w.r.t  $w_6, w_4$ , and  $b_4$





Apply partial derivation w.r.t  $w_1, b_1$



Here we apply partial derivation w.r.t  $w_2, b_2$

### Summary

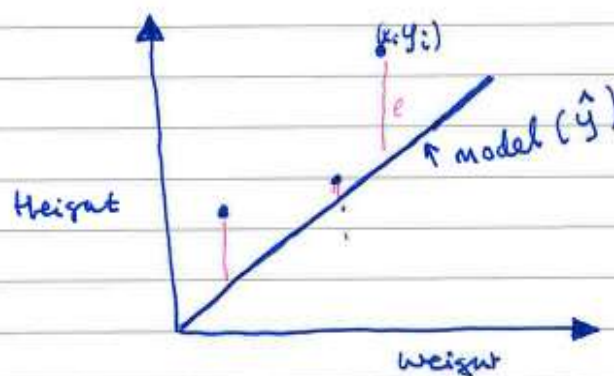
- The above example #1 illustrates how the backward propagation computation process performed through the layers starting from the output until reaching the input.
- Remember that during the ANN modeling you don't need to implement the mathematics from the scratch. The Python library will perform the computation.
- Example #2, In the next page, ~~present~~ numerical example to understand how gradient decent works.

## Example #2. Gradient Decent → Numerical example

Step-by-step ~~how~~ illustration of how gradient decent algorithm works?

→ Let us consider the height and weight dataset.

→ Task : For simplicity, let us just optimize intercept for the known slope = 0.63.



Data #	Height	Weight
1	1.4	0.5
2	1.9	2.3
3	3.2	2.9

The desire is to generate a model / regression line that relates height based on weight as

$$\text{Predicted height} = \text{Slope} * \text{Weight} + \text{Intercept}$$

We assumed slope to be = 0.63

Task! Find "Intercept".

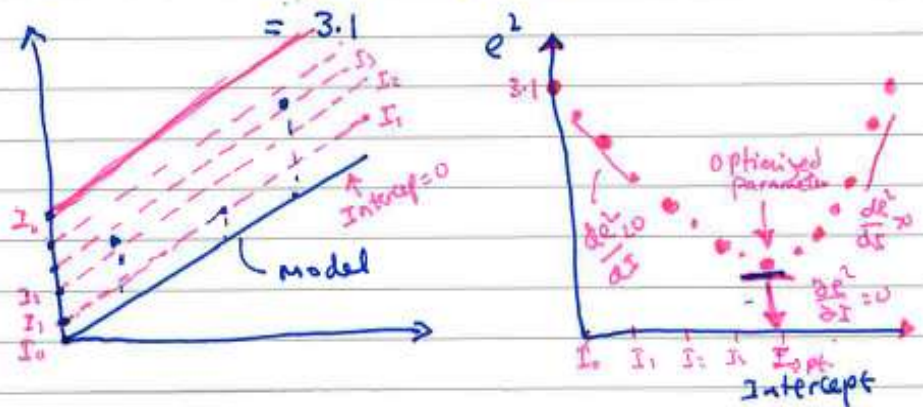


### Step 1: Calculate Residual Sum

→ For a given Predicted model ( $\hat{y}$ ) and data, we will compute the residual sum.

Example → when the intercept = 0, the Residual Sum square is

$$\Rightarrow e^2 = (1.4 - (0 + 0.64 \times 0.5))^2 + \\ (1.9 - (0 + 0.64 \times 2.3))^2 + \\ (3.2 - (0 + 0.64 \times 2.3))^2$$



> Increasing the Intercept, and calculating residual sum square, then plotting, we can see the reduction of  $e^2$  and then increasing  $e^2$ .

>> The Optimized Intercept value associated with minimum residual gives the best-fit Model

⇒ The optimized Parameter is obtained at turning point ⇒  $\frac{\partial e^2}{\partial I} = 0$

## Step 2

The best optimized Parameters are obtained by applying Least Square Error method: i.e

$$\frac{de^2}{d \text{Intercept}} = 0$$

Similarly for ~~slope~~ slope

$$\frac{de^2}{d \text{slope}} = 0$$

Since we already assumed the slope to be 0.64, we will only apply Least Square error for the Intercept.

