PROJECT REPORT

on

MODELLING OF ARTIFICAL NEURAL NETWORK FOR BEALE FUNCTION

Submitted by

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COURSE NAME: Basics & Applications of AI/ML for Process Systems Engineering (PB5230)

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1. INTRODUCTION

This function is used as a test function in order to evaluate the performance of optimization algorithms.

$$f(x,y) = (1.5 - x - xy)^2 + (2.25 - x + xy^2)^2 + (2.625 - x - xy^3)^2$$

where -4.5 < x,y < 4.5. The number of independent variables is 2 (x,y). ANN modelling was performed to develop a functional relationship between the function value and these 2-inputs. The data for the model was generated using the function expression and it was used to build the model.

2. DATA GENERATION

1. Generation of Input and Target Data

The required packages such as *Numpy* and *pandas* were imported into the code. The input data was generated in the range of -4.5 < x,y < 4.5 with a step size of 0.2. These generated data were given as input to the test function and its function value was evaluated.

```
# Defining Beale function
def beale_function(x,y):
   Equation of beale function
   Inputs:
   x and y values
   Outputs:
   Value of beale function at x and y
   return (1.5-x+x*y)**2 + (2.25-x+x*y**2)**2 + (2.625-x+x*y**3)**2
# Generating data for beale function in range in the range -4.5 < x,y < 4.5
with step size 0.2
import numpy as np
X,Y,Z = [],[],[] # Empty lists to store x,y and output values
for i in np.arange(-4.5,4.6,0.2): # -4.5 < x < 4.5
   for j in np.arange(-4.5,4.6,0.2): # -4.5 < y < 4.5
        X.append(i) # Adding x value to list X
        Y.append(j) # Adding y value to list Y
       Z.append(beale_function(i,j)) # Adding beale function value for
respective x and y to list Z
data1 = zip(X,Y,Z) \# Concatenation of inputs and outputs
```

2. Saving and reading the file from excel file

The generated data were then concatenated, and it was assigned to a data frame variable using **DataFrame**. These were then stored in an excel file locally.

```
import pandas as pd
# Creating a dataframe containing inputs and outputs
data2 = pd.DataFrame(data1,columns=['x','y','z'])
# data2 now has 3 columns containing x, y, f(x,y) values for beale function in
the range of -4.5 < x,y < 4.5 with step size 0.2
data2.to_excel('beale_function_data_step=0.2.xlsx',index=False)</pre>
```

The data from excel was read using read_excel and store it in an array for further processing.

```
# Reading data from excel sheetdata3 =
pd.read_excel('beale_function_data_step=0.2.xlsx')
```

3. Normalization of Data

The input and output data were normalized between 0-1. To normalize the data, **MinMaxScaler** tool was imported **skl.Preprocessing** package. Then the normalized data was stored for further usage.

```
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
# Normalizing data between 0 and 1 using MinMaxScaler
scaled_dataset = scaler.fit_transform(data3.values)
```

4. Data for Training, Validation, and Testing

The normalized data was split into input data and target data required for the development of the ANN model. 70% of the data was taken as the input data, 15% as validation and the rest 15 % as testing data.

No.	Process	Data Percentage
1	Training	70
2	Validation	15
3	Testing	15

```
inputs = scaled_dataset[:,0:2] # Splitting inputs from normalized data
output = scaled_dataset[:,-1] # Splitting output from normalized data
from sklearn.model_selection import train_test_split
# Splitting the data into training data and testing data using
train_test_split
inputs_train,inputs_test,output_train,output_test =
train_test_split(inputs,output,train_size=0.7,random_state=0) # train_size=0.7
```

3. ARTIFICIAL NEURAL NETWORK MODELLING

ANN modelling was implemented for the normalized data using *TensorFlow* package in python. *Sequential and Dense* functions were imported from TensorFlow and it was used to create the neural network.

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

1. Neural network using adam optimizer

The network structure is as follows

Layer	Activation Function	No. of nodes
Hidden Layers 1	relu	30
Hidden Layers 2	relu	20
Output Layer	linear	1

```
# Creating ANN model
model = Sequential()
# First layer with 18 nodes and two inputs and "relu" as activation function
model.add(Dense(30,input_dim=2,activation='relu'))
# Second layer with 12 nodes and "relu" as activation function
model.add(Dense(20,activation='relu'))
# Output layer with one output and "linear" as activation function
model.add(Dense(1,activation='linear'))
```

The' **adam'** algorithm was taken as the optimizer and '**Mean Square Error (MSE)'** was taken as the loss function.

```
# Compiling using optimizer "adam" and loss function "MSE"
model.compile(optimizer ='adam',loss='MSE')
```

The number of iterations (epoch) was fixed as 100 and the validation data percentage was assigned as 15% of the dataset.

```
# Training data with 100 epochs and validation split 0.15
history= model.fit(inputs_train,output_train,epochs=100,validation_split=0.15)
```

To validate the predicted results, statistical parameter like Mean Square Error (MSE), R_2 was imported from *sklearn.metrics*.

```
pred_train = model.predict(inputs_train) # Prediction of training data
pred_test = model.predict(inputs_test) # Prediction of testing data
from sklearn.metrics import r2_score
r2_train = r2_score(output_train,pred_train) # R2 score of training data
print(f"R2 Score for training data: {r2_train:.4f}")
r2_test = r2_score(output_test,pred_test) # R2 score of testing data
print(f"R2 Score for testing data: {r2_test:.4f}")
from sklearn.metrics import mean_squared_error
mse_train = mean_squared_error(output_train,pred_train) # MSE of training data
print(f"Mean Squared_error(output_test,pred_test) # MSE of Testing data
print(f"Mean Squared_Error for testing data: {mse_test:.4f}")
```

No. Predicted Data	R^2	MSE
--------------------	-------	-----

1	Training	0.9743	0.0005
2	Testing	0.9707	0.0004

The scatter plot of Predicted data vs True data was plotted using the scatter plot function imported from *matplotlib*.

```
import matplotlib.pyplot as plt
fig,plot = plt.subplots(1,2,figsize=(10,5))
plot[0].plot(output_train,pred_train,'y.')
plot[0].plot(output_train,output_train,'-')
plot[0].set xlabel('True output')
plot[0].set_ylabel('Predicted output')
plot[0].set_ylim(-0.05,1.1)
plot[0].set_xlim(-0.05,1.1)
plot[0].set_title(f'Training Data (adam)')
plot[0].text(0,1,f'R2 = {r2_train:.4f}',fontsize=12,color='magenta')
plot[1].plot(output_test,pred_test,'r*')
plot[1].plot(output_test,output_test,'-')
plot[1].set_ylim(-0.05,1)
plot[1].set_xlim(-0.05,1)
plot[1].set_xlabel('True output')
plot[1].set ylabel('Predicted output')
plot[1].set_title(f'Testing Data (adam)')
plot[1].text(0,0.9,f'R2 = {r2_test:.4f}',fontsize=12,color='magenta')
plt.tight_layout()
plt.show()
```

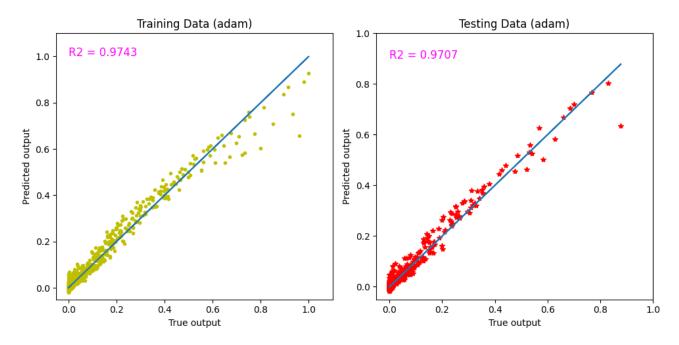


Figure 1: Traning Data Vs Testing Data using adam optimizer

2. Neural network using RMSProp

The same network architecture was now trained with '*RMSProp*' as the optimizer and '*MSE*' as the loss function.

Compiling using optimizer "RMSProp" and loss function "MSE"
model.compile(optimizer ='RMSProp',loss='MSE')

No.	Predicted Data	R^2	MSE
1	Training Data	0.9635	0.0005
2	Testing Data	0.9568	0.0004

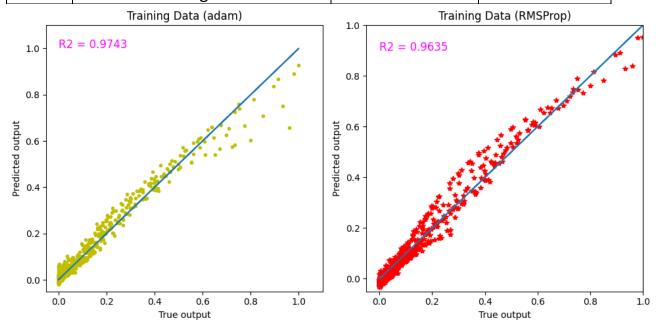


Figure 2: Comparision between adam and RMSProp for Training Data

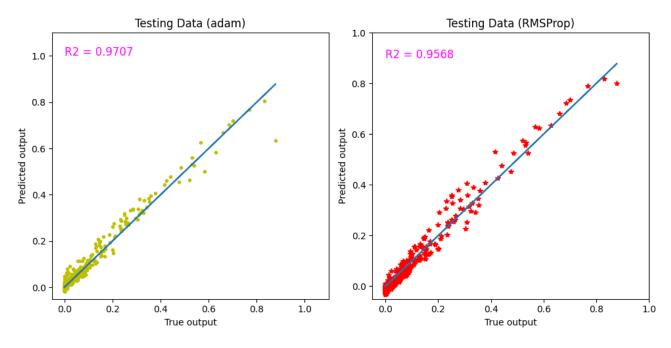


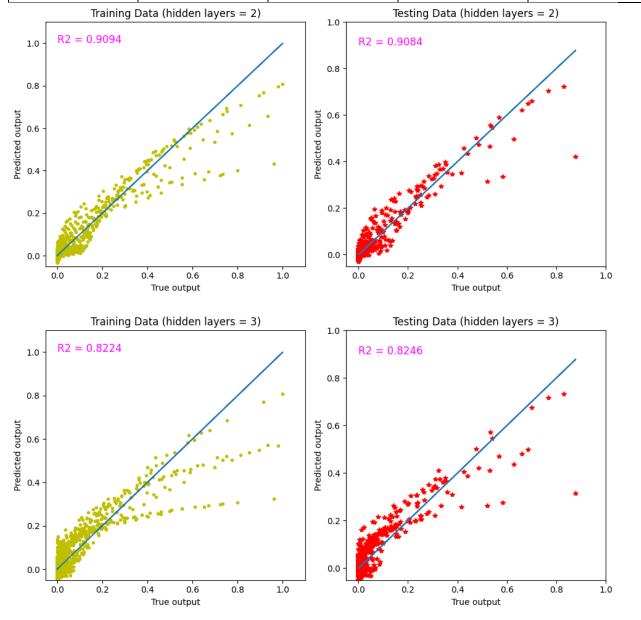
Figure 3: Comparision between adam and RMSProp for Testing Data

