



INFORMATICS INSTITUTE OF TECHNOLOGY

In collaboration with

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5DATA001C.2 Machine Learning and Data Mining

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Abbreviations

Short Form	Long Form	
PCA	Partition Clustering Analysis	
NN	Neural Network	
MLP	Multi-Layer Perceptron	
KM	K-Means (Clustering)	
WSS	Within-Cluster Sum of Squares	
BSS	Between-Cluster Sum of Squares	
СН	Calinski-Harabasz Index	
AR	Autoregressive Model	
MA	Moving Average	
RMSE	Root Mean Squared Error	
MAE	Mean Absolute Error	
MAPE	Mean Absolute Percentage Error	
sMAPE	Symmetric Mean Absolute Percentage Error	
IO	Input / Output	

Partition Clustering

1st Subtask – Before PCA

Z-Score normalization

For preprocessing the given dataset, it was normalized using the **scale()** function in R for the z-score normalization. The reason for this is to ensure that all the features contribute equally to the clustering process – which hence improves the performance of the algorithm. The reason for Z-score is that it could **help in identifying the outliers** and possibly remove them to give an even better output.

dfNormZ <- as.data.frame(scale(Whitewine v6)) # scaling the data

Removal of Outliers

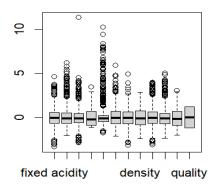
Not all the datasets are perfect – there might be few data that goes too away from the other data. To ensure consistency of the dataset and improve accuracy – removal of outliers was performed.

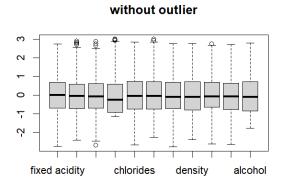
Outlier detection was done using dfNormZ – the z-score normalized data. After inspection, it was decided to use the Tukey's method which is a common method when it comes to removing outliers! It determines the outliers based on the interquartile range (IQR). Interquartile range basically tells you of how disperse the dataset is in the middle half of the distribution. We consider the first and the third quartile range – gets the lowest 25% of the data and the second range is anything above the 75% range.

To do this in R -> using the quatile() method - to get the first and third quartile. We use that to calculate the lower and upper bounds. For lower -> qnt[1] - 1.5 * iqr and the upper bounds -> qnt[2] + 1.5 * iqr. Now whatever data points lies before the lower bound and after the upper bound are considered as outliers and are removed from the dataset.

The following box-plot graphs are to show the comparison of what it was with outliers and how it is now after removing the outliers – almost cleaned dataset.

With Outliers





Now with this cleaned dataset - improves the performance and accuracy of the final output – clustering! Although it is not 100% cleaned as you could inspect a few outliers still available – but just with a few would not have a significant impact so it is all good!

```
# Using Tukey's method to identify outliers

# Function to detect outliers using Tukey's method
detect_outliers_tukey <- function(x) {
    qnt <- quantile(x, probs=c(0.25, 0.75), na.rm = TRUE)
    iqr <- IQR(x, na.rm = TRUE)
    fence_low <- qnt[1] - 1.5 * iqr
    fence_high <- qnt[2] + 1.5 * iqr
    outliers <- which(x < fence_low | x > fence_high)
    return(outliers)
}

# Applying Tukey's method to detect outliers for each variable
outliers_tukey <- apply(dfNormZ, 2, detect_outliers_tukey)

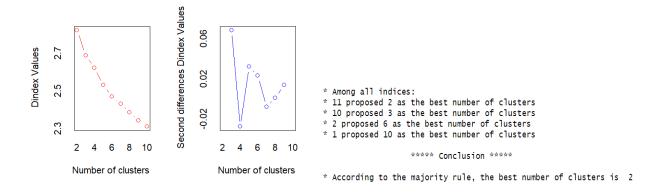
# Combining outliers detected by Tukey's method for all variables
all_outliers <- unique(unlist(outliers_tukey))

# Removing outliers from the dataset
dfNormZ no outliers <- dfNormZ[-all outliers, ]
```