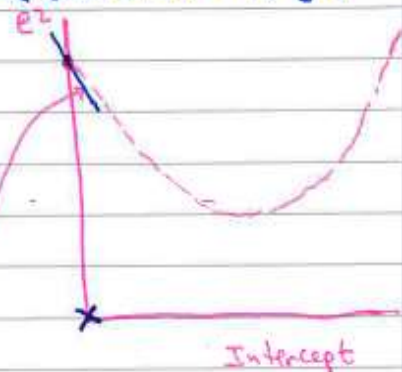
$$\begin{aligned} \Rightarrow \frac{de^2}{d \text{Intercept}} &= -2 (1.4 - (\text{Intercept} + 0.64 \times 0.5)) \\ &\quad + -2 (1.9 - (\text{Intercept} + 0.64 \times 2.3)) \\ &\quad + -2 (3.2 - (\text{Intercept} + 0.64 \times 2.9)) \end{aligned}$$

## Step 3

→ Let us start by setting the Intercept to a random number. In this case, Intercept = 0

→ So, we plug Intercept = 0 in the derivative to get the slope = -5.7

$$\begin{aligned} \frac{de^2}{d \text{Intercept}} &= -2 (1.4 - (0 + 0.64 \times 0.5)) \\ &\quad + -2 (1.9 - (0 + 0.64 \times 2.3)) \\ &\quad + -2 (3.2 - (0 + 0.64 \times 2.9)) \\ &= -5.7 \end{aligned}$$





#### Step 4. Determine Step Size

Gradient decent determines the Step size by multiplying the slope by a small number called Learning rate (Eg, 0.1, 0.01)

→ When the intercept is zero, the Step size

$$\begin{aligned}\Rightarrow \text{Step size} &= \text{Learning rate} \times \text{Slope} \\ &= 0.1 \times (-5.7) \\ &= -0.57\end{aligned}$$

#### Step 5 Compute / Update New Intercept

$$\text{New Intercept} = \text{Old Intercept} - \text{Step size}$$

For the given Step size, the new Intercept

$$\text{New Intercept} : \text{Old Intercept} - \text{Learning rate} \times \text{Slope}$$

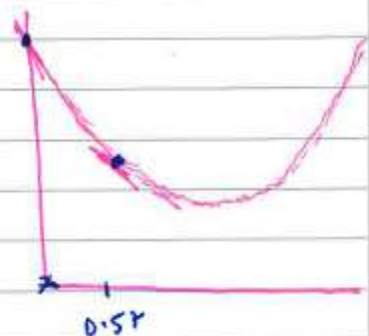
$$\text{New Intercept} : 0 - (-0.57) = 0.57$$

⑨ Now take another Step, we go back to the derivative and plug the new Intercept (0.57)

$$\begin{aligned}\frac{dL}{d\text{Intercept}} &= -2(1.4 - (0.57 + 0.64 \times 0.5)) \\ &+ -2(1.9 - (0.57 + 0.64 \times 2.3)) \\ &+ -2(3.2 - (0.57 + 0.64 \times 2.9)) \\ &= -2.3\end{aligned}$$

$$\begin{aligned}\text{Step size} &= 0.1 \times (-2.3) \\ &= -0.23\end{aligned}$$

$$\begin{aligned}\text{New Intercept} &= 0.57 - (-0.23) \\ &= \underline{0.8}\end{aligned}$$



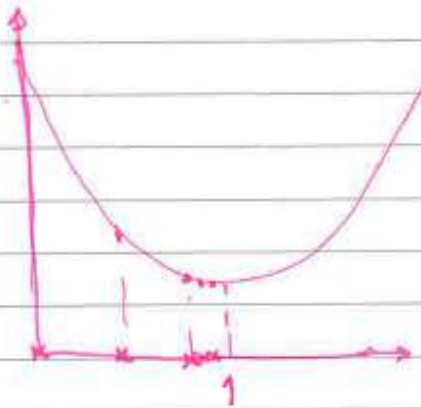


⑤ Repeat for Intercept = 0.8

$$\begin{aligned} d_{\theta^2} &= -2(1.4 - (0.8 + 0.64 \times 0.5)) \\ d_{\text{Intercept}} &+ -2(1.9 - (0.8 + 0.64 \times 2.3)) \\ &+ -2(3.2 - (0.8 + 0.64 \times 2.9)) = \underline{\underline{-0.9}} \end{aligned}$$

$$\begin{aligned} \text{Step Size} &= \text{Learning rate} \times \text{Slope} \\ &= 0.1 \times (-0.9) \\ &= \underline{\underline{-0.09}} \end{aligned}$$

$$\text{New Intercept} = 0.8 - (-0.09) = \underline{\underline{0.89}}$$



→ Again, we take another step, and the new intercept = 0.92

→ And then, we take another step, the new intercept = 0.94

→ we take another step, the new intercept = 0.95

→ After 6 Steps, the gradient decent estimates for the intercept = 0.95

The Least Square estimate for the intercept is also = 0.95

The Question is ~~that~~ how does gradient know stop taking steps?

⇒ When the Step Sizes become closer to zero, the gradient decent process stops.

⇒ Step size close to ZERO occurs when the slope ( $\frac{dL}{d\text{Int}}$ ) close to ZERO

⇒ The minimum step size is 0.001 or smaller is the common practice.