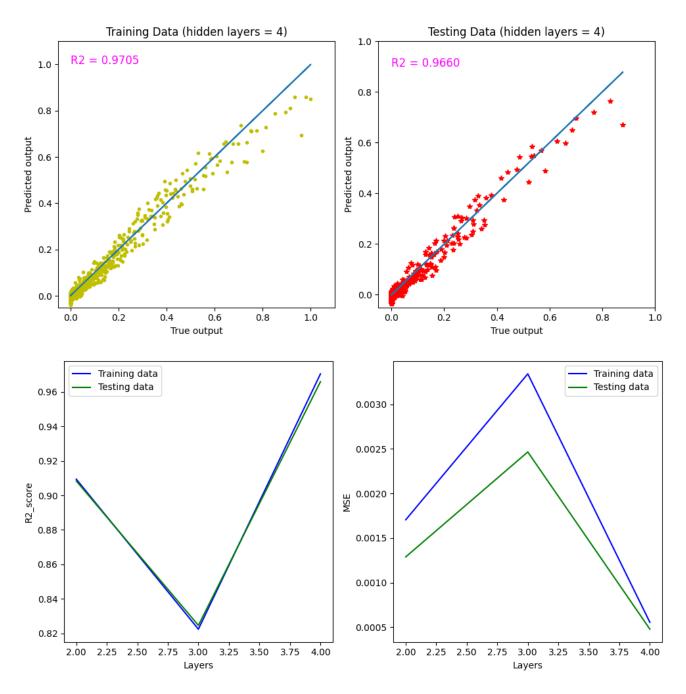
4. RESULTS AND DISCUSSIONS

1. Effect of layers

The number of hidden layers of an ANN model plays an important role in the architecture of the neural network. Additional layers were added to the given layer. Study was conducted using 2,3,4 hidden layers and the results were shown in the table below. Each hidden layer has 'relu' as the activation function.

Number of	Training		Testing	
Hidden Layers	R^2	MSE	R^2	MSE
2	0.9094	0.0017	0.9084	0.0013
3	0.8224	0.0033	0.8246	0.0025
4	0.9705	0.0006	0.9660	0.0005

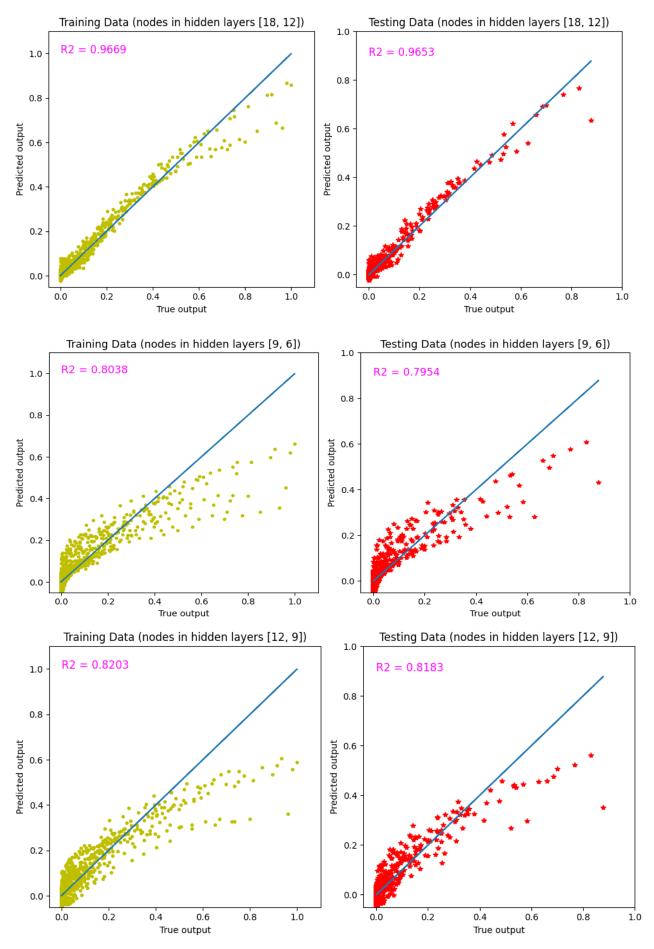


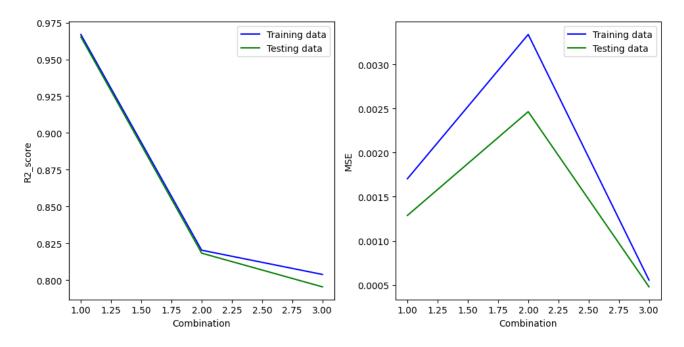


2. Effect of Nodes

The number of Nodes in the hidden layers of the neural network is the important parameter. The number of nodes plays an important role in the performance and predicting capability of the model. The number of nodes in the two hidden layers was varied and the topology which gave the best prediction was found.

Combination	Number of	Training		Testing	
	nodes	R ² MSE		R^2	MSE
1	2-18-12-1	0.9669	0.0006	0.9653	0.0005
2	2-12-9-1	0.8203	0.0034	0.8183	0.0026
3	2-9-6-1	0.8038	0.0037	0.7954	0.0029

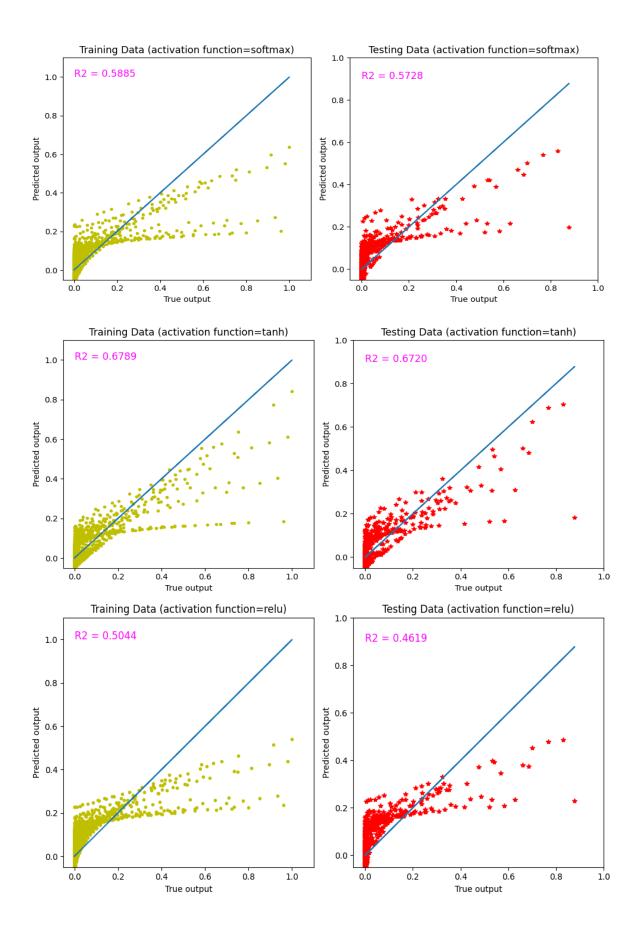


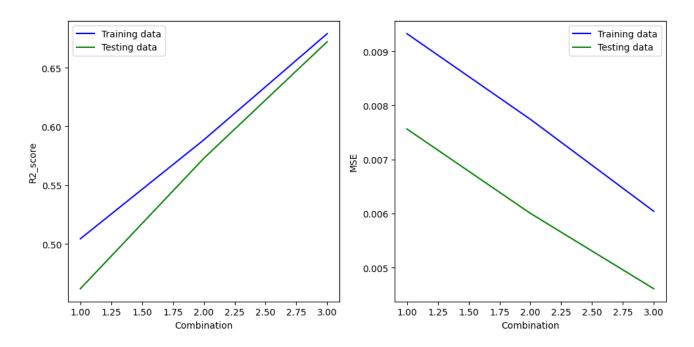


3. Effect of Activation functions

All the other parameter were fixed to study the effect of activation functions. 2 hidden layers were taken. Activation function for both the layers were taken as 'relu','softmax','tanh' respectively. The results observed are given below

Combination	Activation	Training		Testing	
	function	R^2	MSE	R^2	MSE
1	relu-relu-	0.5044	0.0093	0.4613	0.0076
	linear				
2	softmax-	0.5885	0.0077	0.5728	0.0060
	softmax-				
	linear				
3	tanh-tanh-	0.6789	0.0060	0.6720	0.0046
	linear				

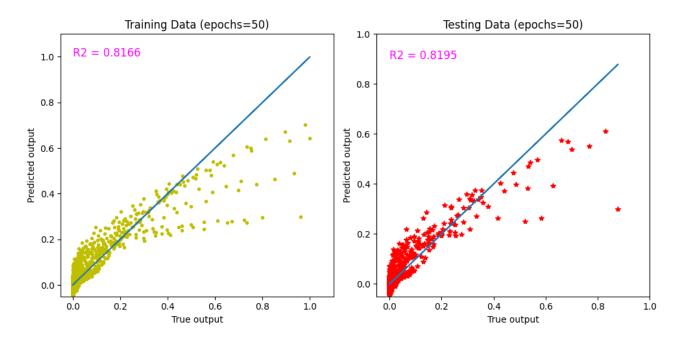


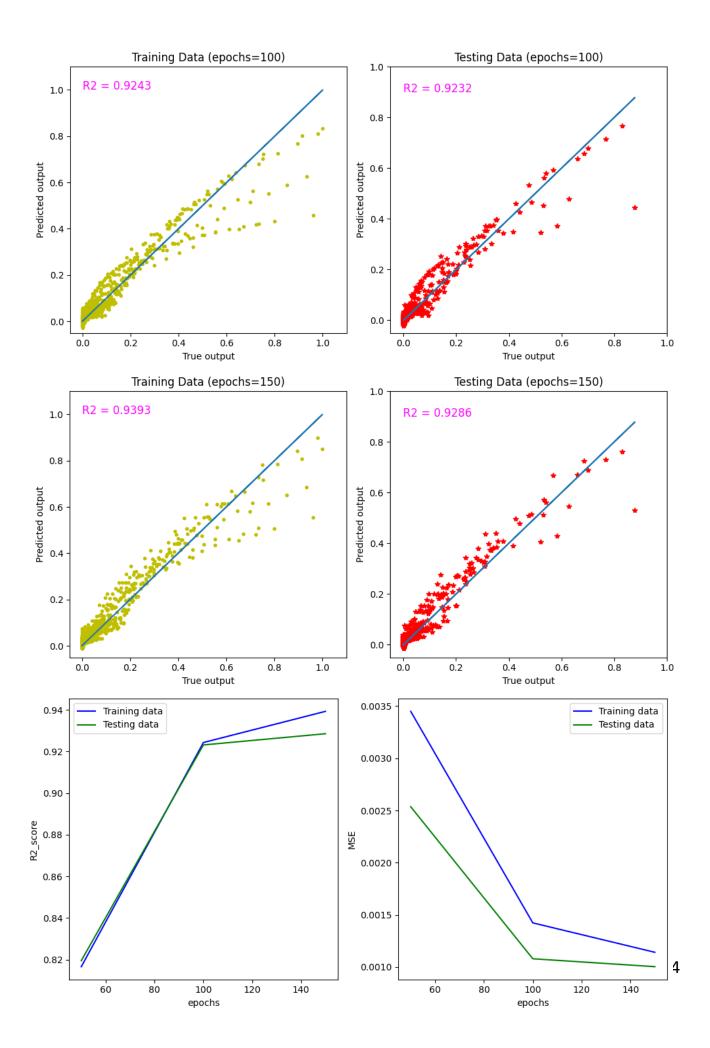


4. Effect of epochs

To study the effect of the Number of Iteration (Epoch) on the prediction performance of the ANN model, the epoch was varied keeping the other parameters fixed as given in the network structure. The results were tabulated below.