Determining K value for clusters

1. NB Clust analysis

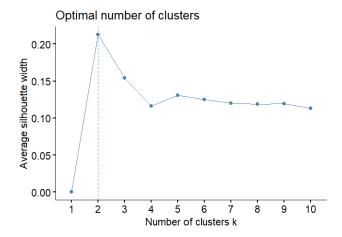
```
# nb clust
set.seed(10)
nb <- NbClust(dfNormZ_no_outliers, distance = "euclidean", min.nc = 2, max.nc = 10, method
= "kmeans", index="all")
```



Over here in the NB Clust – according to the majority tule -> 2 clusters has been selected. 11 are proposed as 2 best number of clusters where with only 1 less proposed which is 3 best number of clusters coming in as second-best number of clusters!

2. Silhouette

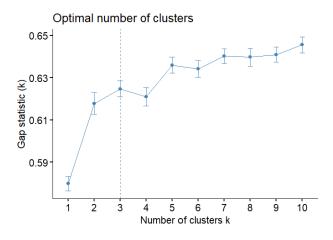
In the silhouette method – it basically determines the clusters by using the silhouette scores. The scores are basically a measure of how similar that specific data is to its own cluster than with the other clusters present.



The above diagram gives us a visual representation of how many clusters could be formed with the scaled dataset. It shows a maximum of 2 clusters while 3 clusters come in second with regards of the optimal number of clusters!

3. Gap Stats

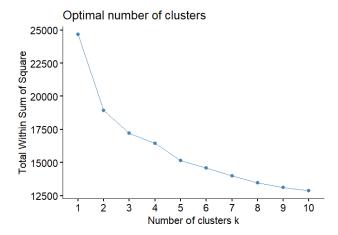
The Gap stats method basically compares the sum of intra-cluster variations of various k values with their expected values under null reference of the data. [citation]



In the gap stats method, we again see clearly a see sudden decrease at point 3 of the number of clusters. This sudden bend in the plot above means that the clustering process becomes less useful/informative after that specific point. Due to this we could come to conclusion that in the gap stats method – the best number of clusters is 3.

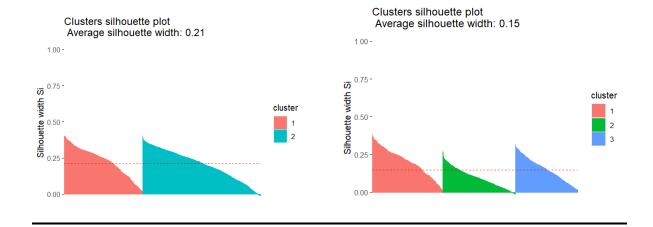
4. Elbow Method

In the elbow method – it basically way to graphically represent the approx. optimal number of clusters in a dataset. It displays the within-cluster-sum-of-square values on the y axis corresponding to various values for k (number of cluster) on the x axis as shown in the below attached plot. The optimal value of clusters (k) is determined by an elbow representation in the plot.



In the above elbow graph – we could clearly see that until the 3rd cluster the lines become steeper meaning that adding more clusters improves the quality of the clustering! But after the 3rd cluster – from the 4th cluster it gets less steep! So, based on the elbow method, we could say in the above elbow diagram – that the optimal number of clusters is 3.

Since it's a tie between the above 4 automated tools -> below explanation has been considered to finalize the cluster k value.



The silhouette plot average with of cluster 2 (width-0.21) is greater than the average plot of cluster 3 (width-0.15) -> so due to this reason – as it was a tie in the auto-mated tools – considering that the greater the width, the better the algorithm has performed clustering -> cluster with the k value 2 wins and is decided to be taken forward with.