⇒ If the Slope is 0.009 and If we plug the Learning rate = 0.1, we get the step size = 0.0009, which is smaller than 0.001, so gradient decent would stop.

⇒ Gradient decent also includes a limit on the number of steps it will take before giving up. In practice the maximum number of steps = 1000 or greater

⇒ On the other hand, if we define the maximum number of steps, the gradient decent will stop even if the Step Size is Large.

### Gradient decent algorithm

We understand how gradient decent can estimate the intercept.

To estimate both slope and intercept.

Step 1: Sum Square Error,  $L = e^2$

Step 2: take derivation of the loss function w.r.t slope and intercept ( $E_1$ ,  $E_2$ )

Step 3: plug random initial value for slope and intercept in the gradient



Step 4: Calculate Step Size = ~~Learning rate \* gradient~~  
= Learning rate \* gradient

Step 5: Calculate New Slope and Intercept

$$\text{New slope} = \text{old slope} - \text{Learning rate} \times \frac{\partial e^L}{\partial \text{slope}}$$

$$\text{New Intercept} = \text{old intercept} - \text{Learning rate} \times \frac{\partial e^L}{\partial \text{intercept}}$$

Go to Step 3:

→ Add/Plug the new slope and new intercept in the gradient.

→ end Step 4. Calculate new Step Size

Step 5 - Calculate new slope/new intercept.

→ Repeat steps 3-5 until the Step Size is small (0.001) or Reaches to the maximum number of steps

The gradient:

Eq. 8

$$\frac{\partial e^L}{\partial \text{slope}} = -2 \times 0.5 (1.5 - (\text{Intercept} + \text{slope} \times 0.5)) \\ + -2 \times 2.9 (3.2 - (\text{Intercept} + \text{slope} \times 2.9)) \\ + -2 \times 2.3 (1.9 - (\text{Intercept} + \text{slope} \times 2.3))$$

Eq. 9

$$\frac{\partial e^L}{\partial \text{Intercept}} = -2 (1.5 - (\text{Intercept} + \text{slope} \times 0.5)) \\ + -2 (3.2 - (\text{Intercept} + \text{slope} \times 2.9)) \\ + -2 (1.9 - (\text{Intercept} + \text{slope} \times 2.3))$$



### 3.2.2 TYPES of Optimizers and How Optimizers work?

→ During<sup>the</sup> backpropagation process, Optimizers are used to update weights and biases.

→ With the updated weight/biases, the forward pass computes to get a reduced error.

→ During the training process of neural network, our aim is to try and minimize the loss function by updating weight/bias as:

$$w_{i+1} = w_i - \eta \cdot \frac{\partial \text{Loss}}{\partial w_i}$$

$$b_{i+1} = b_i - \eta \frac{\partial \text{Loss}}{\partial b_i}$$

where  $\eta$  = learning rate

$\frac{\partial \text{Loss}}{\partial w_i}, \frac{\partial \text{Loss}}{\partial b_i}$  = gradient of error w.r.t weight/bias

$w_i, b_i$  = old weight/bias

$w_{i+1}, b_{i+1} \Rightarrow$  Newly updated weight and bias

→ The detail of the mathematics how gradient descent works, along with numerical example are shown in the previous section

When updating parameter with gradient descent, the learning rate is always constant

$$\theta_{i+1} = \theta_i - \eta \cdot g_t, \quad g_t = \frac{\partial L}{\partial \theta_i}$$

$\eta$  = LR = constant for the whole training process

→ — Researchers came to an idea that an optimizer can change the LEARNING RATE as per previous gradient. By doing so the optimization process CONVERGE FASTER.

(1) Adagrad

→ For this Adagrad was born. → Adaptive gradient

→ The Learning rate becomes

$$\eta' = \frac{\eta}{\sqrt{\alpha_t + \epsilon}}$$

Initialize  $\alpha = 0$

$$\alpha_t = \alpha_{t-1} + g_t^2, \rightarrow g_t^2 = \sum \left( \frac{\partial L}{\partial \theta_i} \right)^2$$

→ In every iteration, we add the square of the gradient in  $\alpha_t$  so that it will have the history of the past gradients.