Epochs	Training		Testing		
	R ² MSE		R^2	MSE	
50	0.8166	0.0035	0.8195	0.0025	
100	0.9243	0.0014	0.9232	0.0011	
150	0.9393	0.0011	0.9286	0.0010	

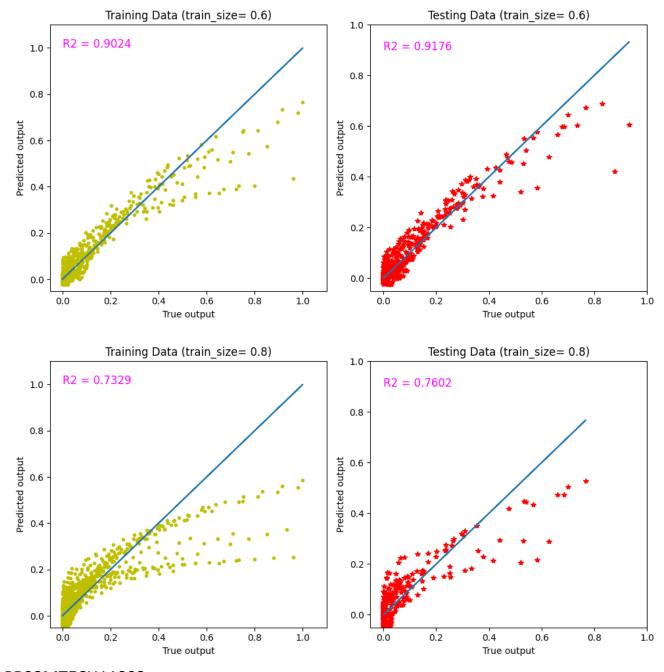


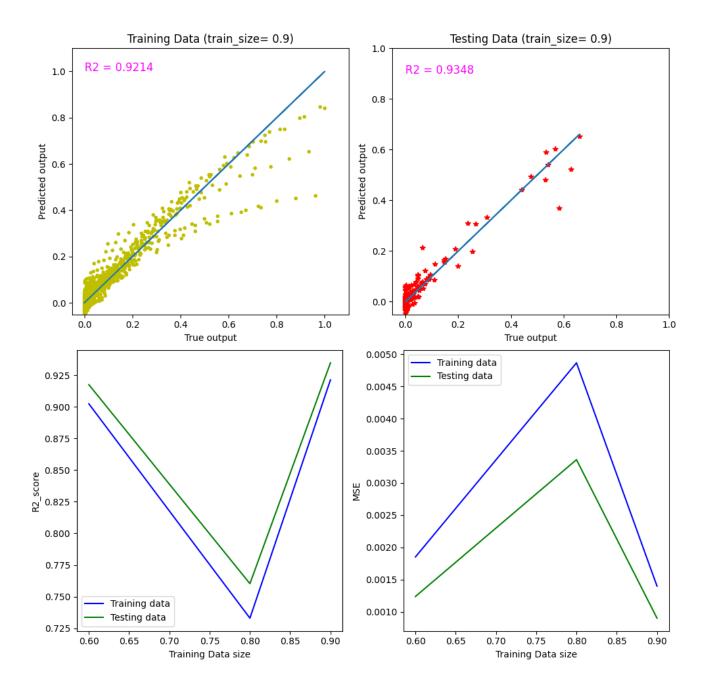


5. Effect of Sample size for training

To study the effect of the sample size taken for training on the prediction performance of the ANN model, the sample size taken for training data was varied keeping the other parameters fixed as given in the network structure. The results were tabulated below.

Size of	Size of	Size of	Training		Tes	ting
Training	Testing	Validation	R^2	MSE	R^2	MSE
Data	Data	data				
51%	40%	9%	0.9024	0.9176	0.9176	0.0012
68%	20%	12%	0.7329	0.0049	0.7062	0.0034
76%	10%	14%	0.9214	0.0014	0.9348	0.0009





5. Conclusion

In our study, we found the best neural network setup for modeling the Beale function. A network with 2 hidden layers, having 64 and 16 nodes respectively, and using ReLU activation functions, performed exceptionally well. We employed the Adam optimizer with a Mean Squared Error (MSE) loss function. Training over 100 epochs, and splitting the data into 70% for training and 15% for both validation and testing, ensured accurate predictions without overfitting. This configuration strikes a balance between complexity and performance, making it the optimal choice for modeling the Beale function.

ANNEXURE

```
In [ ]: # Defining Beale function
        def beale function(x,y):
            Equation of beale function
            Inputs:
            x and y values
            Outputs:
            Value of beale function at x and y
            return (1.5-x+x*y)**2 + (2.25-x+x*y**2)**2 + (2.625-x+x*y**3)**2
        # Generating data for beale function in range in the range -4.5 < x,y < 4.5 with step size 0.2
        import numpy as np
        X,Y,Z = [],[],[] \# Empty lists to store x,y and output values
        for i in np.arange(-4.5,4.6,0.2): # -4.5 < x < 4.5
            for j in np.arange(-4.5,4.6,0.2): # -4.5 < y < 4.5
                X.append(i) # Adding x value to list X
                Y.append(j) # Adding y value to list Y
                Z.append(beale function(i,j)) # Adding beale function value for respective x and y to list Z
        data1 = zip(X,Y,Z) # Concatenation of inputs and outputs
        import pandas as pd
        data2 = pd.DataFrame(data1,columns=['x','y','z']) # Creating a dataframe containing inputs and outputs
        # data2 now has 3 columns containing x, y, f(x,y) values for beale function in the range of -4.5 < x,y < 4.5 with step size 0.2
        data2.head()
        # Saving data to a excel file
        data2.to excel('beale function data step=0.2.xlsx',index=False)
        # Reading data from excel sheet
        data3 = pd.read excel('beale function data step=0.2.xlsx')
```

Normalizing the data - preprocessing

```
from sklearn.model_selection import train_test_split
inputs_train,inputs_test,output_train,output_test = train_test_split(inputs,output,train_size=0.7,random_state=0) # train_size=0.7
```

Creating ANN model

```
from tensorflow.keras import Sequential
from tensorflow.keras.layers import Dense
model = Sequential() # Creating ANN model
model.add(Dense(64,input_dim=2,activation='relu')) # First Layer with 18 nodes and two inputs and "relu" as activation function
model.add(Dense(16,activation='relu')) # Second Layer with 12 nodes and "relu" as activation function
model.add(Dense(1,activation='linear')) # Output Layer with one output and "linear" as activation function
```

Training the model using "adam"

```
In []: model.compile(optimizer ='adam',loss='MSE') # Compiling using optimizer "adam" and loss function "MSE" history = model.fit(inputs_train,output_train,epochs=100,validation_split=0.15) # Training data with 100 epochs and validation split 0.15
```

```
Epoch 1/100
Epoch 2/100
Epoch 3/100
40/40 [============== ] - 0s 3ms/step - loss: 0.0159 - val loss: 0.0177
Epoch 4/100
Epoch 5/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0140 - val loss: 0.0159
Epoch 6/100
Epoch 7/100
Epoch 8/100
Epoch 9/100
Epoch 10/100
40/40 [=============== ] - 0s 5ms/step - loss: 0.0092 - val loss: 0.0103
Epoch 11/100
40/40 [============== ] - 0s 3ms/step - loss: 0.0087 - val loss: 0.0097
Epoch 12/100
Epoch 13/100
40/40 [============== ] - 0s 3ms/step - loss: 0.0077 - val loss: 0.0089
Epoch 14/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0073 - val loss: 0.0084
Epoch 15/100
40/40 [============== ] - 0s 3ms/step - loss: 0.0070 - val loss: 0.0080
Epoch 16/100
Epoch 17/100
Epoch 18/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0061 - val loss: 0.0072
Epoch 19/100
Epoch 20/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0054 - val loss: 0.0064
Epoch 21/100
40/40 [============== ] - 0s 5ms/step - loss: 0.0052 - val loss: 0.0063
Epoch 22/100
```

```
Epoch 23/100
40/40 [=============== ] - 0s 4ms/step - loss: 0.0049 - val loss: 0.0057
Epoch 24/100
Epoch 25/100
40/40 [=============== ] - 0s 5ms/step - loss: 0.0042 - val loss: 0.0056
Epoch 26/100
Epoch 27/100
40/40 [=============== ] - 0s 5ms/step - loss: 0.0041 - val loss: 0.0048
Epoch 28/100
Epoch 29/100
Epoch 30/100
40/40 [=============== ] - 0s 3ms/step - loss: 0.0037 - val loss: 0.0043
Epoch 31/100
Epoch 32/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0035 - val loss: 0.0041
Epoch 33/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0032 - val loss: 0.0041
Epoch 34/100
Epoch 35/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0029 - val loss: 0.0037
Epoch 36/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0029 - val loss: 0.0036
Epoch 37/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0028 - val loss: 0.0036
Epoch 38/100
Epoch 39/100
Epoch 40/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0026 - val loss: 0.0030
Epoch 41/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0023 - val loss: 0.0030
Epoch 42/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0025 - val loss: 0.0032
Epoch 43/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0025 - val loss: 0.0028
Epoch 44/100
```

```
Epoch 45/100
Epoch 46/100
Epoch 47/100
Epoch 48/100
Epoch 49/100
Epoch 50/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0018 - val loss: 0.0024
Epoch 51/100
Epoch 52/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0018 - val loss: 0.0021
Epoch 53/100
Epoch 54/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0017 - val loss: 0.0020
Epoch 55/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0016 - val loss: 0.0020
Epoch 56/100
Epoch 57/100
Epoch 58/100
Epoch 59/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0015 - val loss: 0.0018
Epoch 60/100
Epoch 61/100
Epoch 62/100
Epoch 63/100
Epoch 64/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0012 - val loss: 0.0018
Epoch 65/100
Epoch 66/100
```

```
Epoch 67/100
Epoch 68/100
Epoch 69/100
Epoch 70/100
Epoch 71/100
40/40 [============== ] - 0s 2ms/step - loss: 0.0011 - val loss: 0.0012
Epoch 72/100
40/40 [=============== ] - 0s 2ms/step - loss: 0.0010 - val loss: 0.0014
Epoch 73/100
Epoch 74/100
Epoch 75/100
Epoch 76/100
Epoch 77/100
Epoch 78/100
Epoch 79/100
Epoch 80/100
Epoch 81/100
Epoch 82/100
Epoch 83/100
Epoch 84/100
Epoch 85/100
Epoch 86/100
Epoch 87/100
Epoch 88/100
```

```
Epoch 89/100
Epoch 90/100
Epoch 91/100
Epoch 92/100
Epoch 93/100
Epoch 94/100
Epoch 95/100
Epoch 96/100
Epoch 97/100
Epoch 98/100
Epoch 99/100
Epoch 100/100
```