K-Means Clustering before PCA

Since now we could come to conclusion that the k value could be taken as 2 – we could move on to implementing the k means clustering. The k means clustering is done using the inbuilt function kmeans() with the necessary variables passed in. Move on to getting the clusters of it and finally plotting the graph.

```
### K MEANS CLUSTERING ###

# ASSINGING K VALUE

k_value = 2

# PASSING AND GETTING THE K MEANS

km <- kmeans(dfNormZ_no_outliers, centers= k_value, nstart= 20)

km
```

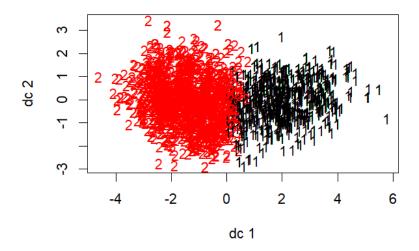
CALCULATING CENTROIDS

centroids <- *km*\$*centers*

PLOTTING

library(fpc)

plotcluster(dfNormZ no outliers, km\$cluster)



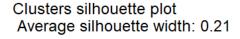
Silhouette Plot for the Width Between Clusters Before PCA

WSS -> the within sum of squares -> gets the total error of the cluster (error meaning the distance between each data point to the cluster centroid) and sum up the squared distance/error within the datapoints of the cluster.

BSS -> the **between cluster sum of squares** -> gets again the squared but this time of the distance between the cluster centroids and the overall centroid of the entire dataset!

Silhouette plot is used to measure the quality of the clustering process during k means. It helps to determine how well a data point fits into its own cluster rather than the other existing clusters within the dataset.

With these values calculated during the clustering k means process -> using *silhouette()* function to get the width for each observation according to the available clusters and the distance between the clusters. Below is the diagram of the silhouette plot using the *fviz_silhouette()* function.



1.00 -

cluster 0.50 - 1 2

Silhouette width is a measure of how similar the datapoints in the dataset to its own cluster compared to other clusters within the dataset. With the above attached image – we could notice that it has a standard average width of 0.21. A width with a higher positive value is a better value whereas a negative width value could indicate an error occurred.

2nd Subtask - PCA

PCA – also known as Principal Component Analysis – is basically a dimensionality reduction of the features to give a similar output by reducing the number of features but also retaining most of the data. This basically helps to use a smaller version of a bigger dataset and gives similar results by maintaining significant patterns. This way it will help in the computational power needed – time taken to do the clustering process but also get similar results with a much time consuming and higher requirement of computational power. [Jaadi, 2024]

In the coursework – to accomplish this – we got to firstly create the covalence matrix along by calculating the eigenvectors and eigenvalues. With this data – we then calculate the cumulative score per principal component and whatever pcs that got at least score greater than 85%. Below is the code for the above-mentioned steps.

```
# calc eigenvalues & eigenvectors

pca <- dfNormZ_no_outliers

wine.cov <- cov(pca)

wine.eigen <- eigen(wine.cov)

str(wine.cov)

phi <- wine.eigen$vectors

phi

# calc scores for all pc -> principal components

PC <- as.matrix(dfNormZ_no_outliers) %*% phi

PC

# calc scores per PC

eigenVal <- wine.eigen$values

cumulative_scores <- cumsum(eigenVal) / sum(eigenVal)

cumulative scores
```

```
select_cumula_scores <- sum(cumulative_scores <= 0.85) +1
select_cumula_scores
```

With the above code – the selected cumulative score is 7. Meaning that out of all the features in the dataset which is 11, depending on the requirement of the scores must be at least 85% - we came down to 7 features.

Determining K value for clusters

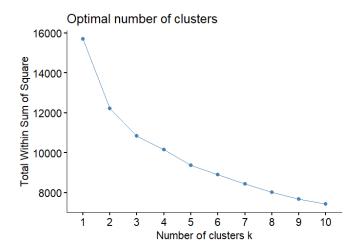
Four "automated" tools to this new pca-based dataset.