→ Now the learning rate will vary for every iterations

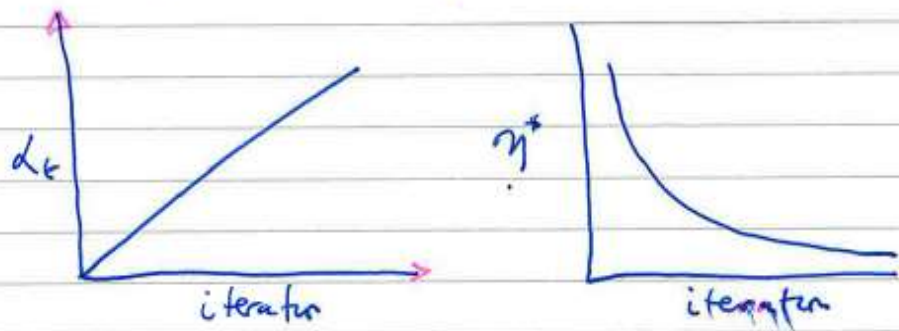
$$\theta_{i+1} = \theta_i - \frac{\eta}{\sqrt{\sum \left( \frac{\partial L}{\partial \theta_i} \right)^2 + \epsilon}} \cdot g_t$$

$\epsilon = 10^{-8}$  in case  $\alpha_t = 0$

## Weakness of Adagrad.

For every iterations, we add  $(\frac{\partial l}{\partial \theta_i})^2$ , thus  $d_t$  will increase. As a result the  $\eta^* = \frac{\eta}{\sqrt{d_t + \epsilon}}$  will be smaller for every iteration.

Thus the continual decay of  $\eta^*$  (LR) is the weakness of Adagrad. Since for small value of  $\eta^*$ , the training process will stop.



## → Adadelta

To overcome the issue of Adagrad, Adadelta was born.

→ Here we don't need to choose learning rate. Adadelta automatically computes the learning rate.

Initialize  $d=0$ ,  $\Delta x=0$

$$x_t = x_{t-1} + g_t^L \quad \text{--- Adagrad}$$

Adadelta  $\rightarrow$  
$$d_t = \rho d_{t-1} + (1-\rho) \cdot g_t^L$$



$$\Delta \theta_t = - \frac{\sqrt{\Delta X_t + \epsilon}}{\sqrt{\alpha_t + \epsilon}} \cdot g_t$$

$$\Delta X_t = \rho \Delta X_{t-1} + (1-\rho) \Delta \theta_t^2$$

$$\theta_{t+1} = \theta_t + \Delta \theta_t$$

$\Delta X$  - is the accumulated rate used to calculate learning rate

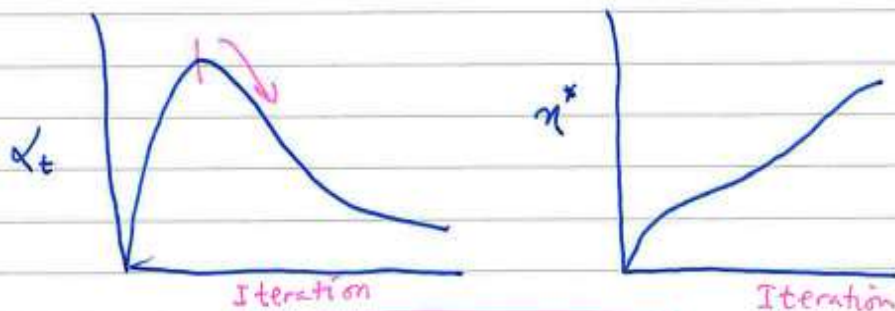
$\rho$  - is used to avoid an infinity increase of  $\alpha_t$  value, as show for Adagrad.

- In case of Adadelta,  $\alpha_t$  value increase upto so iteration then decrease.

- Therefore, there is no problem of  $\eta^*$  decay. This is made possible by  $\rho$  - hyperparameter.

→  $\rho$  is also known as decay constant

→  $\rho$  value is typically = 0.9



$$\theta_{t+1} = \theta_t + \Delta \theta$$

$\Delta \theta$  is calculated by Adadelta

### (3) Adam

Adam stands for adaptive moment estimation

Adam updates / adjust the learning rate adaptively for each parameters in the model based on the history of gradients  
Calculates for each parameters

Adam optimizer

Initialize  $M_0 = 0 \Rightarrow$  1st moment vector  
 $V_0 = 0 \Rightarrow$  2nd " "

$$m_t = \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t \quad g_t = \frac{\partial L}{\partial \theta_i}$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) \cdot g_t^2$$

$$\theta_t = \theta_{t-1} - \frac{\eta \cdot \hat{m}_t}{\sqrt{\hat{v}_t}}$$

$$\text{Where } \hat{m} = \frac{m_t}{1 - \beta_1^t}$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

default, 0.9, 0.999.