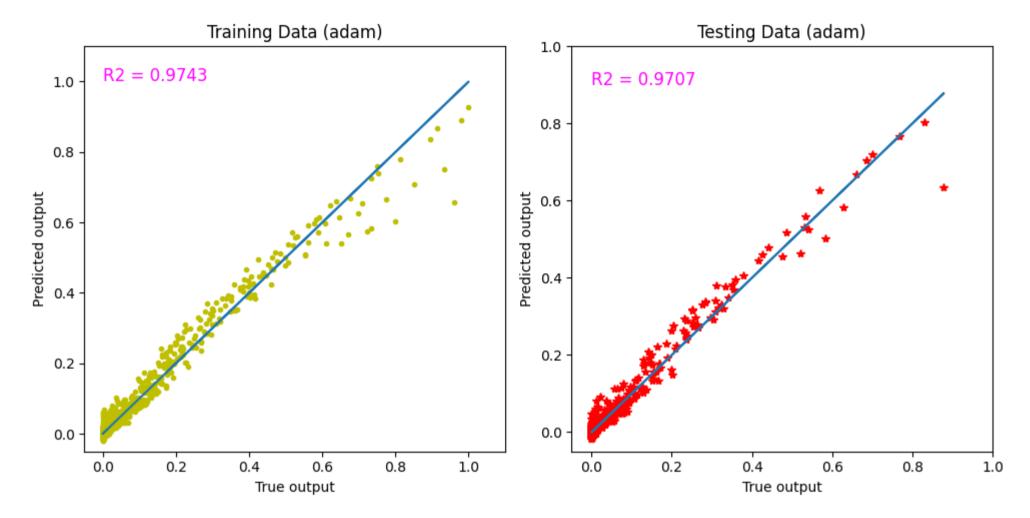
Prediction and analysis

```
In []: pred_train = model.predict(inputs_train) # Prediction of training data
    pred_test = model.predict(inputs_test) # Prediction of testing data
    from sklearn.metrics import r2_score
    r2_train = r2_score(output_train,pred_train) # R2 score of training data
    print(f"R2 Score for training data: {r2_train:.4f}")
    r2_test = r2_score(output_test,pred_test) # R2 score of testing data
    print(f"R2 Score for testing data: {r2_test:.4f}")
    from sklearn.metrics import mean_squared_error
    mse_train = mean_squared_error(output_train,pred_train) # MSE of training data
    print(f"Mean Squared Error for training data: {mse_train:.4f}")
    mse_test = mean_squared_error(output_test,pred_test) # MSE of Testing data
    print(f"Mean Squared Error for testing data: {mse_test:.4f}")
```

```
47/47 [=========] - 0s 953us/step 20/20 [=========] - 0s 1ms/step R2 Score for training data: 0.9743 R2 Score for testing data: 0.9707 Mean Squared Error for training data: 0.0005 Mean Squared Error for testing data: 0.0004
```

Plots - Training Data Vs Testing Data

```
In [ ]: import matplotlib.pyplot as plt
        fig,plot = plt.subplots(1,2,figsize=(10,5))
        plot[0].plot(output train, pred train, 'y.')
        plot[0].plot(output train,output train,'-')
        plot[0].set_xlabel('True output')
        plot[0].set ylabel('Predicted output')
        plot[0].set ylim(-0.05,1.1)
        plot[0].set_xlim(-0.05,1.1)
        plot[0].set_title(f'Training Data (adam)')
        plot[0].text(0,1,f'R2 = {r2 train:.4f}',fontsize=12,color='magenta')
        plot[1].plot(output test,pred test,'r*')
        plot[1].plot(output_test,output_test,'-')
        plot[1].set ylim(-0.05,1)
        plot[1].set xlim(-0.05,1)
        plot[1].set_xlabel('True output')
        plot[1].set_ylabel('Predicted output')
        plot[1].set title(f'Testing Data (adam)')
        plot[1].text(0,0.9,f'R2 = {r2_test:.4f}',fontsize=12,color='magenta')
        plt.tight_layout()
        plt.show()
```



Training the model using "RMSProp"

In []: model.compile(optimizer ='RMSProp',loss='MSE') # Compiling using optimizer "RMSProp" and loss function "MSE"
history = model.fit(inputs_train,output_train,epochs=100,validation_split=0.15) # Training data with 100 epochs and validation split 0.15

```
Epoch 1/100
40/40 [============== ] - 1s 5ms/step - loss: 9.8247e-04 - val loss: 7.2633e-04
Epoch 2/100
Epoch 3/100
Epoch 4/100
Epoch 5/100
Epoch 6/100
Epoch 7/100
Epoch 8/100
Epoch 9/100
Epoch 10/100
Epoch 11/100
Epoch 12/100
Epoch 13/100
Epoch 14/100
Epoch 15/100
Epoch 16/100
Epoch 17/100
Epoch 18/100
Epoch 19/100
Epoch 20/100
Epoch 21/100
Epoch 22/100
```

```
Epoch 23/100
Epoch 24/100
Epoch 25/100
Epoch 26/100
Epoch 27/100
Epoch 28/100
Epoch 29/100
Epoch 30/100
Epoch 31/100
Epoch 32/100
Epoch 33/100
Epoch 34/100
Epoch 35/100
Epoch 36/100
Epoch 37/100
Epoch 38/100
Epoch 39/100
Epoch 40/100
Epoch 41/100
Epoch 42/100
Epoch 43/100
Epoch 44/100
```

```
Epoch 45/100
40/40 [============== ] - 0s 2ms/step - loss: 5.5806e-04 - val loss: 3.7942e-04
Epoch 46/100
Epoch 47/100
Epoch 48/100
Epoch 49/100
Epoch 50/100
Epoch 51/100
Epoch 52/100
Epoch 53/100
Epoch 54/100
Epoch 55/100
Epoch 56/100
Epoch 57/100
Epoch 58/100
Epoch 59/100
Epoch 60/100
Epoch 61/100
Epoch 62/100
Epoch 63/100
Epoch 64/100
Epoch 65/100
Epoch 66/100
```

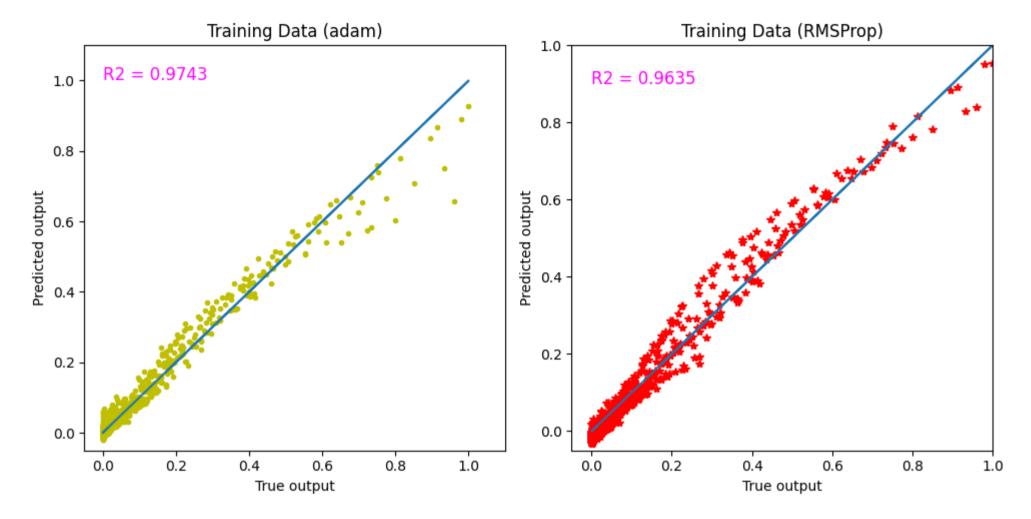
```
Epoch 67/100
Epoch 68/100
Epoch 69/100
Epoch 70/100
Epoch 71/100
Epoch 72/100
Epoch 73/100
Epoch 74/100
Epoch 75/100
Epoch 76/100
Epoch 77/100
Epoch 78/100
Epoch 79/100
Epoch 80/100
Epoch 81/100
Epoch 82/100
Epoch 83/100
Epoch 84/100
Epoch 85/100
Epoch 86/100
Epoch 87/100
Epoch 88/100
```

```
Epoch 89/100
Epoch 90/100
Epoch 91/100
Epoch 92/100
Epoch 93/100
Epoch 94/100
Epoch 95/100
Epoch 96/100
Epoch 97/100
Epoch 98/100
Epoch 99/100
Epoch 100/100
```

Prediction and analysis

```
In []: pred_train2 = model.predict(inputs_train) # Prediction of training data
    pred_test2 = model.predict(inputs_test) # Prediction of testing data
    from sklearn.metrics import r2_score
    r2_train2 = r2_score(output_train,pred_train2) # R2 score of training data
    print(f"R2 Score for training data: {r2_train2:.4f}")
    r2_test2 = r2_score(output_test,pred_test2) # R2 score of testing data
    print(f"R2 Score for testing data: {r2_test2:.4f}")
    from sklearn.metrics import mean_squared_error
    mse_train2 = mean_squared_error(output_train,pred_train2) # MSE of training data
    print(f"Mean Squared Error for training data: {mse_train:.4f}")
    mse_test2 = mean_squared_error(output_test,pred_test2) # MSE of testing data
    print(f"Mean Squared Error for testing data: {mse_test:.4f}")
```

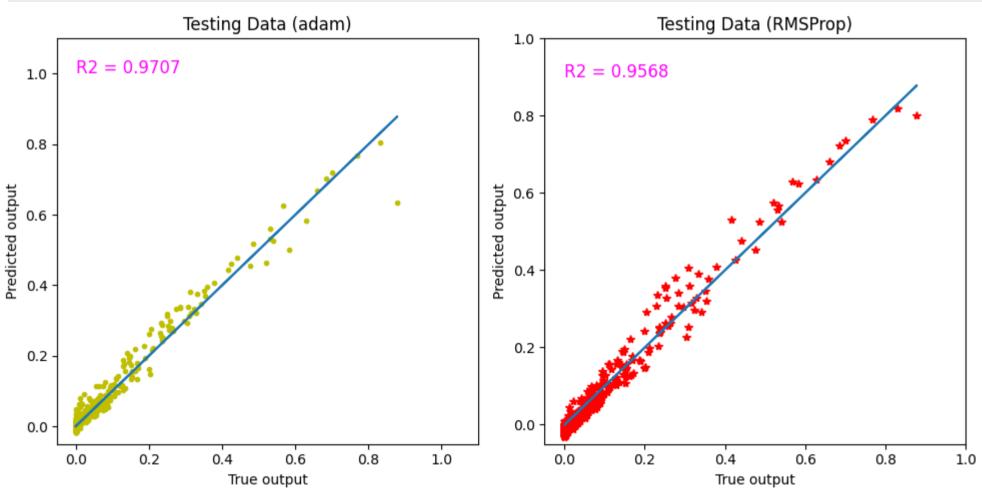
```
In [ ]: # Plot for Training data "adam" Vs "RMSProp"
        import matplotlib.pyplot as plt
        fig,plot2 = plt.subplots(1,2,figsize=(10,5))
        plot2[0].plot(output train,pred train,'y.')
        plot2[0].plot(output train,output train,'-')
        plot2[0].set xlabel('True output')
        plot2[0].set ylabel('Predicted output')
        plot2[0].set_ylim(-0.05,1.1)
        plot2[0].set_xlim(-0.05,1.1)
        plot2[0].set title(f'Training Data (adam)')
        plot2[0].text(0,1,f'R2 = {r2 train:.4f}',fontsize=12,color='magenta')
        plot2[1].plot(output train,pred train2,'r*')
        plot2[1].plot(output train,output train,'-')
        plot2[1].set ylim(-0.05,1)
        plot2[1].set_xlim(-0.05,1)
        plot2[1].set xlabel('True output')
        plot2[1].set ylabel('Predicted output')
        plot2[1].set_title(f'Training Data (RMSProp)')
        plot2[1].text(0,0.9,f'R2 = {r2 train2:.4f}',fontsize=12,color='magenta')
        plt.tight layout()
        plt.show()
```



