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## Machine Learning – Energy Systems Course at University of Calgary

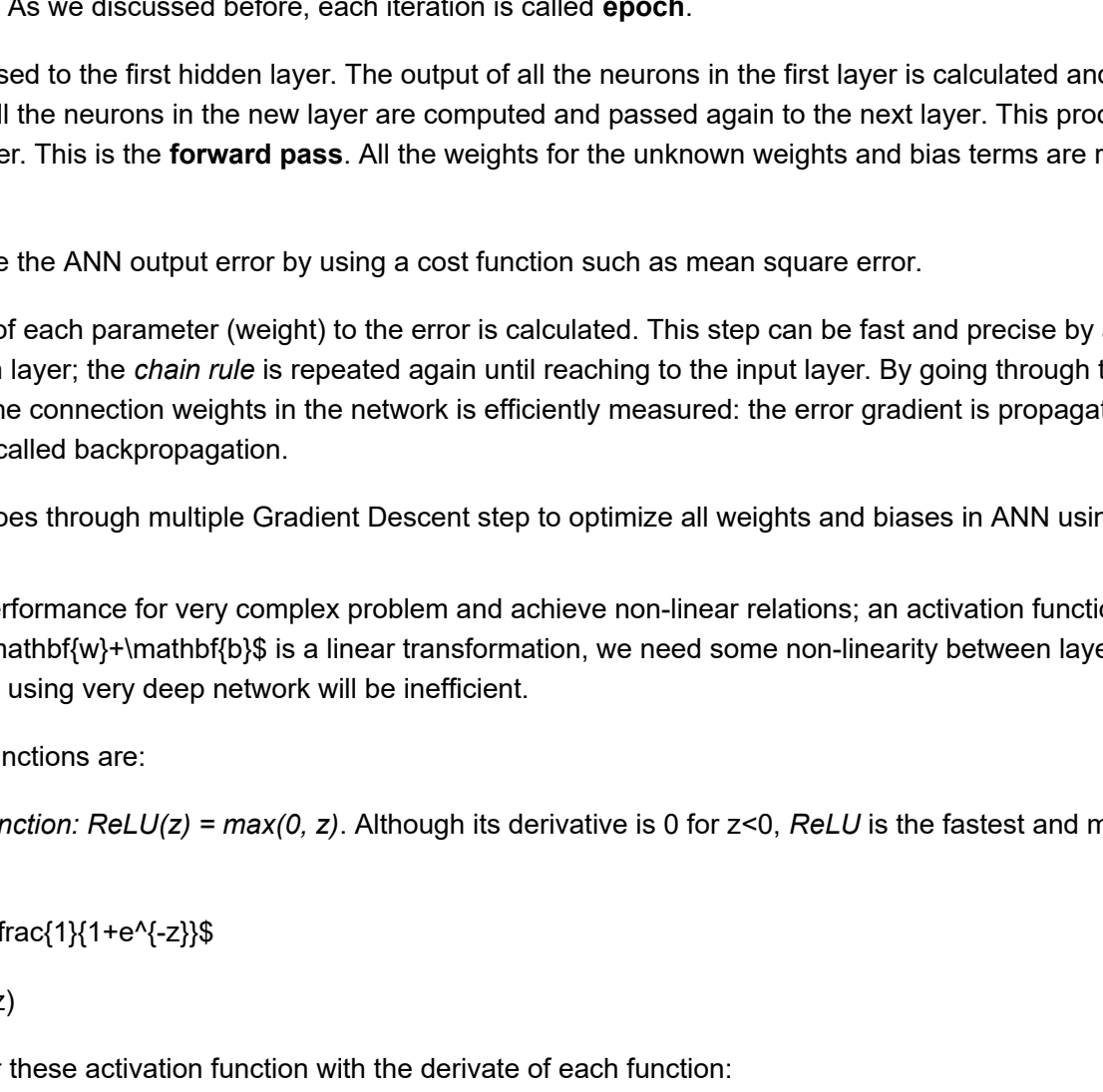
• Instructor: [Metodi Rozendehy](#)

## Artificial Neural Network (ANN)

We are inspired by birds to fly but not exactly doing the same as birds do. planes do not flap their wings. This is the key for Artificial Neural Network (ANN). ANN looks at the human brain's architecture to build an intelligent machine. However, ANN has gradually become quite different from the biological term. ANN is the very core of Deep Learning. Deep Learning usually involves much more successive layers of representations. It is a major field of Machine Learning for tackling very complex problems that Machine Learning is unable to resolve such as classifying billions of images, speech recognition, computer vision. Deep Learning requires big data in order to receive higher performance than Machine Learning and ANN.

## How ANN Works

The Figure below shows a simple ANN architecture. It consists of input layers, hidden layer and output layer. Input layer is number of features in training set. Hidden layer is made up of neurons; here we have two neurons, and final layer is output layer, which is number of target for each training instance. When all the neurons in a layer are connected to every neuron in the previous layer, it is called a **fully connected layer** or a **dense layer**. A bias neuron is also considered for hidden layer and output layer.



The outputs of a layer of artificial neurons for several instances at once is calculated by:

$$SO_i(\text{matrix}(w_{ij}))(\text{matrix}(x))=\text{varphi}(\text{matrix}(w_{ij})\text{matrix}(w_{ij})+\text{matrix}(b_i))\$$$

- $X$  is the matrix of input features.
- $W$  is the connection weights for the neurons except the bias neuron.
- $b$  is the weights for biased neurons.
- $\text{varphi}$  is a universal activation function.

For the ANN architecture above:  $\text{matrix}(w_{ij})=x_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$ ,  $\text{matrix}(w_{ij})=w_{ij}$  and  $\text{matrix}(b_i)=b_i$ ,  $\text{matrix}(b_i)=b_i$ ,  $\text{matrix}(b_i)=b_i$ ,  $\text{matrix}(b_i)=b_i$ .

The weights  $\text{matrix}(w_{ij})$  and  $\text{matrix}(b_i)$  should be optimized by minimizing the calculated error between the calculated output and the target output. The weights  $\text{matrix}(w_{ij})$  and  $\text{matrix}(b_i)$  are updated by using the **backpropagation** algorithm; it is simply Gradient Descent discussed before. Backpropagation algorithm applies two passes through the network (one forward, one backward) to calculate the gradient of the network's error with regard to every single weight. It measures how much each weight and bias term should be tweaked in order to mitigate the error from the actual values. After computing the gradients, simple Gradient Descent is applied by iterating over the entire network until the network converges to the solution.

Lets discuss this approach in more details as below:

1- One mini-batch (mini-batch discussed in previous lecture ) is applied at the time. For example, random selection of 32 training instances can be applied each time. As we discussed before, each iteration is called **epoch**.

2- Each mini-batch is passed to the first hidden layer. The output of all the neurons in the first layer is calculated and then pass on to the next layer. The output of all the neurons in the next layer are computed and passed again to the next layer. This process is repeated until reaching to the output layer. This is the **forward pass**. All the weights for the unknown weights and bias terms are randomly generated in this step.

3- Next step is to calculate the ANN output error by using a cost function such as mean square error.

4- Then, the contribution of each parameter (weight) to the error is calculated. This step can be fast and precise by applying **chain rule**. It starts from the last hidden layer, the **chain rule** is repeated again until reaching to the input layer. By going through this reverse pass, the error gradient across all the connection weights in the network is efficiently measured; the error gradient is propagated backward through the network. That is why it is called **backpropagation**.

5- Finally, the algorithm goes through multiple Gradient Descent step to optimize all weights and biases in ANN using the error gradients.

In order to have higher performance for very complex problem and achieve non-linear relations, an activation function  $\text{varphi}$  should be used. Since  $\text{matrix}(w_{ij})\text{matrix}(x)+\text{matrix}(b_i)$  is a linear transformation, we need some non-linearity between layers to solve complex problems, otherwise even using very deep network will be inefficient.