$\beta_1, \beta_2$  are hyper parameter of adam, are initial decay rates used when estimating the first and the second moment gradients

$m_t$  is the first order moment (i.e. mean of gradients)

$v_t$  is the second order moment, used to adjust the learning rate at time step,  $t$

$\eta$  = global learning rate

$$\epsilon \approx 10^{-8}$$

#### (4) RMSprop

— Root mean square propagation optimizer

→ Use exponentially decay average of squared gradient and discards history from the <sup>extreme</sup> past.

$$\theta_{i+1} = \theta_i - \frac{\eta}{\sqrt{r_i + \epsilon}} \cdot g_i \quad g_i = \frac{\partial \mathcal{L}}{\partial \theta_i}$$

where,  $r$  is exponentially decaying average

$$r_t = \beta r_i + (1 - \beta) \cdot \left( \frac{\partial \mathcal{L}}{\partial \theta_i} \right)^2$$

$\beta$  = tuning / hyper parameter

$$\epsilon = 10^{-8}$$



## Types of optimizers

In keras, a number of optimizers are available

- SGD
- RMSprop
- Adam
- AdamW
- Adadelta
- Adagrad
- Adamax
- Adafactor
- Nadam

- During laboratory exercise, you can test the performance of the optimizers.

→ The most commonly used is Adam.

→ In the following we will review just some of these.

## 4.0 ANN MODELING.

### Workflow - Summary

#### 4.1 Step 1: Data - preprocessing / feature Eng

- Load data file
- Data - Preprocessing
  - cleaning
  - feature selection
- → Standardisation / scaling

#### 4.2 Step 2: ANN Modeling

- Splitting Scaled data into trainig/test
- Creating ANN Model / Fully connected
  - Input layer
  - hidden layer
  - Out put layer
- Compile the model → model.fit()
  - perform optimization
- Fitting ANN with training data

#### 4.3 Step 3: Model prediction

- Perform inverse transform of Scaled data to the original
- Predict with test data
- Compare predicted ( $y_{pred}^{test}$ ) with the true ( $y_{true}$ )

#### 4.4 Step 4: Model Performance accuracy analysis

- Using  $y_{pred.}$  and  $y_{test}$ , perform the goodness fit of the model.

$R^2$ , MSE

→ Following these, the next page present Step by step ANN modeling

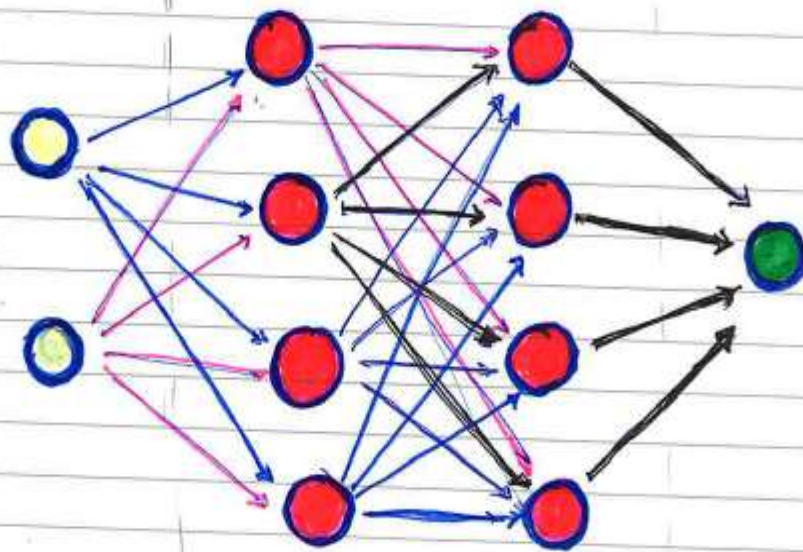
## 4. ANN Modeling

### Laboratory ANN Modeling

Consider the following network.  
We will learn the ANN modeling algorithm.  
In the previous section, we learned the how perceptrons perform the computation to get the output, and based on the loss function, how the gradient decent algorithm performs to update the weights and biases.

In this section we will learn how the built in tensorflow / keras library perform the computation.

We will step-by-step look at how the computation performed.



← Input → ← Hidden layers → ← Output →



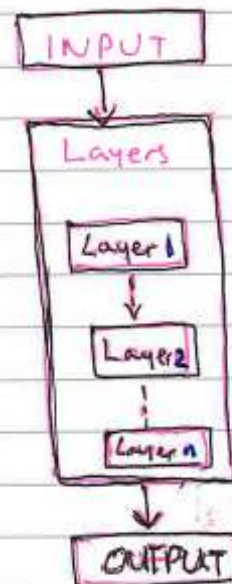
How to build ANN and train data?

Let us examine / describe the model definition

(a) Sequential() → Initialize the ANN

We start the modeling with a Sequential() function. It specifies that the network is a linear stack of layers. Example: → Describe the network

Sequential model



(b) Model.add()

— It allows to add layers

(c) Dense

— It means that neurons between Layers are FULLY CONNECTED

(d) input\_dim

— It defines the number of features in the training dataset

(e) activation

- defines activation function

Example Relu, tanh, Sigmoid...