1. NB Clust.

```
\# nb clust set.seed(10) nb <- NbClust(transformed, distance = "euclidean", min.nc = 2, max.nc = 10, method = "kmeans", index="all")
```

Over here again in the NB Clust – according to the majority rule -> 2 clusters has been selected. 11 are proposed as 2 best number of clusters where with for 5 proposed as 3 best number of clusters coming in as second-best number of clusters!

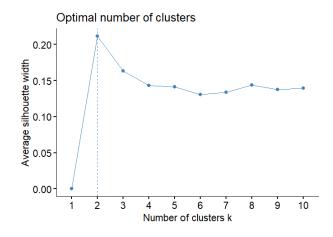
2. Elbow method.



```
\# elbow k = 2:10 set.seed(42) WSS = sapply(k, function(k) \{kmeans(transformed, centers=k)\$tot.withinss\}) plot(k, WSS, type="b", xlab="Number of k", ylab="Within sum of squares")
```

In the above elbow graph – we could clearly see that until the 3rd cluster the lines become steeper meaning that adding more clusters improves the quality of the clustering! But after the 3rd cluster – from the 4th cluster it gets less steep! So, based on the elbow method, we could say in the above elbow diagram – that the optimal number of clusters is 3.

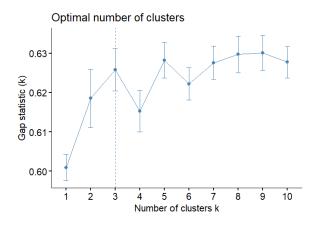
3. Silhouette method.



```
#silhouette
set.seed(12)
silh_nb <- fviz_nbclust(transformed, kmeans, method = "silhouette")
print(silh_nb)
```

In the above plot, we clearly see that there is a sudden bend at point 2 of the number of clusters! This shows that the clusters become less meaningful beyond 2 clusters – so due to this, we could consider 2 as the best number of clusters with the silhouette method.

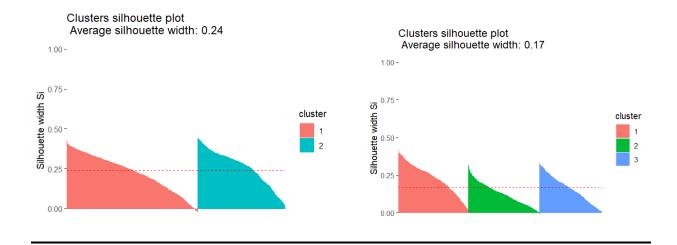
4. Gap Stats method



```
# gap_stat
set.seed(14)
gap_nb <- fviz_nbclust(transformed, kmeans, method = "gap_stat")
print(gap_nb)
I
```

In the gap stats method, we again see clearly a see sudden decrease at point 3 of the number of clusters. This sudden bend in the plot above means that the clustering process becomes less useful/informative after that specific point. Due to this we could come to conclusion that in the gap stats method – the best number of clusters is 3.

Again, like before pca -> even after pca it's a tie between the above 4 automated tools -> below explanation has been considered to finalize the cluster k value.



The silhouette plot average with of cluster 2 (width-0.24) is greater than the average plot of cluster 3(wdith-0.17) -> so due to this reason – as it was a tie in the auto-mated tools – considering that the greater the width, the better the algorithm has performed clustering -> cluster with the k value 2 wins and is decided to be taken forward with.