Plot for Testing data "adam" Vs "RMSProp"

```
import matplotlib.pyplot as plt
fig,plot3 = plt.subplots(1,2,figsize=(10,5))
plot3[0].plot(output_test,pred_test,'y.')
plot3[0].plot(output_test,output_test,'-')
plot3[0].set_xlabel('True output')
plot3[0].set_ylabel('Predicted output')
plot3[0].set_ylim(-0.05,1.1)
plot3[0].set_xlim(-0.05,1.1)
plot3[0].set_title(f'Testing Data (adam)')
plot3[0].text(0,1,f'R2 = {r2_test:.4f}',fontsize=12,color='magenta')
plot3[1].plot(output_test,pred_test2,'r*')
```

```
plot3[1].plot(output_test,output_test,'-')
plot3[1].set_ylim(-0.05,1)
plot3[1].set_xlim(-0.05,1)
plot3[1].set_xlabel('True output')
plot3[1].set_ylabel('Predicted output')
plot3[1].set_title(f'Testing Data (RMSProp)')
plot3[1].text(0,0.9,f'R2 = {r2_test2:.4f}',fontsize=12,color='magenta')
plt.tight_layout()
plt.show()
Testing Data (adam)
```



Effect of variations

```
In [ ]: # Define Beale function
        def beale function(x,y):
            Equation of beale function
            Inputs:
            x and y values
            Outputs:
            Value of beale function at x and y
            return (1.5-x+x*y)**2 + (2.25-x+x*y**2)**2 + (2.625-x+x*y**3)**2
        # Generating data for beale function in range and saving to excel
        def generating data(step,low=-4.5,high=4.6):
            Generates data points on the beale function for all values of x and y in the range -4.5 < x,y < 4.5
            Inputs:
            1) step
            Output:
            1) DataFrame containing values of (x,y,z)
            0.000
            X,Y,Z = [],[],[]
            for i in np.arange(low,high,step):
                for j in np.arange(low,high,step):
                    X.append(i)
                    Y.append(j)
                    Z.append(beale_function(i,j))
            # Creating a dataframe for the data generated above
            data1 = zip(X,Y,Z)
            data2 = pd.DataFrame(data1,columns=['x','y','z'])
            return data2
        # Normarlizing, splitting into inputs and outputs, test splitting
        def split(data,train size:float):
            This function takes the data, normalize it and splits into training dataset and testing dataset
            Input:
            1) data (DataFrame): DataFrame containing labelled data
            2) train_size (float): Fraction of train sample to be split
```

```
Output:
   1) inputs train: input datasets for training
   2) inputs test: input datasets for testing
   2) output test: output datasets for testing
   4) output test: output datasets for training
   # Normallizing the data
   scaler = MinMaxScaler()
   data3 = scaler.fit transform(data.values)
   # Splitting the data
   inputs = data3[:,0:2]
   output = data3[:,-1]
   # Splitting the data
   inputs_train,inputs_test,output_train,output_test = train_test_split(inputs,output,train_size=train_size,random_state=0)
   return inputs train,inputs test,output train,output test
# Structuring ANN with number of hidden layers, nodes and activation functions
def network(layers:int,nodes:list,activation function:str):
   Creates a Artificial Neural Network with linear output layer with one node
   Inputs:
   1) layers (int): Number of layers in the neural network
   2) nodes (list): Number of nodes present in each hidden layer starting from first hidden layer
   3) activation function (str): Optimizer for the hidden layers
   Output:
   1) model: Gives you the nodel as output
   model = Sequential()
   # Add hidden Layers
   for i in range(layers):
       if i == 0:
           # For the first hidden layer
            model.add(Dense(nodes[i], input dim=2, activation=activation function))
        else:
            model.add(Dense(nodes[i], activation=activation function))
   # Output Layer
   model.add(Dense(1,activation='linear'))
   # model.summary()
   return model
# Training
```

```
def training(model,optimizer:str,loss function:str,inputs,output,epoch=100,):
   Trains the data given to the model with given optimizer and loss function with default epochs=100
    Inputs:
    1) model: A model to be trained
   2) optimizer (str): A optimizer for training
   3) loss function (str): Loss function
   4) inputs: All inputs of function
   5) output: All output of function
   6) epoch (int): Number of epochs
   Output:
    1) model: Gives you trained model
    0.00
   model.compile(optimizer =optimizer,loss=loss_function)
   history = model.fit(inputs,output,epochs=epoch,validation split=0.15,verbose=0)
    return model
# Results
def result(predicted,output):
   Takes actual values and predicted values and gives you R2_score and MSE
   Inputs:
   1) predicted: Output that is predicted by model
    2) output: Actual output
    Output:
   1) r2 (float): R2_score of the given data
   2) mse (float): MSE of the given data
   mse = mean_squared_error(output,predicted)
   print(f"Mean Squared Error: {mse:.4f}")
   # Calculating R2 score
   r2 = r2_score(output,predicted)
   print(f"R2 Score: {r2:.4f}")
   return r2,mse
# Plotting Training data vs Testing data
def plotting(splitted data,train prediction,test prediction,tr,te,variation):
    Plots graphs between Predicted output and Actual output for Training and Testing data
```

```
Inputs:
   1) splitted data: Actual data
   2) train prediction: Output predicted by model from training data
   3) test prediction: Output predicted by model from testing data
   4) tr: r2 score of Training data
   4) te: r2 score of Testing data
   5) variation (str): If plotting for multiple variations
   fig,plot = plt.subplots(1,2,figsize=(10,5))
   plot[0].plot(splitted data[2],train prediction,'y.')
   plot[0].plot(splitted data[2],splitted data[2],'-')
   plot[0].set xlabel('True output')
   plot[0].set ylabel('Predicted output')
   plot[0].set ylim(-0.05,1.1)
   plot[0].set xlim(-0.05,1.1)
   plot[0].set_title(f'Training Data ({variation})')
   plot[0].text(0,1,f'R2 = \{tr:.4f\}',fontsize=12,color='magenta')
   plot[1].plot(splitted data[3],test prediction,'r*')
   plot[1].plot(splitted data[3],splitted data[3],'-')
   plot[1].set ylim(-0.05,1)
   plot[1].set xlim(-0.05,1)
   plot[1].set xlabel('True output')
   plot[1].set ylabel('Predicted output')
   plot[1].set title(f'Testing Data ({variation})')
   plot[1].text(0,0.9,f'R2 = \{te:.4f\}',fontsize=12,color='magenta')
   plt.tight layout()
   plt.show()
# Plotting variation
def plotting2(tr r2,tr mse,te r2,te mse,var=[1,2,3],iter='Combination'):
   Plots two graphs for R2 score and MSE for different variations
   Inputs:
   1) tr r2 (list): A list of all r2 score for training data for all variations
   2) tr mse (list): A list of all MSE for training data for all variations
   3) te r2 (list): A list of all r2 score for testing data for all variations
   4) te mse (list): A list of all MSE for testing data for all variations
   5) var (list): A list of number of variations for x-axis
   6) iter (str): Name of the variable that is being studied
   fig,plot = plt.subplots(1,2,figsize=(10,5))
   plot[0].plot(var,tr r2,'b-',label='Training data')
```

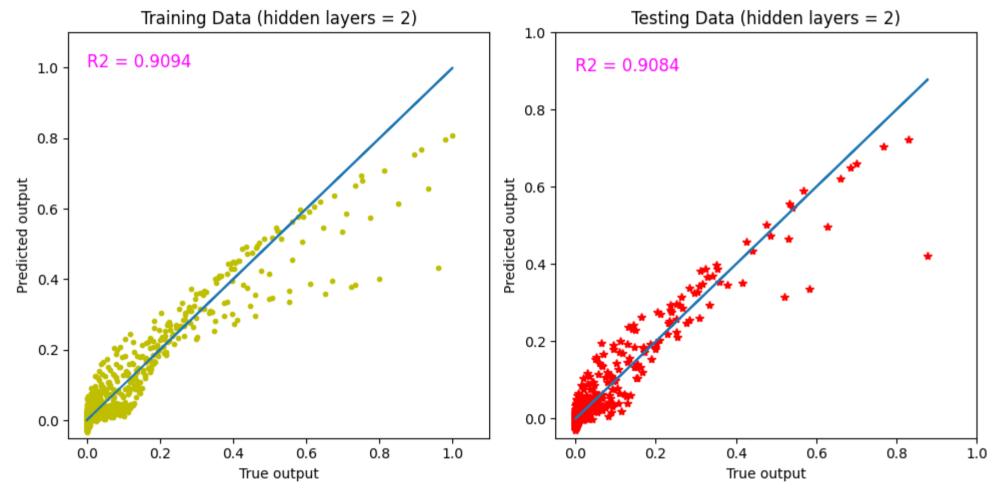
```
plot[0].plot(var,te_r2,'g-',label='Testing data')
            plot[0].set xlabel(iter)
            plot[0].set ylabel('R2 score')
            # plot[0].grid(True)
            plot[0].legend()
            plot[1].plot(var,tr mse,'b-',label='Training data')
            plot[1].plot(var,te mse,'g-',label='Testing data')
            plot[1].set_xlabel(iter)
            plot[1].set ylabel('MSE')
            # plot[1].grid(True)
            plot[1].legend()
            plt.tight_layout()
            plt.show()
        splitted data = split(data3,0.7) # Data for variations
In [ ]: # Variation of parameters
        ex_layers = [2,3,4] # Variation in nodes
        ex nodes = [18,12,9,6] # Variation in Layers
        ex activation functions = ['relu', 'softmax', 'tanh'] # Variations in activation functions of all hidden layers
        ex epochs = [50,100,150] # Variation in epochs
        ex train size = [0.6,0.8,0.9] # Variation in Training size
In [ ]: # Varying number of hidden Layers
        tr r71,tr mse71,te r71,te mse71 = [],[],[],[]
        for a in range(0,3,1):
            iter71 = f'hidden layers = {ex layers[a]}'
            # Creating a network
            ann711 = network(ex_layers[a],ex_nodes,ex_activation_functions[0])
            # Training
            ann712 = training(ann711, 'adam', 'MSE', splitted data[0], splitted data[2], ex epochs[1])
            # Train data
            z71_train = ann712.predict(splitted_data[0],verbose=0)
            # Test data
            z71 test = ann712.predict(splitted data[1], verbose=0)
            # Results
            r71,mse71 = result(z71 train,splitted data[2])
            r711, mse711 = result(z71 test, splitted data[3])
            tr_r71.append(r71)
            tr_mse71.append(mse71)
            te r71.append(r711)
            te_mse71.append(mse711)
            #Plotting
```

```
plotting(splitted_data,z71_train,z71_test,r71,r711,iter71)
plotting2(tr_r71,tr_mse71,te_r71,te_mse71,ex_layers,'Layers')
```