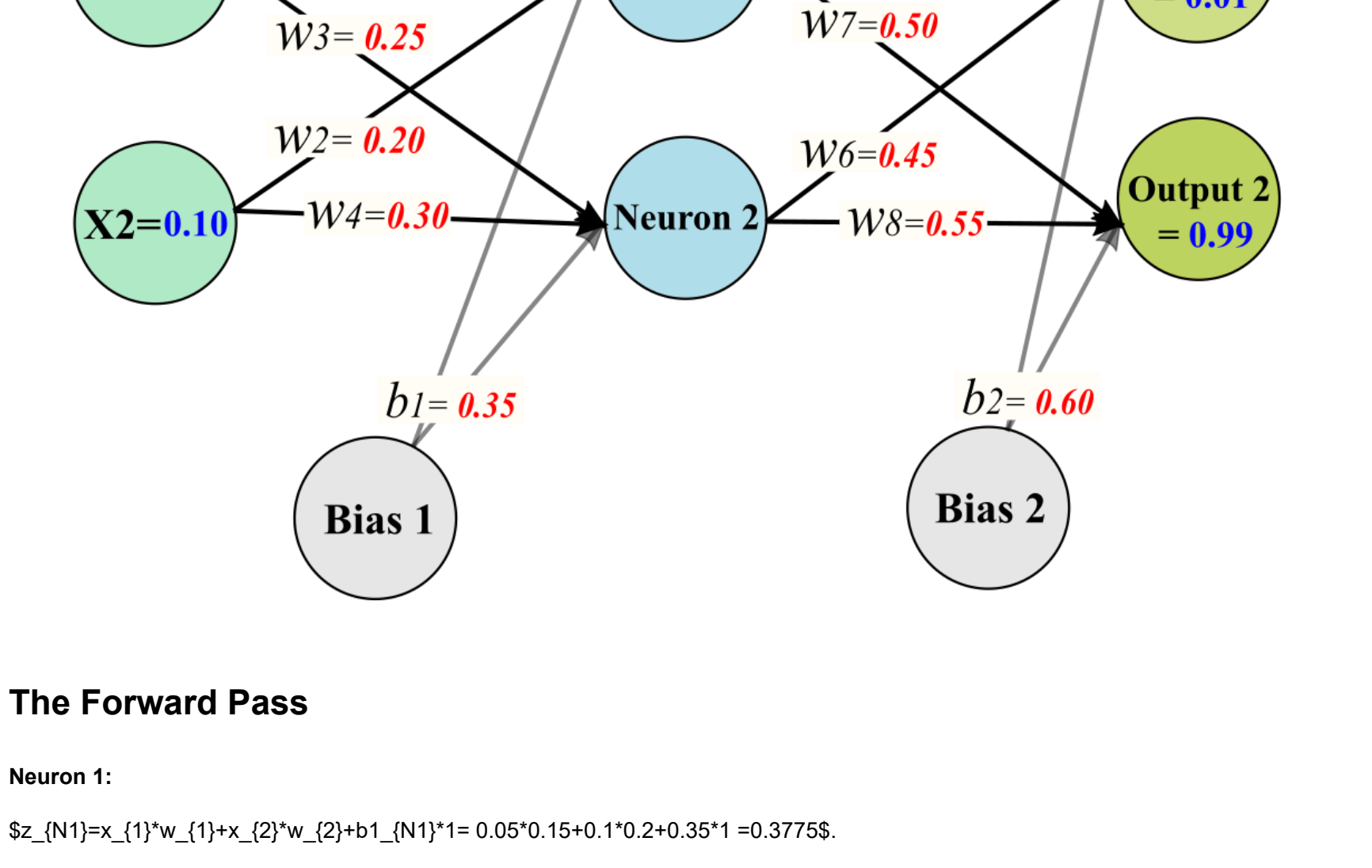
The common activation functions are:

1- **Rectified Linear Unit function:**  $\text{ReLU}(z) = \max(0, z)$ . Although its derivative is 0 for  $z < 0$ ,  $\text{ReLU}$  is the fastest and most popular one activation function.

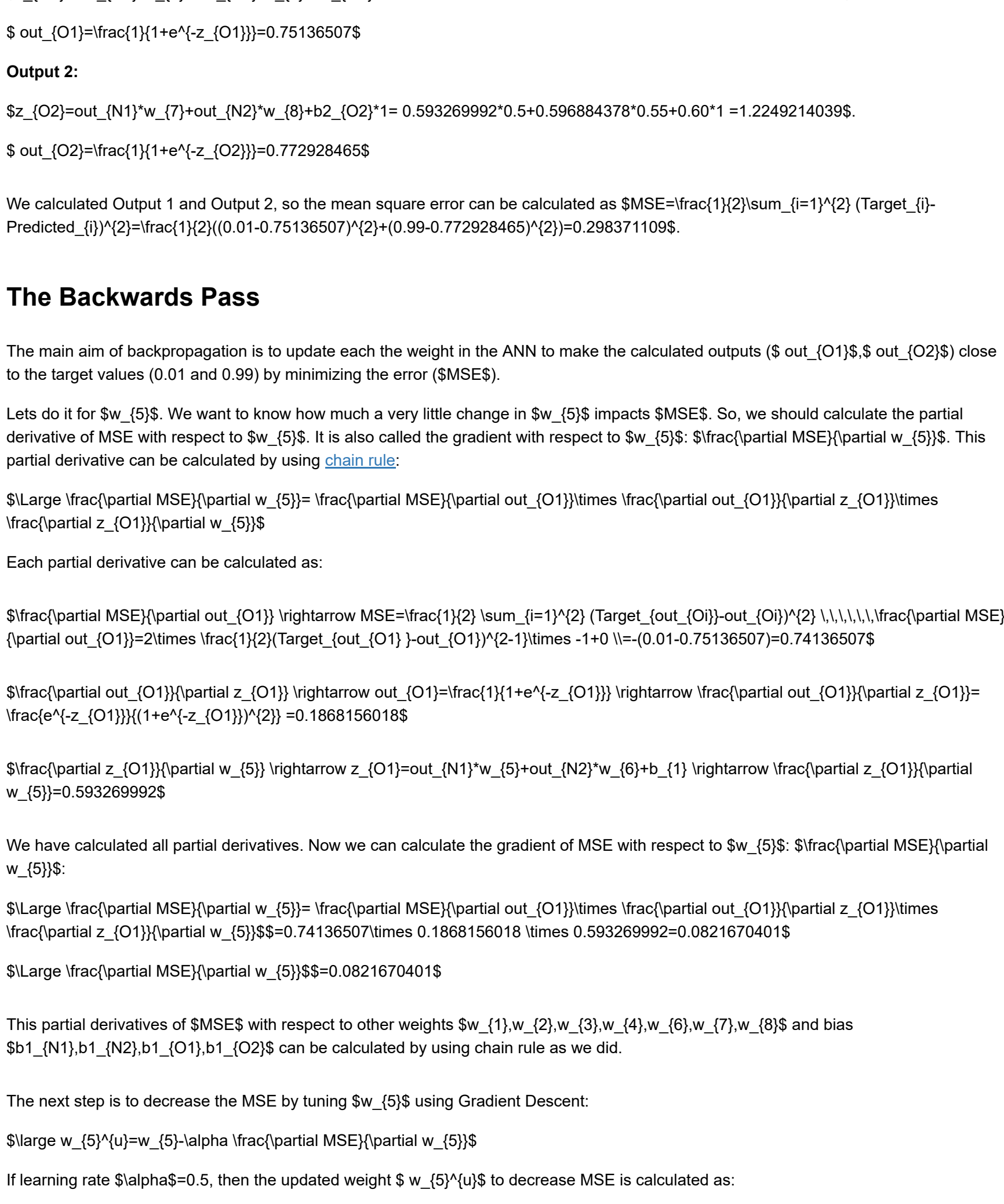
2- **Logistic Regression:**  $\text{Sigmoid}(z) = \frac{1}{1 + e^{-z}}$

3- **Tangent function:**  $\text{tanh}(z)$

See the following plots for these activation function with the derivate of each function:



Lets apply ANN for a simple example below. Assume for one training instance, we have the value  $X_1=0.05$ ,  $X_2=0.10$  for features  $X_1$  and  $X_2$  respectively. And we have two outputs 0.01 and 0.99. The activation function is logistic regression. First, the weights  $W_{11}, W_{12}, W_{21}, W_{22}, W_{31}, W_{32}, W_{41}, W_{42}, W_{51}, W_{52}, W_{61}, W_{62}, W_{71}, W_{72}, W_{81}, W_{82}, W_{91}, W_{92}$  are randomly generate between 0 to 1 as below:



## The Forward Pass

Neuron 1:

$$z_1 = w_{11}x_1 + w_{12}x_2 + b_1 = 0.05 \times 0.15 + 0.10 \times 0.20 + 0.35 = 0.3775$$

$$\text{out}_1 = \frac{1}{1 + e^{-z_1}} = 0.5932699925$$

Neuron 2:

$$z_2 = w_{21}x_1 + w_{22}x_2 + b_2 = 0.05 \times 0.25 + 0.10 \times 0.30 + 0.60 = 0.39245$$

$$\text{out}_2 = \frac{1}{1 + e^{-z_2}} = 0.5968843785$$

Output 1:

$$z_3 = w_{31}\text{out}_1 + w_{32}\text{out}_2 + b_3 = 0.5932699925 \times 0.5968843785 + 0.60 \times 0.10 = 0.10590596675$$

$$\text{out}_3 = \frac{1}{1 + e^{-z_3}} = 0.751365075$$

Output 2:

$$z_4 = w_{41}\text{out}_1 + w_{42}\text{out}_2 + b_4 = 0.5932699925 \times 0.5968843785 + 0.55 \times 0.10 = 0.122492140395$$

$$\text{out}_4 = \frac{1}{1 + e^{-z_4}} = 0.7729284655$$

We calculated Output 1 and Output 2, so the mean square error can be calculated as  $\text{MSE} = \frac{1}{2} \sum (\text{Target}_i - \text{Predicted}_i)^2 = \frac{1}{2} ((0.01 - 0.751365075)^2 + (0.99 - 0.7729284655)^2) = 0.2983711095$ .