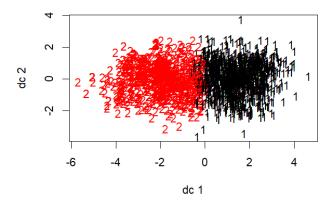
K-Means Clustering using PCA Processed Data

Since now we could come to conclusion that the k value could be taken as 2 – we could move on to implementing the k means clustering. The k means clustering is done using the inbuilt function kmeans() with the necessary variables passed in. Move on to getting the clusters of it and finally plotting the graph.

```
# k means cluster
k_value = 2

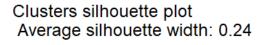
pca_km <- kmeans(transformed, centers= k_value, nstart= 20)
pca_km

# calc centroids
pca_km$centers
fviz cluster(pca_km,data=transformed)</pre>
```

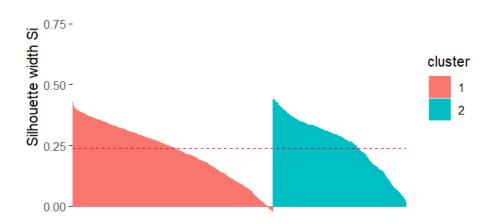


Silhouette Plot for the Width Between Clusters

Below is the diagram of the silhouette plot using the *fviz silhouette()* function.



1.00 -



With the above attached image – we could notice that it has a standard average width of 0.24. The average silhouette width has increased after performing pca -> meaning that it has now clustered even better before performing pca which is a good sign. The higher the average width -> a better gap between clusters (BSS) -> meaning clustering performance has increased.

Calinski Harabasz Index Calculation

Calinski-Harabasz (CH) Index is a metrics utilized to evaluate the performance of clustering models. Meanwhile, the CH Index (also known as Variance ratio criterion) is a ratio of how of basically BSS and WSS. The ratio of how well the clusters points is separate between clusters and within clusters. Therefore, this index could be used when the data has partitioned in a clustering algorithm that has no external validation like in silhouette plots. [Unknown Wrtier, 2024]

```
> # CALINSKI HARABASZ INDEX CALCULATION
> library(fpc)
>
> calin_Harab_index <- cluster.stats(transformed, pca_km$cluster)$ch
> print(calin_Harab_index)
[1] 639.0902
```

The above screenshot – result shows that the CH index for the clustering after performing PCA is 639.0902 -> meaning that the ratio of BSS to WSS is high. This is a good sign so now it clearly shows that the clustering process has been performed exceptionally do the better separation value – width between clusters. Overall, a good high CH value is expected for a well clustered dataset!

Financial Forecasting Part

Input variables used in MLP models for exchanges rates forecasting.

- a) Exchange rate forecasting is crucial especially for businesses so that they can tract and make decisions in the global market. For predicting the future exchange rates MLP models could play a powerful tool for doing it as they could be used to identify and learn complex patterns in historical data. In MLP models, input vectors play a huge role in the accuracy in predicting the rates and for exchange rate forecasting a few could be considered as crucial factors.
 - **AR Approach** Autoregressive (AR) approach is when it considers time-delayed values of the exchange rate as the input variables. Basically, in AR it understands the pattern of the past exchange rates learning from the data over time.
 - Exogenous variables along with the lagged values as mentioned above (past exchange rates) it is also important to consider the variable that could affect the exchange rates. Variables like inflation rates, interest rates and more could potentially have an impact on the flow of the exchange rates pattern over time.
 - MA Approach Moving Average (MA) approach is like AR but not the same. In MA approach, it does not consider the past values but the past forecast errors to predict the current value. By considering the previous inaccuracies in terms of predictions the model adjusts and improves the prediction accuracy with the past forecast errors.
 - Regularization Techniques when training models it is vital to check whether it
 does not overfit and even underfit but train properly for a accurate output for similar
 but unseen data! Regularization could help prevent the overfitting which will
 eventually improve the model's capabilities to generalize against similar but unseen
 data that it is very important in forecasting models as accuracy is key especially
 when dealing with currency ratings!