R2 Score: 0.9094

Mean Squared Error: 0.0013

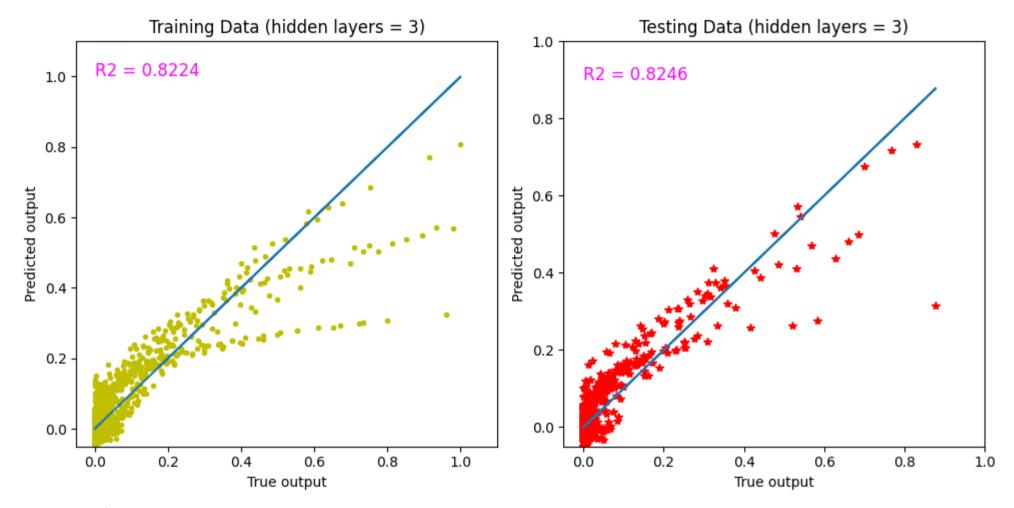
R2 Score: 0.9084



Mean Squared Error: 0.0033

R2 Score: 0.8224

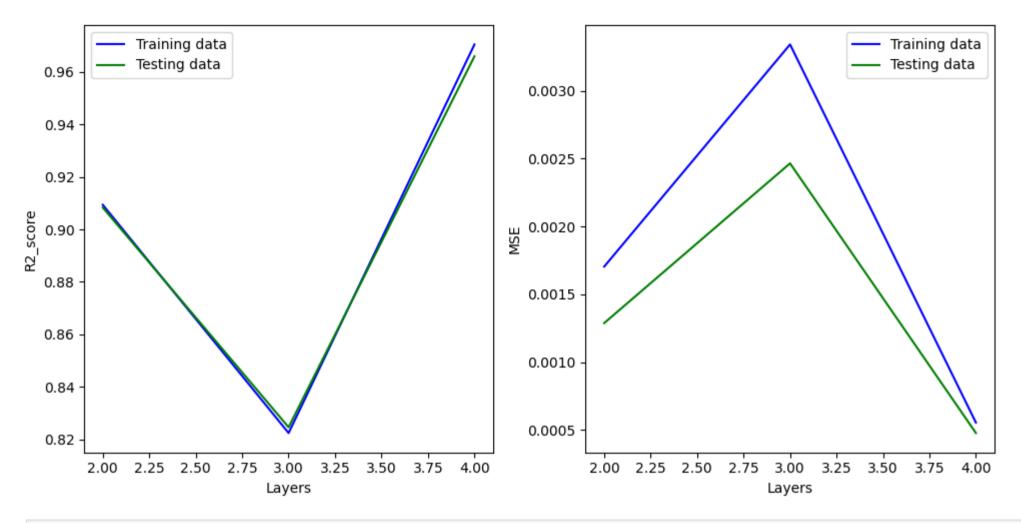
Mean Squared Error: 0.0025



R2 Score: 0.9705

Mean Squared Error: 0.0005



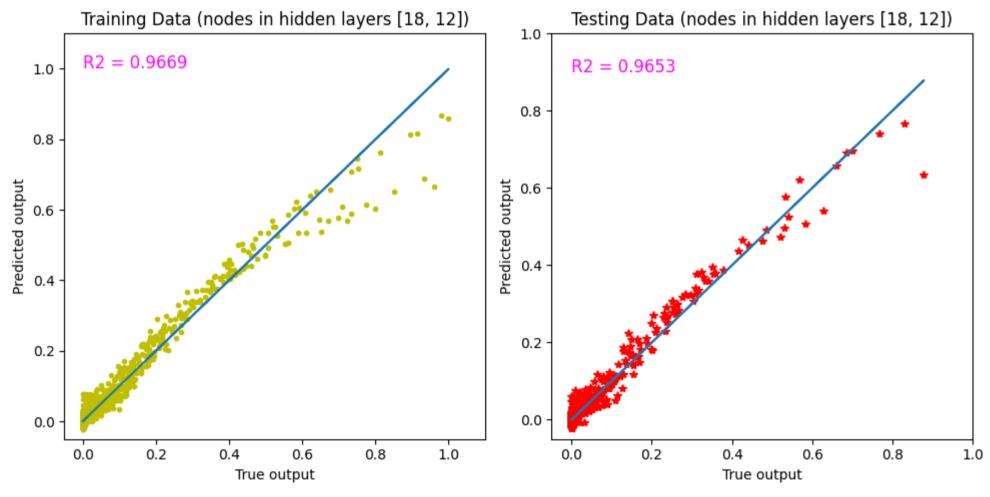


```
In []: # Varying nodes
tr_r72,tr_mse72,te_r72,te_mse72 = [],[],[],[]
for b in range(0,3,1):
    iter72 = f'nodes in hidden layers {ex_nodes[b:b+2]}'
    # ex_nodes2.append(ex_nodes[b:b+2])
    #Creating a network
    ann721 = network(ex_layers[0],ex_nodes[b:b+2],ex_activation_functions[0])
    # Training
    ann722 = training(ann721, 'adam', 'MSE',splitted_data[0],splitted_data[2],ex_epochs[1])
# Train data results
z72_train = ann722.predict(splitted_data[0],verbose=0)
# Test data results
z72_test = ann722.predict(splitted_data[1],verbose=0)
# Results
```

```
r72,mse72 = result(z72_train,splitted_data[2])
r722,mse722 = result(z72_test,splitted_data[3])
tr_r72.append(r72)
tr_mse72.append(mse72)
te_r72.append(r722)
te_mse72.append(mse722)
#Plotting
plotting(splitted_data,z72_train,z72_test,r72,r722,iter72)
plotting2(tr_r72,tr_mse71,te_r72,te_mse71)
```