## The Backwards Pass

The main aim of Backpropagation is to update each the weight in the ANN to make the calculated outputs ( $\text{out}_1, \text{out}_2$ ) close to the target values (0.01 and 0.99) by minimizing the error (MSE).

Lets do it for  $W_{51}$ . We want to know how much a very little change in  $W_{51}$  impacts  $\text{MSE}$ . So, we should calculate the partial derivative of MSE with respect to  $W_{51}$ . It is also called the gradient with respect to  $W_{51}$ . The partial derivative can be calculated by using [chain rule](#):

$$\frac{\partial \text{MSE}}{\partial W_{51}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \frac{\partial \text{out}_1}{\partial W_{51}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \frac{\partial (w_{51}\text{out}_1 + w_{52}\text{out}_2 + b_5)}{\partial W_{51}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \text{out}_1$$

Each partial derivative can be calculated as:

$$\frac{\partial \text{MSE}}{\partial \text{out}_1} = \frac{\partial \text{MSE}}{\partial (w_{31}\text{out}_1 + w_{32}\text{out}_2 + b_3)} \times \frac{\partial (w_{31}\text{out}_1 + w_{32}\text{out}_2 + b_3)}{\partial \text{out}_1} = \frac{\partial \text{MSE}}{\partial (w_{31}\text{out}_1 + w_{32}\text{out}_2 + b_3)} \times w_{31}$$

$$\frac{\partial \text{MSE}}{\partial \text{out}_1} = \frac{\partial \text{MSE}}{\partial (w_{41}\text{out}_1 + w_{42}\text{out}_2 + b_4)} \times \frac{\partial (w_{41}\text{out}_1 + w_{42}\text{out}_2 + b_4)}{\partial \text{out}_1} = \frac{\partial \text{MSE}}{\partial (w_{41}\text{out}_1 + w_{42}\text{out}_2 + b_4)} \times w_{41}$$

$$\frac{\partial \text{MSE}}{\partial \text{out}_1} = \frac{\partial \text{MSE}}{\partial (w_{51}\text{out}_1 + w_{52}\text{out}_2 + b_5)} \times \frac{\partial (w_{51}\text{out}_1 + w_{52}\text{out}_2 + b_5)}{\partial \text{out}_1} = \frac{\partial \text{MSE}}{\partial (w_{51}\text{out}_1 + w_{52}\text{out}_2 + b_5)} \times 1$$

We have calculated all partial derivatives. Now we can calculate the gradient of MSE with respect to  $W_{51}$ .  $\frac{\partial \text{MSE}}{\partial W_{51}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \text{out}_1 = 0.5932699925 \times 0.01 = 0.005932699925$ .

Lets calculate the partial derivative of MSE with respect to  $W_{52}$ .  $\frac{\partial \text{MSE}}{\partial W_{52}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \frac{\partial \text{out}_1}{\partial W_{52}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \frac{\partial (w_{51}\text{out}_1 + w_{52}\text{out}_2 + b_5)}{\partial W_{52}} = \frac{\partial \text{MSE}}{\partial \text{out}_1} \times \text{out}_2 = 0.5932699925 \times 0.5968843785 = 0.35390596675$ .

The next step is to decrease the MSE by tuning  $W_{51}$  using Gradient Descent:

$$W_{51} = W_{51} - \alpha \times \frac{\partial \text{MSE}}{\partial W_{51}} = 0.5932699925 - 0.01 \times 0.005932699925 = 0.5932699925$$

If learning rate  $\alpha = 0.01$ , then the updated weight  $W_{51}$  to decrease MSE is calculated as:

$$W_{51} = 0.5932699925 - 0.01 \times 0.005932699925 = 0.5932699925$$

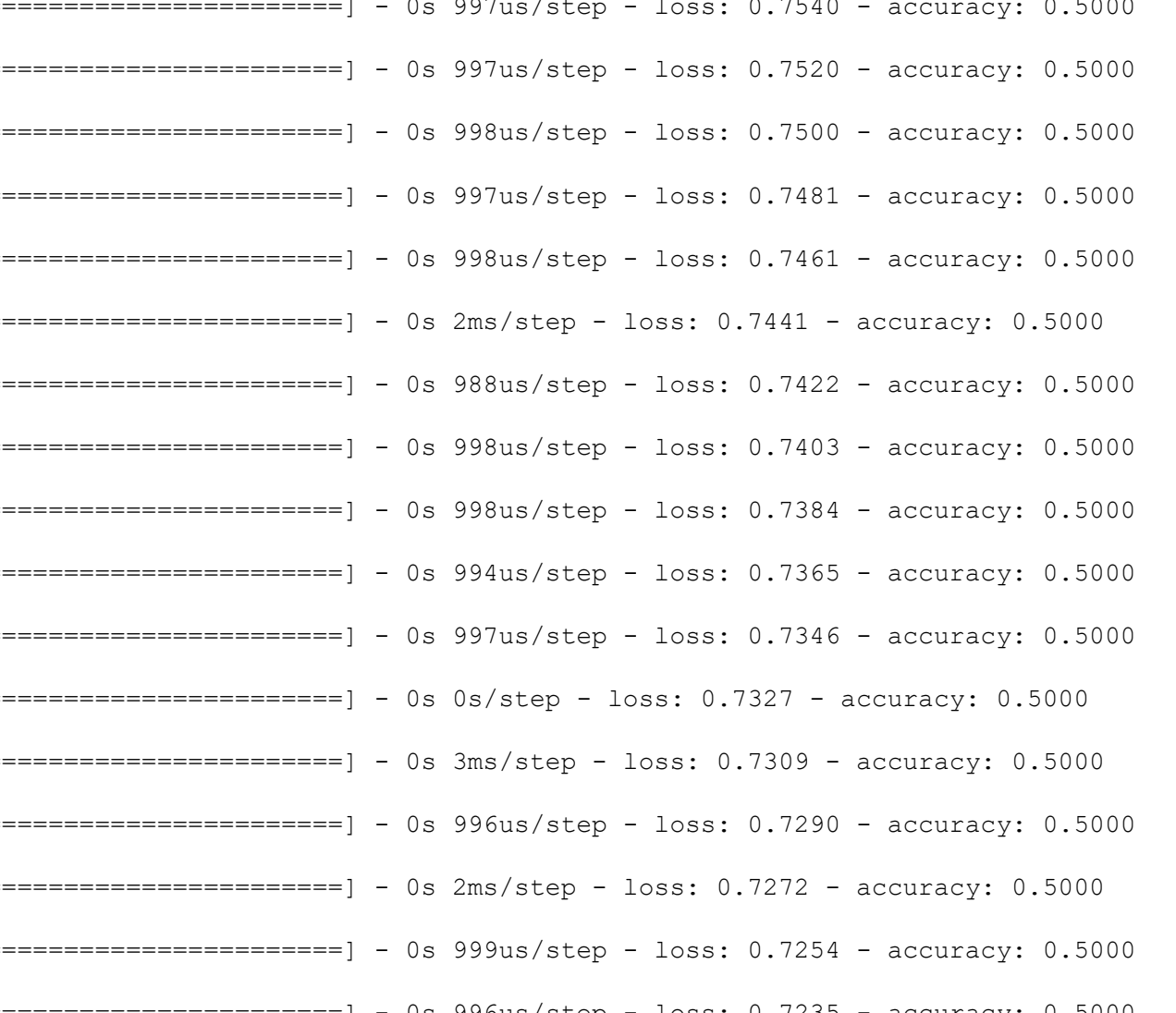
This process should be repeated for many iteration to optimize  $W_{51}$ . See lecture before for more information about Gradient Descent. The entire process should be applied to optimize other weights  $W_{11}, W_{12}, W_{21}, W_{22}, W_{31}, W_{32}, W_{41}, W_{42}, W_{61}, W_{62}, W_{71}, W_{72}, W_{81}, W_{82}, W_{91}, W_{92}$ .