IO Matrix

To build the IO (input / output) matrices -> we **firstly build the input vectors**. In the coursework, it is mentioned to use the last column of the data set as the input variables and up to t-4 is recommended. So, using the lag() function -> the **lagged values of the first 4 of the 3rd column** is taken as input vectors!

```
lagged_output_1 <- lag(output_col_og_dataset, 1)
lagged_output_2 <- lag(output_col_og_dataset, 2)
lagged_output_3 <- lag(output_col_og_dataset, 3)
lagged_output_4 <- lag(output_col_og_dataset, 4)
```

Using the lagged values – we **bind all** the values together along **with the actual data** of the 3rd column of dataset to **one IO matrices**. By mixing up the lagged values -> four different IO matrices are built to be used in the latter process of the code!

```
IO_matrix_1 <- cbind(lagged_output_1, lagged_output_2, lagged_output_3, lagged_output_4,
output_col_og_dataset)</pre>
```

```
IO_matrix_2 <- cbind(lagged_output_2, lagged_output_1, lagged_output_3, lagged_output_4,
output col og dataset)</pre>
```

```
IO_matrix_3 <- cbind(lagged_output_4, lagged_output_3, lagged_output_2, lagged_output_1,
output_col_og_dataset)</pre>
```

IO_matrix_4 <- cbind(lagged_output_3, lagged_output_4, lagged_output_2, lagged_output_1,
output col og dataset)</pre>

Why normalize data before using in MLP

As in MLP – it is all about learning patterns and understanding how a set of inputs could correspond to an output. Normalizing the data at the start before passing it to the MLP model for training will generally help in speeding up the learning process which will lead to a fast and a more efficient process. It will also eventually improve the performance of the network as it will lead to an increase in the accuracy of the output. Not only accuracy, but it will help in stabilizing the training process. How stabilize? Basically, before normalization – the data points in the dataset could vary in scale – making the model harder to understand patterns. But after normalizing – it is then basically brought up to a certain low scale which now the model can easily learn the patterns in a faster and efficient way.

Following the creation of IO matrix -> firstly before normalizing with min max function -> all the NA rows are removed as it would become an issue when doing min max on a matrices that contains NA values.

```
IO_matrix_1 <- IO_matrix_1[complete.cases(IO_matrix_1),]
IO_matrix_2 <- IO_matrix_2[complete.cases(IO_matrix_2),]
IO_matrix_3 <- IO_matrix_3[complete.cases(IO_matrix_3),]
IO_matrix_4 <- IO_matrix_4[complete.cases(IO_matrix_4),]
```

After successfully removing all the NA value rows as required -> normalize (min max) has been applied to all the four matrices.

```
IO_matrix_1_normz <- normalize(IO_matrix_1)
IO_matrix_2_normz <- normalize(IO_matrix_2)
IO_matrix_3_normz <- normalize(IO_matrix_3)
IO_matrix_4_normz <- normalize(IO_matrix_4)
```

Now with the processed IO matrix -> 14 different models have been created by changing the hidden state nodes/ layers, activation function used and the linear or nonlinear output!

Understanding of the four stat. indices

1. RMSE

RMSE, short form for – Root Mean Square Error – is a widely utilized metrics for forecasting models like the one above. It is calculated by getting the square root of the average of squared error – difference – between the prediction and the actual value. So, the lower the error rate value – the better the model predicts the output!

2. MAE

MAE is another performance metric used to measure the accuracy of a model. It measures the average size/magnitude of the errors got in a sample of predictions and its observations. It is one of the most common loss functions for regression problems. [Unknown Writer, 2024] So, the lower the error rate value – the better the model predicts the output!

3. **MAPE**

MAPE is one of the many performance metrics utilized to get to know/measure how good a model is in making predictions. Basically, a measure of the model's accuracy. How it does it – it measures the average percentage of difference/errors made by the model tested with. In simple words, how inaccurate the predictions are on average. So, MAPE of 5% means – the average absolute percentage difference between the predicted values tested to its actual values is 5%. [Roberts, 2023] So, the lower the error rate value – the better the model predicts the output!