(f) loss

- It allows us to select the cost/loss function

Ex. MSE

(g) Optimizers

→ It allows to select the learning algorithm

Ex. adam, SGD, RMSopt, adagrad,

(h) metrics

- It allows to select the performance metrics to be saved for further analysis

Ex.  $R^2$ , MSE

(i) model.fit()

→ To initialize the training

(j) kernel\_initializer

→ This allow to initialize weight and bias

Feature scaling is also known as data normalization. is part of data-preprocessing

It is reported that when using gradient-decent-based optimization algorithm, feature-scaling can help speedup convergence and improve model performance. - (both accuracy and stability of ML model)

→ For regression problem, it is often desirable to scale / or / transform both

\* → Input features and

\* → Target variables

The two most popular techniques for scaling numerical data prior to modelling are

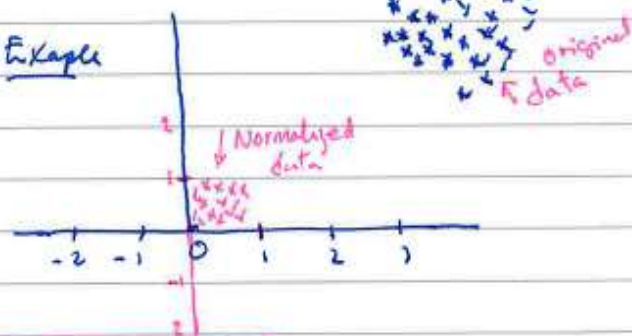
(1) Normalization

(2) Standardization

(A) Normalization:

→ Normalization is rescaling of data from the original range so that all values are within the new range of 0 and 1

Example



$$X_{\text{Norm}} = \frac{X - X_{\min}}{X_{\max} - X_{\min}} \Rightarrow X_{\text{Norm}} = [0, 1]$$

If we want  $X_{\text{Norm}}$  to be between  $[a, b]$

$$X_{\text{Norm}} = a + \frac{(X - X_{\min})(b - a)}{X_{\max} - X_{\min}}$$



### (\*) Example : Data normalization

Assume, For a data set, the min and max observable values are 30 and -10

What is the normalized value of 18.8?

$$y = \frac{x - x_{\min}}{x_{\max} - x_{\min}}$$

$$= \frac{18.8 - (-10)}{30 - (-10)}$$

$$= \underline{0.72}, \text{ which is in } [0, 1]$$

→ We can normalize dataset using the Skikit-learn object MinMaxScaler

→ The default scale for the MinMaxScaler is to rescale variables into the range  $[0, 1]$ .

Example:

$x = df.iloc[:, 1:5].values$

~~from sklearn import preprocessing~~  
~~min\_max\_scaler = preprocessing.MinMaxScaler~~

Example

```
import sklearn import preprocessing  
min_max_scaler = preprocessing.MinMaxScaler(feature_range=(0,1))
```

# Scaled feature

```
scaled_x = min_max_scaler.fit_transform(x)
```

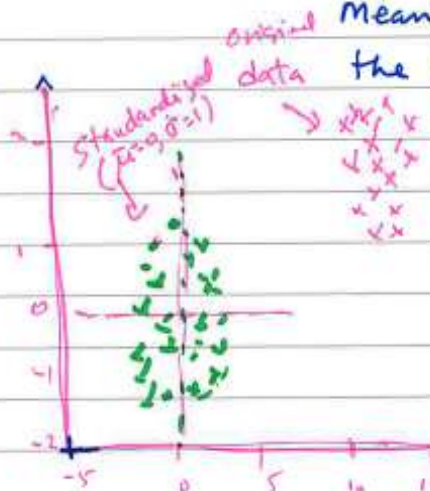
# Display

```
print("After min max scaling: \n", scaled_x)
```

## (2) Standardization

Feature standardization makes the value of each feature in the data have zero mean and unit variance.

→ The method calculates the statistical mean and standard deviation of the attribute values, subtract the mean ( $\bar{x}$ ) from each value, and divide the result by the Standard deviation ( $\sigma$ )



$$x_{std} = \frac{x - \bar{x}}{\sigma}$$

→ Subtracting the mean from the data is called Centering

→ whereas dividing by the standard deviation is called Scaling

— The method sometimes called 'center scaling'

Mean →

$$\bar{x} = \frac{\sum x_i}{\text{Count}(x)}$$

Standard deviation →

$$\sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{\text{Count}(x)}}$$

Example:

Assume that  $\bar{x} = 10$ ,  $\sigma = 5$ .