## Small Examples

We start to build a ANN using tensorflow library.

```
In [2]: import tensorflow as tf
from tensorflow import keras
```

We want to build a neural network structure for a binary classification and regression. The network structure has 1 hidden layers with 6 neurons (see Figure below).



## Classification (binary)

Here is a synthetic data set with two features and only 4 training instances.

```
In [3]: X=[[1.5,2.1],
[1.1,1.6],
[1.4,1.8],
[3.1,2.5]]
y=[1,
0,
0,
1]
```

```
In [4]: np.random.seed(42)
tf.random.set_seed(42)
keras.backend.clear_session() # Clear the previous model
```

```
# create model
model = keras.models.Sequential()

# Input & Hidden Layer
model.add(keras.layers.Dense(6, input_dim=np.array(X).shape[1], activation='sigmoid'))

# Output Layer
model.add(keras.layers.Dense(1, activation='sigmoid'))

# Compile model
model.compile(optimizer='sgd', loss='binary_crossentropy', metrics=['accuracy'])
```

```
# Use stochastic gradient descent
# loss='binary_crossentropy' is for binary classification
# use loss='sparse_categorical_crossentropy' for multiclass classification
history=model.fit(X,y,verbose=1,epochs=200)
```

```
Epoch 1/200
1/1 [=====] - loss: 1.0000 - accuracy: 0.0000
Epoch 2/200
1/1 [=====] - loss: 0.9980 - accuracy: 0.0000
Epoch 3/200
1/1 [=====] - loss: 0.9960 - accuracy: 0.0000
Epoch 4/200
1/1 [=====] - loss: 0.9940 - accuracy: 0.0000
Epoch 5/200
1/1 [=====] - loss: 0.9920 - accuracy: 0.0000
Epoch 6/200
1/1 [=====] - loss: 0.9900 - accuracy: 0.0000
Epoch 7/200
1/1 [=====] - loss: 0.9880 - accuracy: 0.0000
Epoch 8/200
1/1 [=====] - loss: 0.9860 - accuracy: 0.0000
Epoch 9/200
1/1 [=====] - loss: 0.9840 - accuracy: 0.0000
Epoch 10/200
1/1 [=====] - loss: 0.9820 - accuracy: 0.0000
Epoch 11/200
1/1 [=====] - loss: 0.9800 - accuracy: 0.0000
Epoch 12/200
1/1 [=====] - loss: 0.9780 - accuracy: 0.0000
Epoch 13/200
1/1 [=====] - loss: 0.9760 - accuracy: 0.0000
Epoch 14/200
1/1 [=====] - loss: 0.9740 - accuracy: 0.0000
Epoch 15/200
1/1 [=====] - loss: 0.9720 - accuracy: 0.0000
Epoch 16/200
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Epoch 17/200
1/1 [=====] - loss: 0.9680 - accuracy: 0.0000
Epoch 18/200
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Epoch 19/200
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Epoch 20/200
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Epoch 21/200
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Epoch 22/200
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1/1 [=====] - loss: 0.7140 - accuracy: 0.0000
Epoch 145/200
1/1 [=====] - loss: 0.7120 - accuracy: 0.0000
Epoch 146/200
1/1 [=====] - loss: 0.7100 - accuracy: 0.0000
Epoch 147/200
1/1 [=====] - loss: 0.7080 - accuracy: 0.0000
Epoch 148/200
1/1 [=====] - loss: 0.7060 - accuracy: 0.0000
Epoch 149/200
1/1 [=====] - loss: 0.7040 - accuracy: 0.0000
Epoch 150/200
1/1 [=====] - loss: 0.7020 - accuracy: 0.0000
Epoch 151/200
1/1 [=====] - loss: 0.7000 - accuracy: 0.0000
Epoch 152/200
1/1 [=====] - loss: 0.6980 - accuracy: 0.0000
Epoch 153/200
1/1 [=====] - loss: 0.6960 - accuracy: 0.0000
Epoch 154/200
1/1 [=====] - loss: 0.6940 - accuracy: 0.0000
Epoch 155/200
1/1 [=====] - loss: 0.6920 - accuracy: 0.0000
Epoch 
```



```
In [6]: weights_input = mml.layers[i].get_weights()[0]
print('Weights: ',weights_input)
Bias = model.layers[i].get_weights()[1]
print('Bias:',Bias)

w0Weights: [[ 0.37828332]
 [ 0.57736015]
 [-0.59459901]
 [ 0.02347528]
 [ 0.78492385]]
Bias: [-0.2640285]
```

```
In [7]: pred=model.predict(X)
pred
```

```
Out[7]: array([[0.6444869 ],
 [0.53500885],
 [0.42337704],
 [0.6769317 ]], dtype=float32)
```

The predict function gives probability of each class. We can simply convert to integer:

```
In [8]: pred=[1 if i >= 0.5 else 0 for i in pred]
pred
```

```
Out[8]: [1, 1, 0, 1]
```