4. **SMAPE** (symmetric MAPE)

With the name itself – sMAPE is like MAPE but not! It rather calculates the mean percentage error/difference symmetrically around zero. It is widely used in predicting and forecasting models

models with both positive and negative values in the dataset samples. So, the lower the error rate
 value – the better the model predicts the output!

Comparison Table of Testing Performances

```
> # PRINTING THE DATA FRAME FOR A TABLE PORMAT - EAST TO DO COMPAN
> error_stats_df
    MLP_MODEL
                    RMSE
                                 MAE
                                            MAPE
  model - 1 0.006095409 0.004521968 0.003421270 0.003423940
   model - 2 0.006110399 0.004517073 0.003417456 0.003419622
3 model - 3 0.006165682 0.004669948 0.003531184 0.003534666
4 model - 4 0.006245512 0.004677452 0.003537087 0.003539669
   model - 5 0.006191635 0.004659528 0.003522638 0.003526435
6 model - 6 0.006290856 0.004858592 0.003671178 0.003675920
   model - 7 0.006181300 0.004733746 0.003578312 0.003581876
   model - 8 0.006202858 0.004726766 0.003571719 0.003575773
   model - 9 0.006156254 0.004587161 0.003470686 0.003473613
10 model - 10 0.006217388 0.004788007 0.003618653 0.003623087
11 model - 11 0.006083447 0.004512063 0.003414040 0.003416356
12 model - 12 0.006222788 0.004717673 0.003566824 0.003570934
13 model - 13 0.006178757 0.004704432 0.003556723 0.003560144
14 model - 14 0.006389065 0.004947045 0.003737845 0.003742729
```

The above comparison table is a collection of all the error stat indices of all the models separately! Below is the table of how the models were built.

Model	Inputs	Hidden state layer	Activation function
mlp_model1	lagged1, lagged2, lagged3, lagged4	1-c(5)	no function
mlp_model2	lagged1, lagged2, lagged3, lagged4	2-c(4, 6)	no function
mlp_model3	lagged1, lagged3, lagged4, lagged2	2-c(6, 8)	no function
mlp_model4	lagged1, lagged3, lagged2, lagged4	3 - c(4, 6, 8)	logistic
mlp_model5	lagged1, lagged4, lagged3, lagged2	2-c(8, 6)	tanh
mlp_model6	lagged1, lagged4, lagged3, lagged2	2-c(6, 8)	logistic
mlp_model7	lagged2, lagged1, lagged3", lagged4	3-c(4, 8, 4)	logistic
mlp_model8	lagged2, lagged3, lagged4, lagged1	2-c(6,4)	tanh
mlp_model9	lagged2, lagged4, lagged1, lagged3	3 - c(4, 6, 8)	tanh
mlp_model10	lagged4, lagged3, lagged2, lagged1	4 - c(6, 6, 9)	tanh

mlp_model11	lagged4, lagged1, lagged3,	3 - c(6, 4, 8)	logistic
4 445	lagged2	(0)	
mlp_model12	Lagged3, lagged4, lagged2,	3 - c(8)	tanh
	lagged1		
mlp_model13	lagged3, lagged1, lagged4,	2-c(8,4,6)	no function
	lagged2		
mlp_model14	lagged3, lagged2, lagged1,	3 - c(10, 6, 8)	tanh
	lagged4	·	

Above is the table of all the MLP models created along with the inputs – hidden state layer and node count and the activation function used. Let's consider the MVP model 1 and MVP model 11 as we could take both of them as the best and second best as both them have the lower values compared to other models.

Parameter counts for the hidden state.

MVP model1 -> 1 layer with 5 nodes -> 5params.