Using Standardization, what is the standard value of 20.7?

$$y_{std} = \frac{x - \bar{x}}{\sigma} = \frac{20.7 - 10}{5}$$

$$y = 2.14$$

You can Standardize your dataset using  
Scikit-learn object StandardScaler

Example

```
x = df.iloc[:, 1:5].values
```

Import preprocessing library

```
from sklearn import preprocessing
```

```
Standardisation = preprocessing.StandardScaler()
```

```
# Scaled feature
```

```
Standardized_x = Standardisation.fit_transform(x)
```

```
# Display
```

```
print('After Standardisation : \n', Standardized_x)
```

Note:

→ The split data NEEDS to be standardised  
before ML modeling

→



4.0

Example

ANN: Modeling Application

- Regression

Assume dataset

X | y

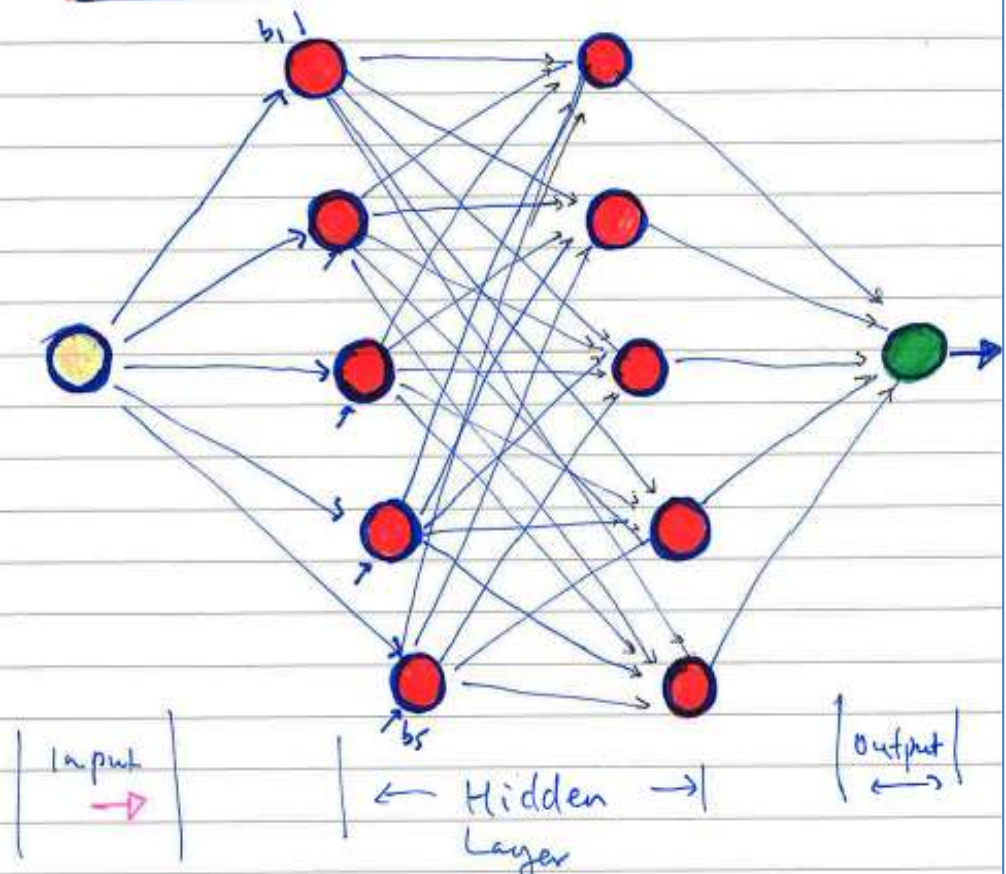
- a single feature
- a single target

- 2 hidden layers with 5 nodes each
- Activation = Relu.
- Loss = mse
- Optimizer = adam.

Task → ① Create the ANN model

② Show Step-by-step modeling/performance evaluation

~~ANN Model~~



## 4. ANN - Modeling

### Step 1: Data Preprocessing

Before modeling, data must be cleaned, appropriate features must be selected and finally, it will be scaled for the better <sup>model</sup> performance.

- This section has been done during Lab#. You must run the process and the final cleaned data saved in excel will be loaded here.

#### a) # Load cleaned data

Import Pandas as pd

Import numpy as np

logData = pd.read\_excel('ballistic.xlsx')

logData.head()

Out:      Vo      ang      Time R

0      -      -      -      -

1      -      -      -      -

2      -      -      -      -

3      -      -      -      -

4      -      -      -      -

#### b) Separate Target and Predictor variables

TargetVariable = ['Time']

or # TargetVariable = ['R']

Predictors = ['Vo', 'ang']

X = logData[Predictors].value

y = logData[TargetVariable].value

## (c) Standardise and split data for training/test

> (C1) # Scaling / standardisation of dataset  
from sklearn.preprocessing import StandardScaler

PredictorScaler = StandardScaler()

TargetVarScaler = StandardScaler()