## Regression

```
In [9]: X=[1.5,2.1],
[-1.1,1.6],
[-2.7,-0.5],
[0.2347528]
y=[1.6,
0.4,
-0.4,
0.3]
```

```
In [10]: np.random.seed(42)
tf.random.set_seed(42)
```

```
keras.backend.clear_session() # Clear the previous model

# Create model
model = keras.models.Sequential()
# Input Layer
model.add(keras.layers.Dense(6, input_dim=np.array(X).shape[1], activation='relu'))
# Output Layer
model.add(keras.layers.Dense(1))

# Compile model
model.compile(optimizer='sgd',loss='mse')
history=model.fit(X,y,verbose=1,epochs=300)

Epoch 1/300
1/1 [=====] - 0s 2ms/step - loss: 0.2352
Epoch 2/300
1/1 [=====] - 0s 987us/step - loss: 0.2024
Epoch 3/300
1/1 [=====] - 0s 2ms/step - loss: 0.1784
Epoch 4/300
1/1 [=====] - 0s 2ms/step - loss: 0.1604
Epoch 5/300
1/1 [=====] - 0s 997us/step - loss: 0.1467
Epoch 6/300
1/1 [=====] - 0s 998us/step - loss: 0.1361
Epoch 7/300
1/1 [=====] - 0s 996us/step - loss: 0.1278
Epoch 8/300
1/1 [=====] - 0s 2ms/step - loss: 0.1211
Epoch 9/300
1/1 [=====] - 0s 998us/step - loss: 0.1157
Epoch 10/300
1/1 [=====] - 0s 997us/step - loss: 0.1113
Epoch 11/300
1/1 [=====] - 0s 997us/step - loss: 0.1076
Epoch 12/300
1/1 [=====] - 0s 0s/step - loss: 0.1045
Epoch 13/300
1/1 [=====] - 0s 997us/step - loss: 0.1019
Epoch 14/300
1/1 [=====] - 0s 998us/step - loss: 0.0996
Epoch 15/300
1/1 [=====] - 0s 997us/step - loss: 0.0977
Epoch 16/300
1/1 [=====] - 0s 997us/step - loss: 0.0960
Epoch 17/300
1/1 [=====] - 0s 2ms/step - loss: 0.0944
Epoch 18/300
1/1 [=====] - 0s 997us/step - loss: 0.0931
Epoch 19/300
1/1 [=====] - 0s 996us/step - loss: 0.0919
Epoch 20/300
1/1 [=====] - 0s 998us/step - loss: 0.0908
Epoch 21/300
1/1 [=====] - 0s 998us/step - loss: 0.0898
Epoch 22/300
1/1 [=====] - 0s 998us/step - loss: 0.0889
Epoch 23/300
1/1 [=====] - 0s 1ms/step - loss: 0.0881
Epoch 24/300
1/1 [=====] - 0s 994us/step - loss: 0.0873
Epoch 25/300
1/1 [=====] - 0s 0s/step - loss: 0.0866
Epoch 26/300
1/1 [=====] - 0s 998us/step - loss: 0.0859
Epoch 27/300
1/1 [=====] - 0s 984us/step - loss: 0.0853
Epoch 28/300
1/1 [=====] - 0s 999us/step - loss: 0.0848
Epoch 29/300
1/1 [=====] - 0s 0s/step - loss: 0.0842
Epoch 30/300
1/1 [=====] - 0s 997us/step - loss: 0.0837
Epoch 31/300
1/1 [=====] - 0s 998us/step - loss: 0.0833
Epoch 32/300
1/1 [=====] - 0s 998us/step - loss: 0.0828
Epoch 33/300
1/1 [=====] - 0s 993us/step - loss: 0.0824
Epoch 34/300
1/1 [=====] - 0s 997us/step - loss: 0.0820
Epoch 35/300
1/1 [=====] - 0s 996us/step - loss: 0.0817
Epoch 36/300
1/1 [=====] - 0s 997us/step - loss: 0.0813
Epoch 37/300
1/1 [=====] - 0s 997us/step - loss: 0.0810
Epoch 38/300
1/1 [=====] - 0s 986us/step - loss: 0.0806
Epoch 39/300
1/1 [=====] - 0s 996us/step - loss: 0.0803
Epoch 40/300
1/1 [=====] - 0s 999us/step - loss: 0.0800
Epoch 41/300
1/1 [=====] - 0s 2ms/step - loss: 0.0798
Epoch 42/300
1/1 [=====] - 0s 996us/step - loss: 0.0795
Epoch 43/300
1/1 [=====] - 0s 998us/step - loss: 0.0792
Epoch 44/300
1/1 [=====] - 0s 999us/step - loss: 0.0790
Epoch 45/300
1/1 [=====] - 0s 958us/step - loss: 0.0788
Epoch 46/300
1/1 [=====] - 0s 995us/step - loss: 0.0785
Epoch 47/300
1/1 [=====] - 0s 998us/step - loss: 0.0783
Epoch 48/300
1/1 [=====] - 0s 2ms/step - loss: 0.0781
Epoch 49/300
1/1 [=====] - 0s 997us/step - loss: 0.0779
Epoch 50/300
1/1 [=====] - 0s 997us/step - loss: 0.0777
Epoch 51/300
1/1 [=====] - 0s 995us/step - loss: 0.0775
Epoch 52/300
1/1 [=====] - 0s 998us/step - loss: 0.0773
Epoch 53/300
1/1 [=====] - 0s 996us/step - loss: 0.0771
Epoch 54/300
1/1 [=====] - 0s 2ms/step - loss: 0.0770
Epoch 55/300
1/1 [=====] - 0s 0s/step - loss: 0.0768
Epoch 56/300
1/1 [=====] - 0s 998us/step - loss: 0.0767
Epoch 57/300
1/1 [=====] - 0s 1ms/step - loss: 0.0765
Epoch 58/300
1/1 [=====] - 0s 0s/step - loss: 0.0764
Epoch 59/300
1/1 [=====] - 0s 2ms/step - loss: 0.0762
Epoch 60/300
1/1 [=====] - 0s 995us/step - loss: 0.0761
Epoch 61/300
1/1 [=====] - 0s 998us/step - loss: 0.0759
Epoch 62/300
1/1 [=====] - 0s 995us/step - loss: 0.0758
Epoch 63/300
1/1 [=====] - 0s 997us/step - loss: 0.0757
Epoch 64/300
1/1 [=====] - 0s 994us/step - loss: 0.0756
Epoch 65/300
1/1 [=====] - 0s 997us/step - loss: 0.0754
Epoch 66/300
1/1 [=====] - 0s 0s/step - loss: 0.0753
Epoch 67/300
1/1 [=====] - 0s 997us/step - loss: 0.0752
Epoch 68/300
1/1 [=====] - 0s 997us/step - loss: 0.0751
Epoch 69/300
1/1 [=====] - 0s 0s/step - loss: 0.0750
Epoch 70/300
1/1 [=====] - 0s 994us/step - loss: 0.0749
Epoch 71/300
1/1 [=====] - 0s 992us/step - loss: 0.0748
Epoch 72/300
1/1 [=====] - 0s 2ms/step - loss: 0.0747
Epoch 73/300
1/1 [=====] - 0s 2ms/step - loss: 0.0746
Epoch 74/300
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Epoch 75/300
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1/1 [=====] - 0s 2ms/step - loss: 0.0743
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Epoch 79/300
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Epoch 80/300
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Epoch 86/300
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Epoch 87/300
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Epoch 88/300
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Epoch 91/300
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Epoch 92/300
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Epoch 95/300
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Epoch 162/300
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Epoch 225/300
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Epoch 239/300
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Epoch 240/300
1/1 [=====] - 0s 997us/step - loss: 0.0676
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Epoch 242/300
1/1 [=====] - 0s 2ms/step - loss: 0.0676
Epoch 243/300
1/1 [=====] - 0s 996us/step - loss: 0.0675
Epoch 244/300
1/1 [=====] - 0s 995us/step - loss: 0.0675
Epoch 245/300
1/1 [=====] - 0s 1ms/step - loss: 0.0675
Epoch 246/300
1/1 [=====] - 0s 927us/step - loss: 0.0674
Epoch 247/300
1/1 [=====] - 0s 996us/step - loss: 0.0674
Epoch 248/300
1/1 [=====] - 0s 998us/step - loss: 0.0674
Epoch 249/300
1/1 [=====] - 0s 998us/step - loss: 0.0673
Epoch 250/300
1/1 [=====] - 0s 996us/step - loss: 0.0673
Epoch 251/300
1/1 [=====] - 0s 995us/step - loss: 0.0673
Epoch 252/300
1/1 [=====] - 0s 998us/step - loss: 0.0673
Epoch 253/300
1/1 [=====] - 0s 997us/step - loss: 0.0672
Epoch 254/300
1/1 [=====] - 0s 996us/step - loss: 0.0672
Epoch 255/300
1/1 [=====] - 0s 998us/step - loss: 0.0672
Epoch 256/300
1/1 [=====] - 0s 2ms/step - loss: 0.0672
Epoch 257/300
1/1 [=====] - 0s 998us/step - loss: 0.0671
Epoch 258/300
1/1 [=====] - 0s 3ms/step - loss: 0.0670
Epoch 259/300
1/1 [=====] - 0s 998us/step - loss: 0.0671
Epoch 260/300
1/1 [=====] - 0s 2ms/step - loss: 0.0670
Epoch 261/300
1/1 [=====] - 0s 2ms/step - loss: 0.0670
Epoch 262/300
1/1 [=====] - 0s 995us/step - loss: 0.0669
Epoch 263/300
1/1 [=====] - 0s 995us/step - loss: 0.0669
Epoch 264/300
1/1 [=====] - 0s 996us/step - loss: 0.0669
Epoch 265/300
1/1 [=====] - 0s 997us/step - loss: 0.0669
Epoch 266/300
1/1 [=====] - 0s 2ms/step - loss: 0.0668
Epoch 267/300
1/1 [=====] - 0s 997us/step - loss: 0.0668
Epoch 268/300
1/1 [=====] - 0s 997us/step - loss: 0.0668
Epoch 269/300
1/1 [=====] - 0s 0s/step - loss: 0.0668
Epoch 270/300
1/1 [=====] - 0s 996us/step - loss: 0.0667
Epoch 271/300
1/1 [=====] - 0s 0s/step - loss: 0.0667
Epoch 272/300
1/1 [=====] - 0s 1ms/step - loss: 0.0667
Epoch 273/300
1/1 [=====] - 0s 998us/step - loss: 0.0667
Epoch 274/300
1/1 [=====] - 0s 999us/step - loss: 0.0666
Epoch 275/300
1/1 [=====] - 0s 997us/step - loss: 0.0666
Epoch 276/300
1/1 [=====] - 0s 0s/step - loss: 0.0666
Epoch 277/300
1/1 [=====] - 0s 996us/step - loss: 0.0666
Epoch 278/300
1/1 [=====] - 0s 1000us/step - loss: 0.0665
Epoch 279/300
1/1 [=====] - 0s 997us/step - loss: 0.0665
Epoch 280/300
1/1 [=====] - 0s 995us/step - loss: 0.0664
Epoch 281/300
1/1 [=====] - 0s 2ms/step - loss: 0.0664
Epoch 282/300
1/1 [=====] - 0s 996us/step - loss: 0.0664
Epoch 283/300
1/1 [=====] - 0s 999us/step - loss: 0.0664
Epoch 284/300
1/1 [=====] - 0s 994us/step - loss: 0.0663
Epoch 285/300
1/1 [=====] - 0s 965us/step - loss: 0.0663
Epoch 286/300
1/1 [=====] - 0s 997us/step - loss: 0.0662
Epoch 287/300
1/1 [=====] - 0s 999us/step - loss: 0.0662
Epoch 288/300
1/1 [=====] - 0s 2ms/step - loss: 0.0662
Epoch 289/300
1/1 [=====] - 0s 997us/step - loss: 0.0661
Epoch 290/300
1/1 [=====] - 0s 999us/step - loss: 0.0661
Epoch 291/300
1/1 [=====] - 0s 996us/step - loss: 0.0660
Epoch 292/300
1/1 [=====] - 0s 997us/step - loss: 0.0660
Epoch 293/300
1/1 [=====] - 0s 998us/step - loss: 0.0660
Epoch 294/300
1/1 [=====] - 0s 0s/step - loss: 0.0660
Epoch 295/300
1/1 [=====] - 0s 968us/step - loss: 0.0659
Epoch 296/300
1/1 [=====] - 0s 998us/step - loss: 0.0659
Epoch 297/300
1/1 [=====] - 0s 996us/step - loss: 0.0659
Epoch 298/300
1/1 [=====] - 0s 2ms/step - loss: 0.0659
Epoch 299/300
1/1 [=====] - 0s 998us/step - loss: 0.0658
```

```
In [11]: pred=model.predict(X)
pred
```

```
Out[11]: array([1.10544993],
 [0.5455201 ],
 [0.9749805 ],
 [1.5648493 ]], dtype=float32)
```

You can see by increasing number of epochs, the model will greatly overfit training data. The easiest technique is to apply early stopping as we discussed before, it stops iteration when error in validation set start to increase while error in training set keep decreasing. So, first you need to divide data into training set and test set, then the training set should be divided to smaller training set and validation. The test set should be applied in the end only for measuring the error of the model.