R2 Score: 0.9669

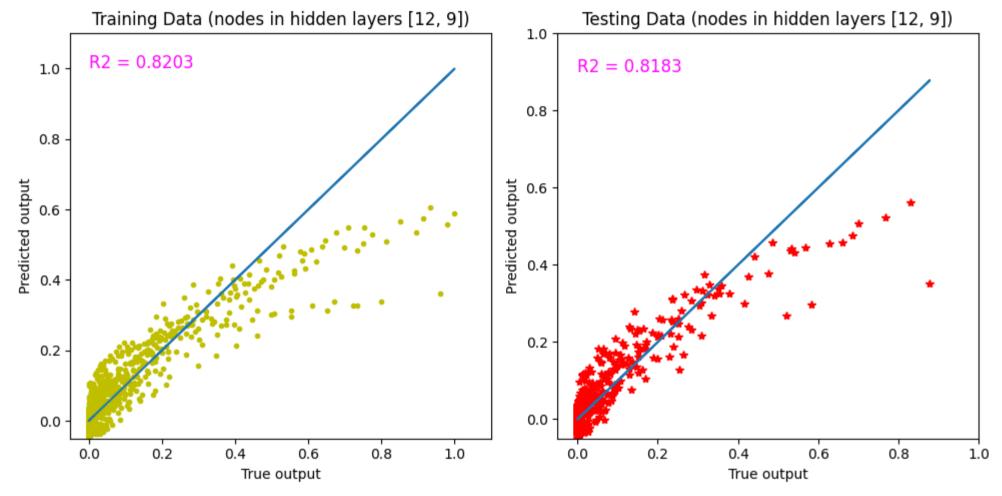
Mean Squared Error: 0.0005



R2 Score: 0.8203

Mean Squared Error: 0.0026

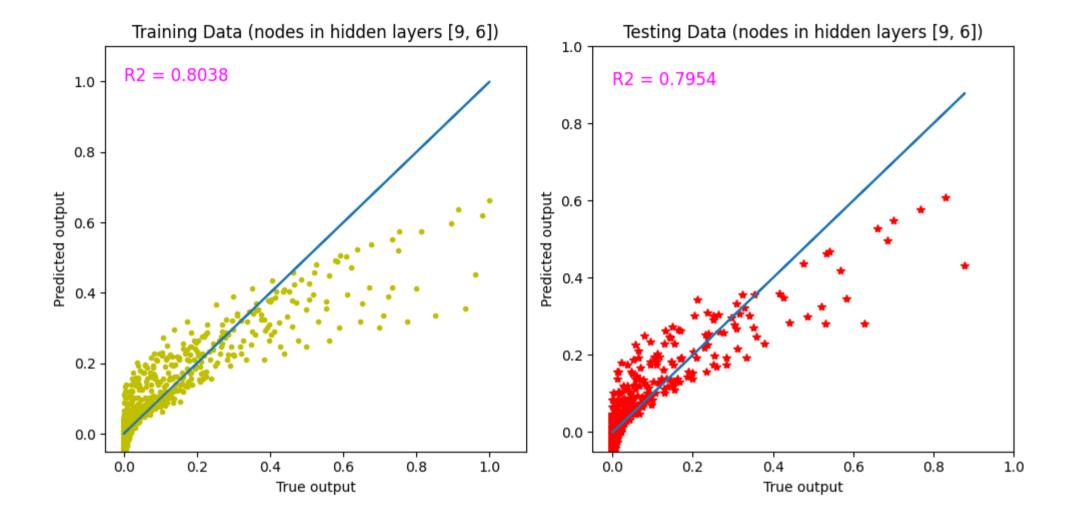
R2 Score: 0.8183

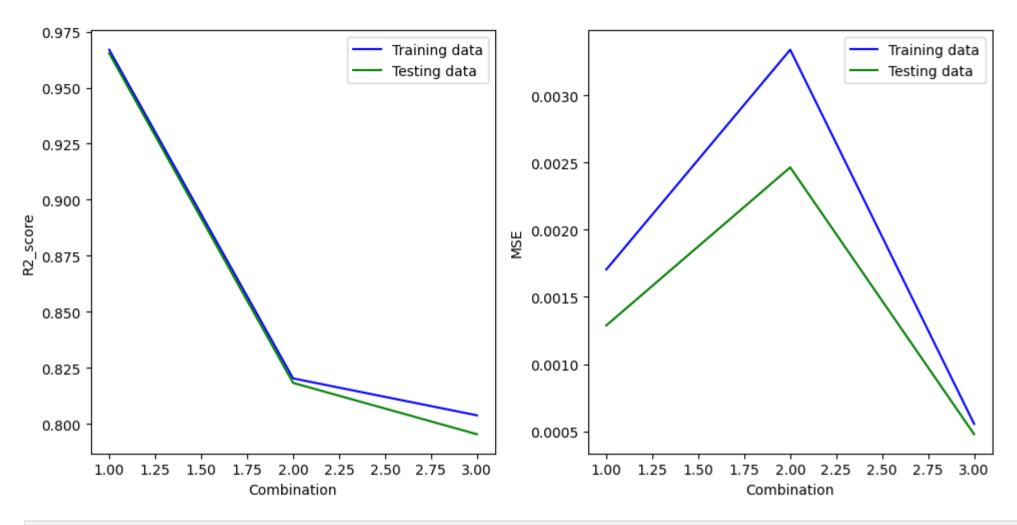


Mean Squared Error: 0.0037

R2 Score: 0.8038

Mean Squared Error: 0.0029





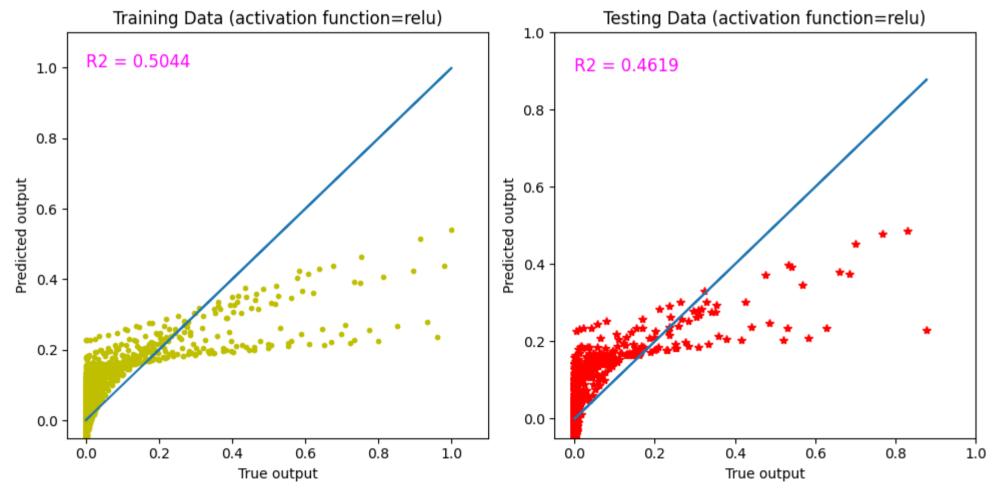
```
In []: # Varying activation functions
tr_r73,tr_mse73,te_r73,te_mse73 = [],[],[],[]
for c in range(0,3,1):
    iter73 = f'activation function={ex_activation_functions[c]}'
    ann731 = network(ex_layers[0],ex_nodes,ex_activation_functions[c])
    ann732 = training(ann732, 'adam', 'MSE',splitted_data[0],splitted_data[2],ex_epochs[1])
    # Train data
    z73_train = ann732.predict(splitted_data[0],verbose=0)
# Test data
    z73_test = ann732.predict(splitted_data[1],verbose=0)
# Results
    r73,mse73 = result(z73_train,splitted_data[2])
    r733,mse733 = result(z73_test,splitted_data[3])
    tr_r73.append(r73)
```

```
tr_mse73.append(mse73)
  te_r73.append(r733)
  te_mse73.append(mse733)
  #Plotting
  plotting(splitted_data,z73_train,z73_test,r73,r733,iter73)
plotting2(tr_r73,tr_mse73,te_r73,te_mse73)
```

R2 Score: 0.5044

Mean Squared Error: 0.0076

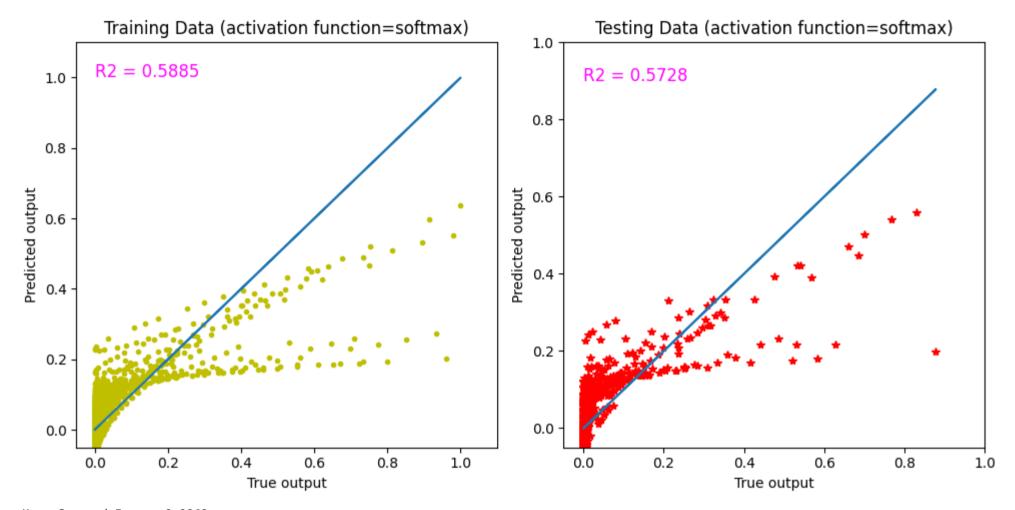
R2 Score: 0.4619



Mean Squared Error: 0.0077

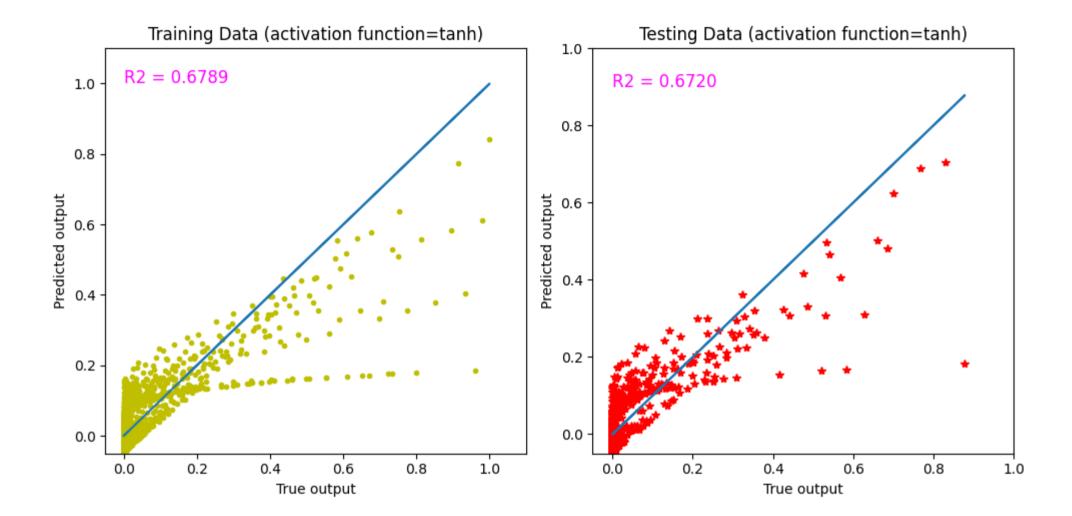
R2 Score: 0.5885

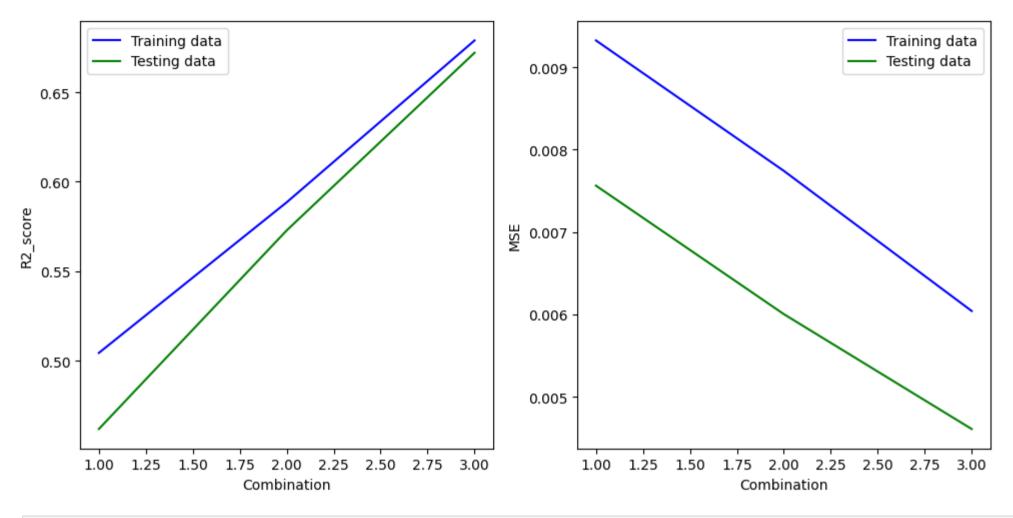
Mean Squared Error: 0.0060



R2 Score: 0.6789

Mean Squared Error: 0.0046





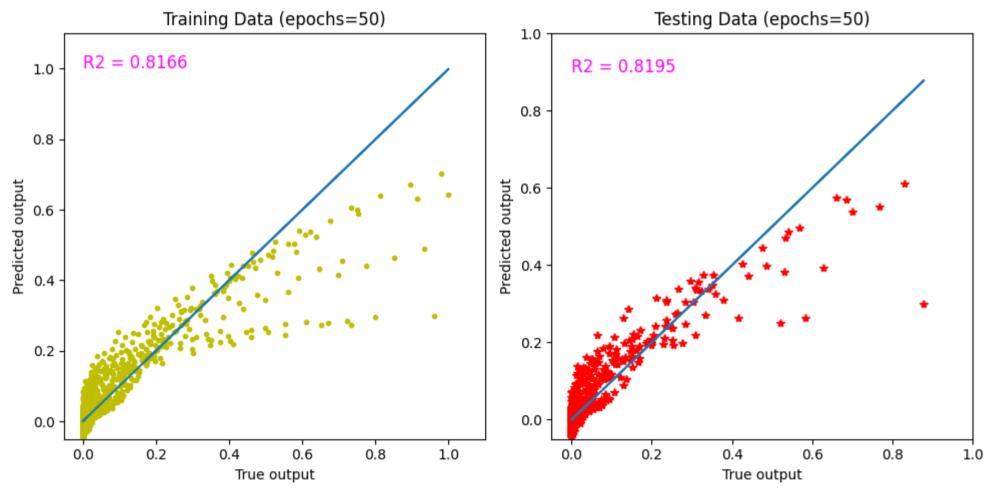
```
In []: # Varying epochs
tr_r74,tr_mse74,te_r74,te_mse74 = [],[],[],[]
for d in range(0,3,1):
    iter74 = f'epochs={ex_epochs[d]}'
    ann741 = network(ex_layers[0],ex_nodes,ex_activation_functions[0])
    ann742 = training(ann741, 'adam', 'MSE', splitted_data[0], splitted_data[2],ex_epochs[d])
    # Train data
    z74_train = ann742.predict(splitted_data[0],verbose=0)
    # Test data
    z74_test = ann742.predict(splitted_data[1],verbose=0)
# Results
    r74,mse74 = result(z74_train,splitted_data[2])
    r744,mse744 = result(z74_test,splitted_data[3])
    tr_r74.append(r74)
```

```
tr_mse74.append(mse74)
  te_r74.append(r744)
  te_mse74.append(mse744)
  #Plotting
  plotting(splitted_data,z74_train,z74_test,r74,r744,iter74)
plotting2(tr_r74,tr_mse74,te_mse74,ex_epochs,'epochs')
```