(C2) # Storing the fit object

PredictorScalerFit = PredictorScaler.fit()

TargetVarScalerFit = TargetVarScaler.fit()

(C3) # Generating the Standardised values of  
X and y

X = PredictorScalerFit.transform(X)

y = TargetVarScalerFit.transform(y)

(C4) # Split the scaled data into training / Test

> from sklearn.model\_selection import train\_test\_split

X\_train, X\_test, y\_train, y\_test = train\_test\_split(X, y, test\_size=0.3,  
random\_state=42)

(C5) Quick sanity check with the shape of training  
and testing dataset

print('X\_train:', X\_train.shape)

print('y\_train:', y\_train.shape)

print('X\_test:', X\_test.shape)

print('y\_test:', y\_test.shape)

Out: X\_train: (210, 2)

y\_train: (210, 1)

X\_test: (90, 2)

y\_test: (90, 1)



## STEP 2: ANN Modeling

### (2a) Import the libraries

```
from keras.models import Sequential  
from keras.layers import Dense
```

### (2b) Creating ANN

→ `model = Sequential()`

#### (2b-I) Defining Input layer / First hidden layer (5 nodes)

→ `model.add(Dense(unit=5, input_dim=1, kernel_initializer='normal', activation='relu'))`

#### (2b-II) Defining the second hidden layer (5 nodes)

∴ NB. [ After the first hidden layer, we don't have to specify input-dim as keras configures it automatically ]

→ `model.add(Dense(unit=5, kernel_initializer='normal', activation='relu'))`

#### (2b-III) Define the output neuron

[ output neuron is a single fully connected node ]

→ `model.add(Dense(1, kernel_initializer='normal'))`  
↑  
`units=1`

STEP(2c) Compile the model → • `compile()`

→ `Model.compile(loss='mean_squared_error',  
optimizer='adam')`

[other optimizers: SGD, RMSopt, ...]

STEP(2d) Fitting the ANN to the training data  
• `fit()`

→ `model.fit(X_train, y_train, batch_size=20, epochs=1000,  
verbose=0)`

# here we define the model bit  
as history thinking that the model  
performance history parameter will be  
displayed at the end.

→ `history = model.fit(X_train, y_train, batch_size=20,  
epochs=1000, verbose=0)`  
`verbose=0` = ~~training progress~~  
(silent) = will not be seen  
`verbose=1` = will be seen.  
(animation) for each epoch.  
(progress bar)  
`verbose=2` → one line per  
epochs.

Step 2e: Model Summary

To display model Summary → • `summary()`

→ `model.summary()`

Output	Layer (type)	Output Shape	Param #
	dense_1 (Dense)	(None, 5)	15
	dense_2 (Dense)	(None, 5)	30
	dense_3 (Dense)	(None, 1)	6



### STEP 3: Model Prediction

→ # Fitting ANN to the training data • fit()  
model.fit(X\_train, y\_train, batch\_size=20, epochs=100,  
Verbose=0)

# Generating (y-pred) Predictions on testing data  
• Predict()  
→ Predictions = model.Predict(X\_test)

# Scaling the predicted data back to the original dataset  
• inverse\_transform()  
\* → Predictions = TargetVarScalarFit.inverse\_transform(Predictions)

# Scaling the y\_test data back to the original dataset  
\* → y\_test\_orig = TargetVarScalarFit.inverse\_transform(y\_test)

# Scaling the X\_test data back to the original dataset

→ Test\_Data = PredictorScalarFit.inverse\_transform(X\_test)

→ Display data → Create Data Frame ( )

TestingData = pd.DataFrame(data=Test\_Data, columns=  
Predictors)

TestingData['True data'] = y\_test\_orig

TestingData['ANN-predicted'] = Predictions

TestingData.head()



Out put:

	Vo	ang	True data	ANN Predicted
0	-	-	-	-
1	-	-	-	-
2	-	-	-	-
3	-	-	-	-
4	-	-	-	-

Display Predicted and true data

```
import matplotlib.pyplot as plt  
from matplotlib.pyplot import figure
```

```
figure(figsize=(8, 6), dpi=380)
```

```
plt.plot(y_test_orig)
```

```
plt.plot(predictions)
```

```
plt.ylabel(
```

```
plt.xlabel(
```

```
plt.legend(
```

```
plt.show()
```

## 5 Summary

In this chapter both the concept how the ANN computation performed and the ANN modeling in Keras.

In chapter 4, the step-by-step process of ANN is presented.

During Lab class, you will use synthetic data that is computed from the physics model. Then, you will use the data to train/model with ANN. From the result, you will learn how ANN predict/recover the physics data.

After testing the ~~say~~ ANN with the synthetic data, you will use field data that you have performed data preprocessing during Lab 1.

From these two exercises, you will have good understanding how ANN works.