Visit the TensorFlow Playground at <https://playground.tensorflow.org/>, play with the parameters, change Hidden layers, Neurons, choose regression and classification task to understand the problem

## Energy Efficiency Data Set

Let's apply ANN for Energy Efficiency data set for both regression and classification. First get training data:

### Binary Classification

```
In [12]: import pandas as pd
import numpy as np
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import train_test_split

df=pd.read_csv('..Data/building_
```

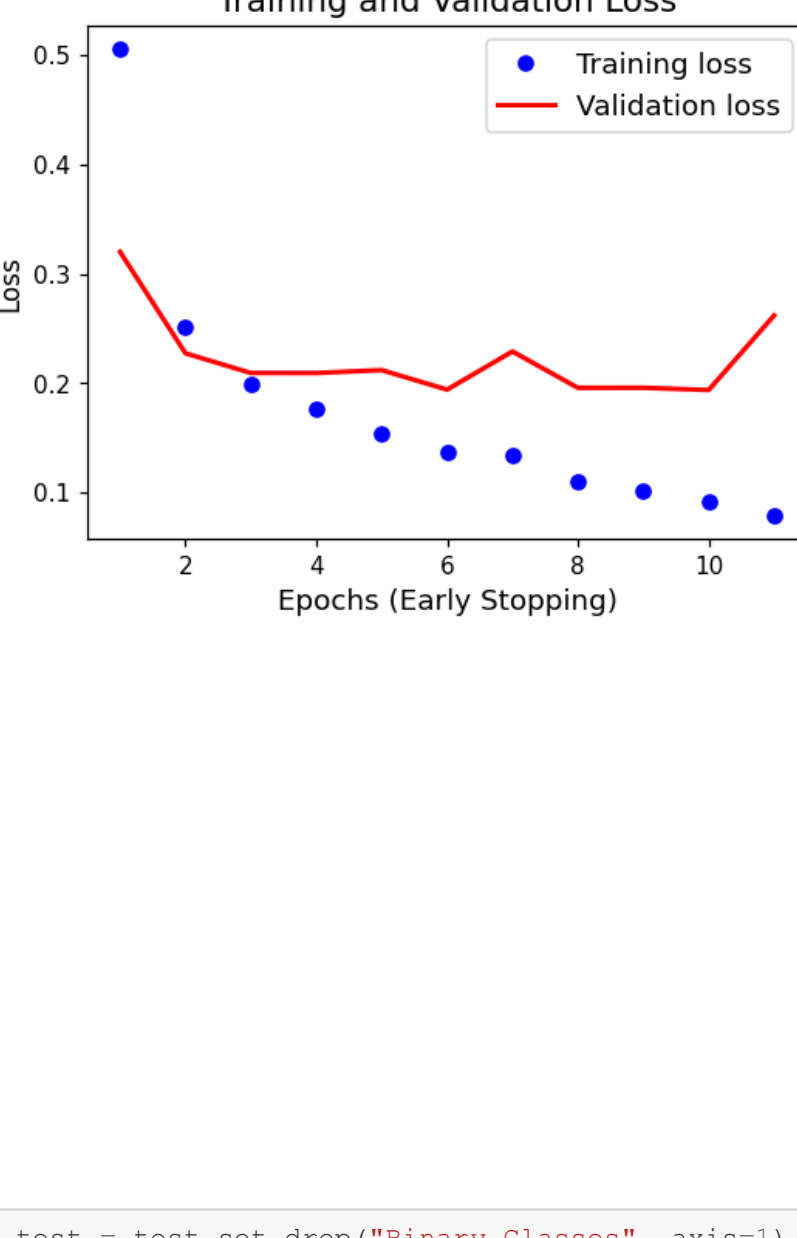




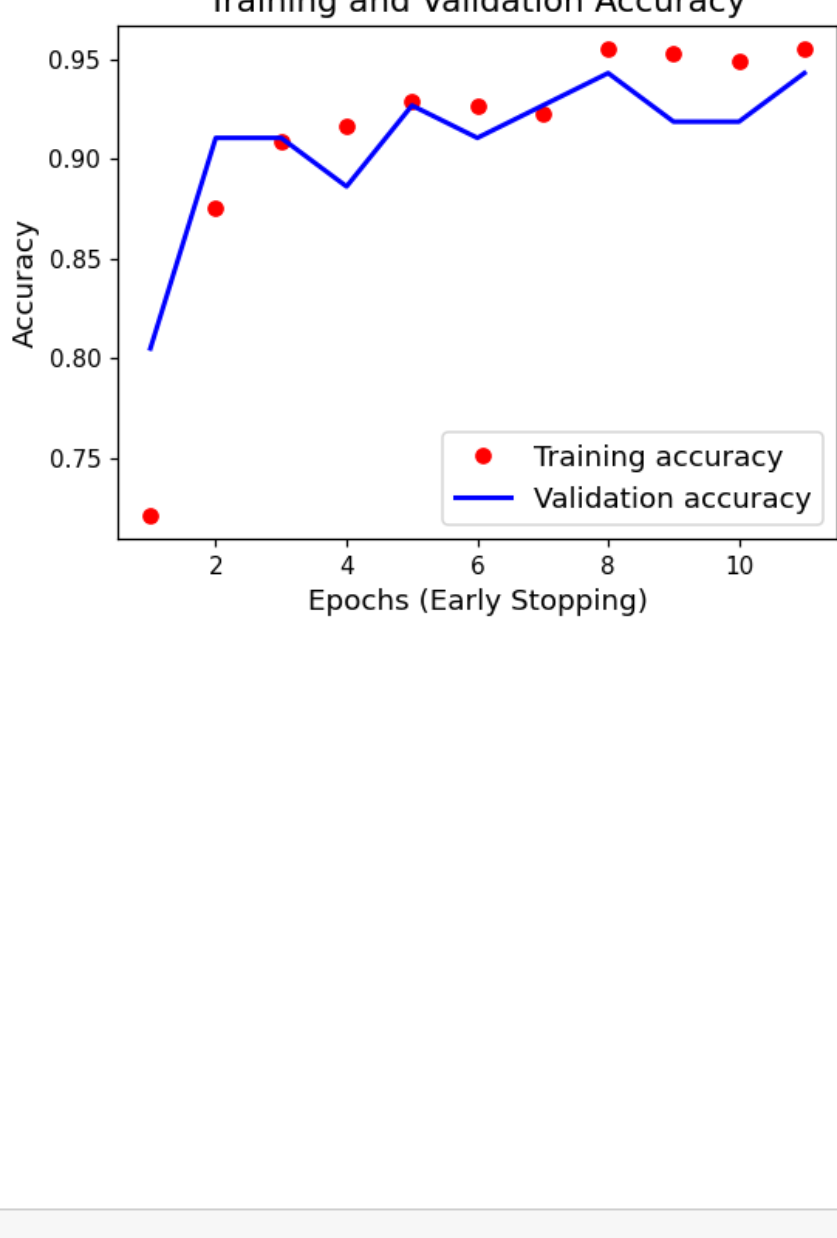


In [41]: plot(history)

Training and Validation Loss



Training and Validation Accuracy



```
In [42]: X_test = test_set.drop("Binary Classes", axis=1)
         y_test = test_set["Binary Classes"].values
         #
         X_test_std=scaler.transform(X_test)
```

```
In [43]: from sklearn.metrics import accuracy_score
```

```
pred=model_ft.predict(X_test_std)
grid_result = [1 if i >= 0.5 else 0 for i in pred]
acr=accuracy_score(y_test, pred)
print(acr)
0.9675324675324676
```