R2 Score: 0.8166

Mean Squared Error: 0.0025

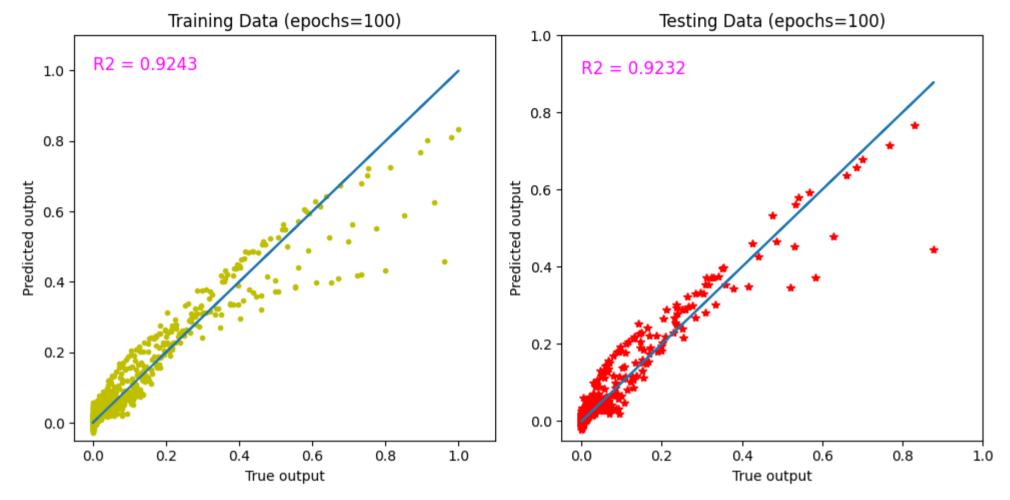
R2 Score: 0.8195



Mean Squared Error: 0.0014

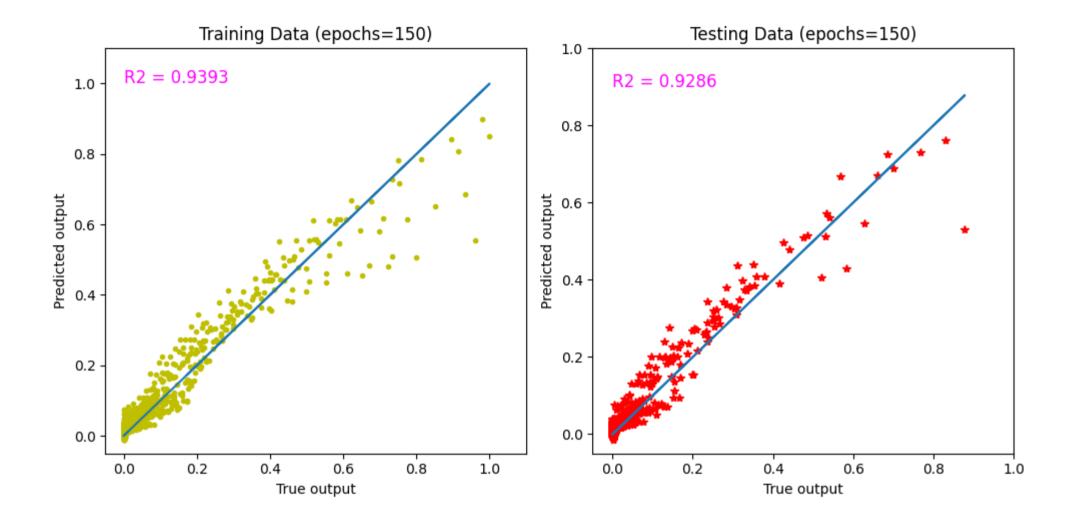
R2 Score: 0.9243

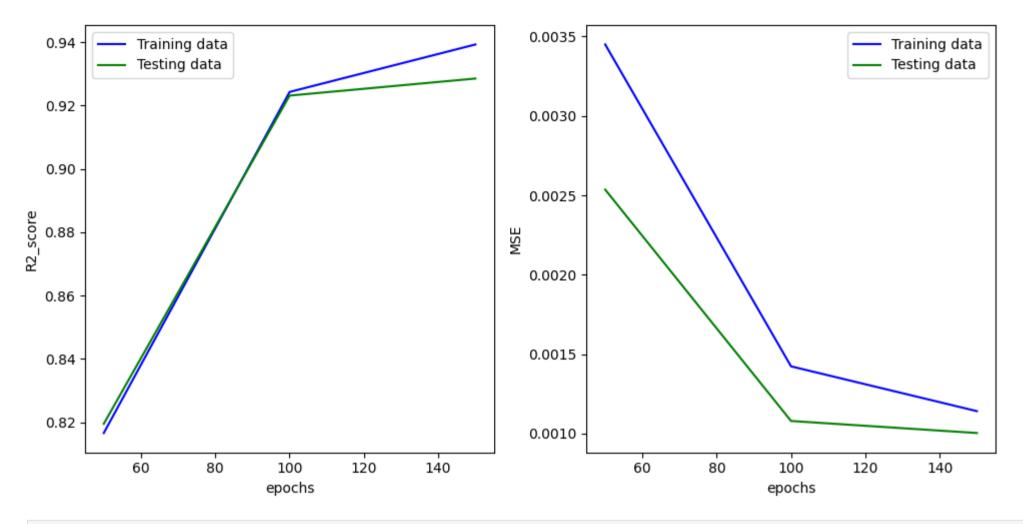
Mean Squared Error: 0.0011



R2 Score: 0.9393

Mean Squared Error: 0.0010



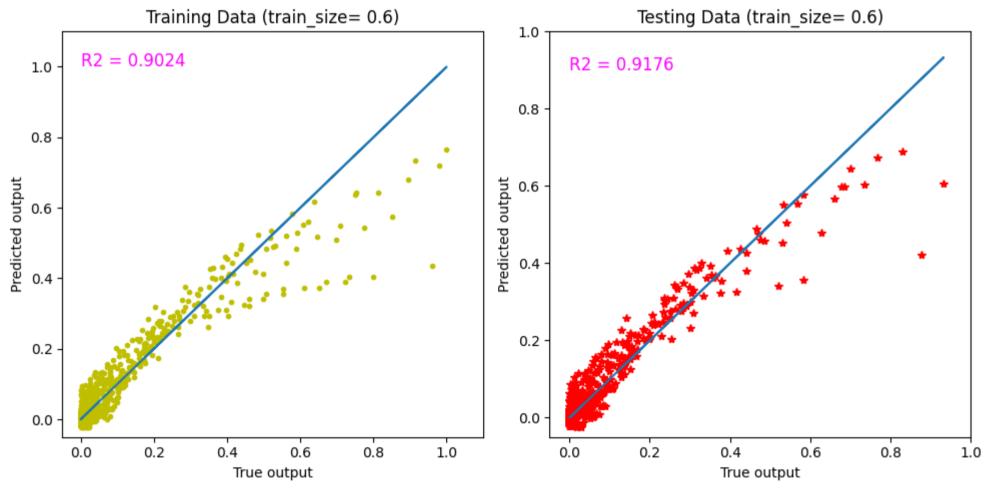


```
In []: # Varying sample size
tr_r75,tr_mse75,te_r75,te_mse75 = [],[],[],[]
for e in range(0,3,1):
    iter75 = f'train_size= {ex_train_size[e]}'
    sp_data = split(data3,ex_train_size[e]) |
    ann751 = network(ex_layers[0],ex_nodes,ex_activation_functions[0])
    ann752 = training(ann751,'adam','MSE',sp_data[0],sp_data[2],ex_epochs[1])
    # Train data
    z75_train = ann752.predict(sp_data[0],verbose=0)
    # Test data
    z75_test = ann752.predict(sp_data[1],verbose=0)
# Results
    r75,mse75 = result(z75_train,sp_data[2])
    r755,mse755 = result(z75_test,sp_data[3])
```

```
tr_r75.append(r75)
  tr_mse75.append(mse75)
  te_r75.append(r755)
  te_mse75.append(mse755)
  #Plotting
  plotting(sp_data,z75_train,z75_test,r75,r755,iter75)
plotting2(tr_r75,tr_mse75,te_mse75,ex_train_size,'Training Data size')
```

R2 Score: 0.9024

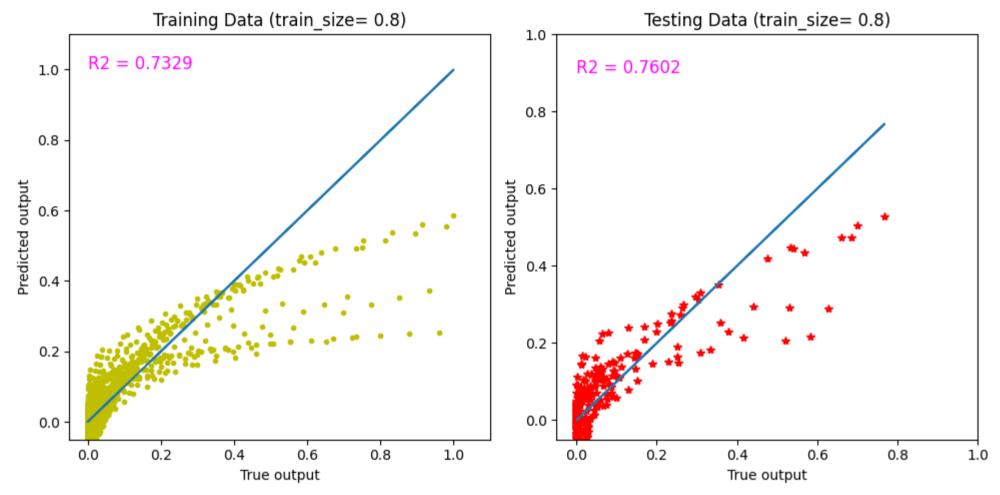
Mean Squared Error: 0.0012



R2 Score: 0.7329

Mean Squared Error: 0.0034

R2 Score: 0.7602



Mean Squared Error: 0.0014

R2 Score: 0.9214

Mean Squared Error: 0.0009