You can see the accuracy you calculated is higher than "grid\_result.score" because of some overfitting. So, it is always a good idea

In [ ] :

## Regression: GridSearchCV

```
In [44]: df_reg=df.copy()
         df_reg.drop(["Binary Classes", "Multi-Classes"], axis=1, inplace=True)

         # Training and Test
         train_set, test_set = train_test_split(df_reg, test_size=0.2, random_state=42)

         X_train = train_set.drop("Heating Load", axis=1)
         y_train = train_set["Heating Load"].values
         #
         scaler = StandardScaler()
         X_train_std=scaler.fit_transform(X_train)

         # Smaller Training
         # You need to divid your data to smaller training set and validation set for early stopping.
         Training=np.concatenate((X_train_std,np.array(y_train).reshape(-1,1)),axis=1)
         Smaller_Training, Validation = train_test_split(Training, y_test_size=0.2, random_state=100)
         #
         Smaller_Training_Target=Smaller_Training[:, :-1]
         Smaller_Training_Target[:, -1]
         Validation_Target=Validation[:, :-1]
         Validation_Target[:, -1]
```

In [ ] :

```
In [45]: from keras.wrappers.scikit_learn import KerasRegressor
```

```
# Define the grid search parameters
param_grid = {'neurons': [50,100,150]}

# Run Keras Classifier
model = KerasRegressor(build_fn=ANN, input_dim=Smaller_Training.shape[1], loss='mse',
                        metrics=None, activation_out=None)
#model._estimator_type = "Regressor"

# Apply Scikit Learn GridSearchCV
grid = GridSearchCV(estimator=model, param_grid=param_grid, cv=2)

# Early stopping to avoid overfitting
monitor= keras.callbacks.EarlyStopping(min_delta=1e-3, patience=5, verbose=0)
grid_result = grid.fit(Smaller_Training, Smaller_Training_Target, batch_size=32, validation_data=
                      (Validation, Validation_Target), callbacks=[monitor],
                      verbose=0, epochs=1000)
```

```
8/8 [=====] - 0s 628us/step - loss: 3.2498
8/8 [=====] - 0s 502us/step - loss: 10.2170
8/8 [=====] - 0s 623us/step - loss: 5.1038
8/8 [=====] - 0s 499us/step - loss: 8.7048
8/8 [=====] - 0s 624us/step - loss: 3.0345
8/8 [=====] - 0s 628us/step - loss: 6.0309
```

```
In [46]: # Best result
         print("Best parameters: %f using %s" % (-1*grid_result.best_score_, grid_result.best_params_))
```

Best parameters: 4.532704 using {'neurons': 150}

You can tune any ANN hyperparameter. Then call the function using fine-tuned neurons.

```
In [47]: # Call Function with fined-tune numbre of neurons
         model_ft=ANN (input_dim=Smaller_Training.shape[1], neurons=150, loss='mse', metrics=None, activation_out=None)
         # Early stopping to avoid overfitting
         monitor= keras.callbacks.EarlyStopping(min_delta=1e-3, patience=5)
         grid_result = grid.fit(Smaller_Training, Smaller_Training_Target, batch_size=32, validation_data=
                               (Validation, Validation_Target), callbacks=[monitor], verbose=1, epochs=1000)
```

```
Epoch 1/1000
16/16 [=====] - 0s 7ms/step - loss: 496.0419 - val_loss: 411.0409
Epoch 2/1000
16/16 [=====] - 0s 2ms/step - loss: 189.4804 - val_loss: 69.1375
Epoch 3/1000
16/16 [=====] - 0s 2ms/step - loss: 61.8730 - val_loss: 30.8594
Epoch 4/1000
16/16 [=====] - 0s 2ms/step - loss: 33.7987 - val_loss: 29.8524
Epoch 5/1000
16/16 [=====] - 0s 2ms/step - loss: 26.3349 - val_loss: 21.3596
Epoch 6/1000
16/16 [=====] - 0s 2ms/step - loss: 22.6852 - val_loss: 21.2456
Epoch 7/1000
16/16 [=====] - 0s 2ms/step - loss: 19.7035 - val_loss: 16.8350
Epoch 8/1000
16/16 [=====] - 0s 2ms/step - loss: 17.5764 - val_loss: 16.0825
Epoch 9/1000
16/16 [=====] - 0s 2ms/step - loss: 15.4212 - val_loss: 12.5194
Epoch 10/1000
16/16 [=====] - 0s 2ms/step - loss: 14.0032 - val_loss: 11.0032
Epoch 11/1000
16/16 [=====] - 0s 2ms/step - loss: 12.4288 - val_loss: 9.8423
Epoch 12/1000
16/16 [=====] - 0s 2ms/step - loss: 11.0770 - val_loss: 9.3910
Epoch 13/1000
16/16 [=====] - 0s 2ms/step - loss: 10.1157 - val_loss: 8.4061
Epoch 14/1000
16/16 [=====] - 0s 2ms/step - loss: 9.3192 - val_loss: 8.0439
Epoch 15/1000
16/16 [=====] - 0s 2ms/step - loss: 8.6984 - val_loss: 7.5356
Epoch 16/1000
16/16 [=====] - 0s 2ms/step - loss: 8.3997 - val_loss: 7.2205
Epoch 17/1000
16/16 [=====] - 0s 2ms/step - loss: 7.6843 - val_loss: 6.8987
Epoch 18/1000
16/16 [=====] - 0s 2ms/step - loss: 7.2509 - val_loss: 6.3502
Epoch 19/1000
16/16 [=====] - 0s 2ms/step - loss: 7.4151 - val_loss: 6.8005
Epoch 20/1000
16/16 [=====] - 0s 2ms/step - loss: 6.6192 - val_loss: 5.8998
Epoch 21/1000
16/16 [=====] - 0s 2ms/step - loss: 6.5088 - val_loss: 5.8347
Epoch 22/1000
16/16 [=====] - 0s 2ms/step - loss: 6.1192 - val_loss: 6.1785
Epoch 23/1000
16/16 [=====] - 0s 2ms/step - loss: 6.3020 - val_loss: 3.4689
Epoch 24/1000
16/16 [=====] - 0s 2ms/step - loss: 5.9191 - val_loss: 5.5249
Epoch 25/1000
16/16 [=====] - 0s 2ms/step - loss: 5.5505 - val_loss: 4.8241
Epoch 26/1000
16/16 [=====] - 0s 2ms/step - loss: 5.4321 - val_loss: 5.1484
Epoch 27/1000
16/16 [=====] - 0s 2ms/step - loss: 5.2984 - val_loss: 4.9999
Epoch 28/1000
16/16 [=====] - 0s 2ms/step - loss: 5.0261 - val_loss: 5.7480
Epoch 29/1000
16/16 [=====] - 0s 2ms/step - loss: 5.2190 - val_loss: 4.9393
Epoch 30/1000
16/16 [=====] - 0s 2ms/step - loss: 5.0271 - val_loss: 4.9039
Epoch 31/1000
16/16 [=====] - 0s 2ms/step - loss: 4.7875 - val_loss: 4.6973
Epoch 32/1000
16/16 [=====] - 0s 2ms/step - loss: 4.5833 - val_loss: 4.6911
Epoch 33/1000
16/16 [=====] - 0s 2ms/step - loss: 4.6143 - val_loss: 4.5598
Epoch 34/1000
16/16 [=====] - 0s 2ms/step - loss: 4.4251 - val_loss: 4.5542
Epoch 35/1000
16/16 [=====] - 0s 2ms/step - loss: 4.4548 - val_loss: 5.1642
Epoch 36/1000
16/16 [=====] - 0s 2ms/step - loss: 4.8674 - val_loss: 4.9474
Epoch 37/1000
16/16 [=====] - 0s 2ms/step - loss: 5.5750 - val_loss: 5.7298
Epoch 38/1000
16/16 [=====] - 0s 2ms/step - loss: 5.4152 - val_loss: 5.5497
Epoch 39/1000
16/16 [=====] - 0s 2ms/step - loss: 4.3875 - val_loss: 4.9470
Epoch 40/1000
16/16 [=====] - 0s 2ms/step - loss: 4.2398 - val_loss: 4.1655
Epoch 41/1000
16/16 [=====] - 0s 2ms/step - loss: 4.2398 - val_loss: 4.1655
Epoch 42/1000
16/16 [=====] - 0s 2ms/step - loss: 4.1187 - val_loss: 4.5292
Epoch 43/1000
16/16 [=====] - 0s 2ms/step - loss: 4.0220 - val_loss: 4.1258
Epoch 44/1000
16/16 [=====] - 0s 2ms/step - loss: 4.0955 - val_loss: 4.8214
Epoch 45/1000
16/16 [=====] - 0s 2ms/step - loss: 3.7867 - val_loss: 3.9332
Epoch 46/1000
16/16 [=====] - 0s 2ms/step - loss: 3.3985 - val_loss: 3.6392
Epoch 47/1000
16/16 [=====] - 0s 2ms/step - loss: 3.3016 - val_loss: 3.7124
Epoch 48/1000
16/16 [=====] - 0s 2ms/step - loss: 3.2104 - val_loss: 3.6684
Epoch 49/1000
16/16 [=====] - 0s 2ms/step - loss: 3.0862 - val_loss: 3.5787
Epoch 50/1000
16/16 [=====] - ETA: 0s - loss: 1.752 - 0s 2ms/step - loss: 3.0164 - val_loss: 3.4757
Epoch 50/1000
16/16 [=====] - 0s 2ms/step - loss: 2.9203 - val_loss: 3.4317
Epoch 51/1000
16/16 [=====] - 0s 2ms/step - loss: 3.0320 - val_loss: 3.4689
Epoch 52/1000
16/16 [=====] - 0s 2ms/step - loss: 2.7935 - val_loss: 3.2752
Epoch 53/1000
16/16 [=====] - 0s 2ms/step - loss: 2.7513 - val_loss: 3.4164
Epoch 54/1000
16/16 [=====] - 0s 2ms/step - loss: 2.6770 - val_loss: 3.3035
Epoch 55/1000
16/16 [=====] - 0s 2ms/step - loss: 2.5766 - val_loss: 3.2466
Epoch 56/1000
16/16 [=====] - 0s 2ms/step - loss: 2.5639 - val_loss: 3.3499
Epoch 57/1000
16/16 [=====] - 0s 2ms/step - loss: 2.3649 - val_loss: 3.0051
Epoch 58/1000
16/16 [=====] - 0s 2ms/step - loss: 2.1905 - val_loss: 3.4642
Epoch 59/1000
16/16 [=====] - 0s 2ms/step - loss: 2.4544 - val_loss: 3.2325
Epoch 60/1000
16/16 [=====] - 0s 2ms/step - loss: 2.2106 - val_loss: 3.8061
Epoch 61/1000
16/16 [=====] - 0s 2ms/step - loss: 2.1582 - val_loss: 3.9797
Epoch 62/1000
16/16 [=====] - 0s 2ms/step - loss: 2.1414 - val_loss: 2.7830
Epoch 63/1000
16/16 [=====] - 0s 2ms/step - loss: 2.1931 - val_loss: 2.5126
Epoch 64/1000
16/16 [=====] - 0s 2ms/step - loss: 2.3123 - val_loss: 3.1691
Epoch 65/1000
16/16 [=====] - 0s 2ms/step - loss: 1.9668 - val_loss: 2.5556
Epoch 66/1000
16/16 [=====] - 0s 2ms/step - loss: 1.7030 - val_loss: 2.5010
Epoch 67/1000
16/16 [=====] - 0s 2ms/step - loss: 1.7079 - val_loss: 2.7022
Epoch 68/1000
16/16 [=====] - 0s 2ms/step - loss: 1.8957 - val_loss: 2.5126
Epoch 69/1000
16/16 [=====] - 0s 2ms/step - loss: 1.8670 - val_loss: 2.5414
Epoch 70/1000
16/16 [=====] - 0s 2ms/step - loss: 1.6417 - val_loss: 2.4126
Epoch 71/1000
16/16 [=====] - 0s 2ms/step - loss: 1.5892 - val_loss: 2.3989
Epoch 72/1000
16/16 [=====] - 0s 2ms/step - loss: 1.4380 - val_loss: 2.0954
Epoch 73/1000
16/16 [=====] - 0s 2ms/step - loss: 1.2311 - val_loss: 2.2355
Epoch 74/1000
16/16 [=====] - 0s 2ms/step - loss: 1.1962 - val_loss: 1.9829
Epoch 75/1000
16/16 [=====] - 0s 2ms/step - loss: 1.1219 - val_loss: 2.0183
Epoch 76/1000
16/16 [=====] - 0s 2ms/step - loss: 1.0019 - val_loss: 1.8860
Epoch 77/1000
16/16 [=====] - 0s 3ms/step - loss: 0.9830 - val_loss: 1.7563
Epoch 78/1000
16/16 [=====] - 0s 2ms/step - loss: 0.9107 - val_loss: 2.3790
Epoch 79/1000
16/16 [=====] - 0s 2ms/step - loss: 1.0232 - val_loss: 1.9398
Epoch 80/1000
16/16 [=====] - 0s 2ms/step - loss: 0.8119 - val_loss: 1.4614
Epoch 81/1000
16/16 [=====] - 0s 2ms/step - loss: 0.7030 - val_loss: 1.9426
Epoch 82/1000
16/16 [=====] - 0s 2ms/step - loss: 0.7883 - val_loss: 1.6369
Epoch 83/1000
16/16 [=====] - 0s 2ms/step - loss: 0.7123 - val_loss: 1.5083
Epoch 84/1000
16/16 [=====] - 0s 2ms/step - loss: 0.6877 - val_loss: 1.3337
Epoch 85/1000
16/16 [=====] - 0s 2ms/step - loss: 0.6299 - val_loss: 1.3608
Epoch 86/1000
16/16 [=====] - 0s 2ms/step - loss: 0.5525 - val_loss: 1.1083
Epoch 87/1000
16/16 [=====] - 0s 2ms/step - loss: 0.4475 - val_loss: 1.0157
Epoch 88/1000
16/16 [=====] - 0s 2ms/step - loss: 0.4745 - val_loss: 1.0285
Epoch 89/1000
16/16 [=====] - 0s 2ms/step - loss: 0.4305 - val_loss: 0.9644
Epoch 90/1000
16/16 [=====] - 0s 2ms/step - loss: 0.3969 - val_loss: 0.9314
Epoch 91/1000
16/16 [=====] - 0s 2ms/step - loss: 0.3768 - val_loss: 0.8610
Epoch 92/1000
16/16 [=====] - 0s 2ms/step - loss: 0.3506 - val_loss: 0.8625
Epoch 93/1000
16/16 [=====] - 0s 2ms/step - loss: 0.3450 - val_loss: 0.8950
Epoch 94/1000
16/16 [=====] - 0s 2ms/step - loss: 0.3313 - val_loss: 0.8003
Epoch 95/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2967 - val_loss: 0.8246
Epoch 96/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2823 - val_loss: 0.7612
Epoch 97/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2723 - val_loss: 0.7157
Epoch 98/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2665 - val_loss: 0.7039
Epoch 99/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2620 - val_loss: 0.6482
Epoch 100/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2504 - val_loss: 0.7040
Epoch 101/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2573 - val_loss: 0.6372
Epoch 102/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2572 - val_loss: 0.6856
Epoch 103/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2301 - val_loss: 0.6433
Epoch 104/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2233 - val_loss: 0.6034
Epoch 105/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1974 - val_loss: 0.6036
Epoch 106/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1832 - val_loss: 0.6474
Epoch 107/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1815 - val_loss: 0.5545
Epoch 108/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1682 - val_loss: 0.5798
Epoch 109/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1837 - val_loss: 0.6729
Epoch 110/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1784 - val_loss: 0.5668
Epoch 111/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1533 - val_loss: 0.5680
Epoch 112/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1482 - val_loss: 0.5305
Epoch 113/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1654 - val_loss: 0.5589
Epoch 114/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1782 - val_loss: 0.5042
Epoch 115/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1684 - val_loss: 0.5456
Epoch 116/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1734 - val_loss: 0.6055
Epoch 117/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1625 - val_loss: 0.4919
Epoch 118/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1517 - val_loss: 0.6197
Epoch 119/1000
16/16 [=====] - 0s 2ms/step - loss: 0.2609 - val_loss: 0.5866
Epoch 120/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1842 - val_loss: 0.6176
Epoch 121/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1672 - val_loss: 0.5615
Epoch 122/1000
16/16 [=====] - 0s 2ms/step - loss: 0.1937 - val_loss: 0.5411
```

```
In [48]: plot_NN(model_ft, history, Smaller_Training, Smaller_Training_Target)
```

Training and validation loss



Prediction vs Expected for Training



```
In [49]: X_test = test_set.drop("Heating Load", axis=1)
         y_test = test_set["Heating Load"].values
         X_test_std=scaler.transform(X_test)
```

```
In [50]: pred=model_ft.predict(X_test_std)
         mse = mean_squared_error(y_test, pred)
         rmse = np.sqrt(mse)
```

Out[50]: 0.5701598221707747

In [ ] :