MVP model11 -> 3 layers with 6 to 4 to 8 nodes ratio -> 24+32 -> 56 params.

```
> # GETTING THE ENNOW VALUES INDIVIDUALET MONTH
> calc_error_values_helper(predicted_values_c
                                                 > calc_error_values_helper(predicted_values_der
$RMSE
                                                 $RMSE
[1] 0.006095409
                                                 [1] 0.006083447
[1] 0.004521968
                                                 [1] 0.004512063
$MAPE
                                                 $MAPE
[1] 0.00342127
                                                 [1] 0.00341404
                                                 $SMAPE
[1] 0.00342394
                                                 [1] 0.003416356
```

Model1 got 5 number of params in hidden state while model11 got 56. Both the models have lower error values compared to others but obviously since model11 has more params than model1 – eventually making it learn better and have a lower loss rate lower than that of model1 as in average.

```
0.00436564675 - model 1
```

0.0043564765 - model 11

Meaning model11 is the better model as now it is prone to error less likely than compared to model1. The image on the left hand is for model1 and the image at the right hand is for model1.

Model11 is taken as the best model due to having the lowest average error values compared to all the other models trained!

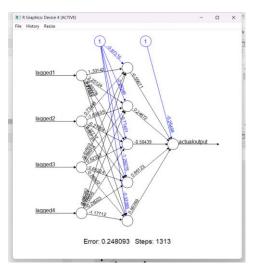
Efficiency Explanation Using One and Two Hidden Layer MLP Models

** I did not consider the activation function when calculating the parameters (cazt too much calculation) – just the parameters within the hidden state **

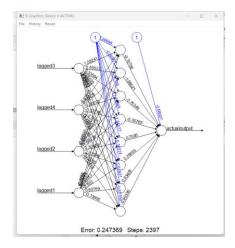
One hidden layer MLP models

Calculating Number of Params

Model1



5 nodes in node layer -> 5 params in nodes + bias as 1 -> so total 10 params $\mathbf{Model12}$



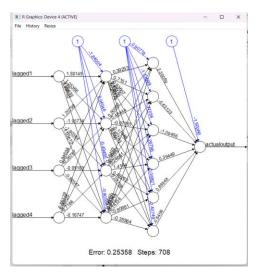
8 nodes in node layer -> 8 params in nodes + bias as 1 -> so total 16 params

For the MLP model with one hidden layer -> **model1 is more efficient** than model12 as in model1 it has less params than model12.

Two hidden layer MLP models

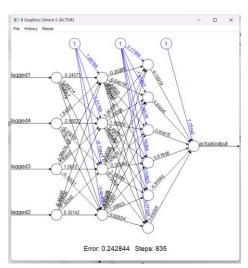
Calculating Number of Params

Model2



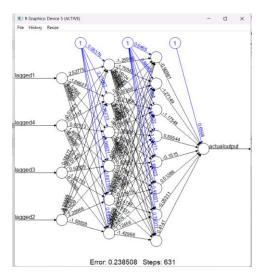
2 node layer -> 4 to 6 ratio -> so 24 params in node layer + bias as 1 -> 24 + 4 + 6 -> so total 34 params

Model5



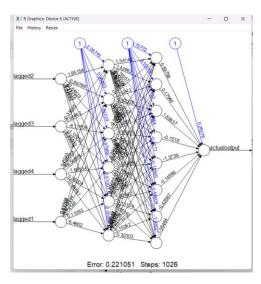
2 node layer -> 4 to 6 ratio -> so 24 params in node layer + bias as 1 -> 24 + 4 + 6 -> so total 34 params

Model6



2 node layer -> 6 to 8 ratio -> so 48 params in node layer + bias as 1 -> 48 + 6 + 8 -> so total 60 params

Model8



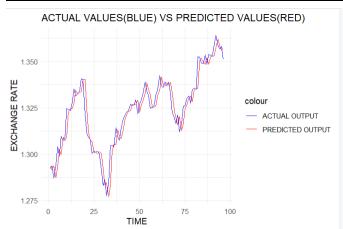
2 node layer -> 6 to 8 ratio -> so 48 params in node layer + bias as 1 -> 48 + 6 + 8 -> so total 60 params

For the MLP model with two hidden layers -> model2 and model3 is more efficient than model6 and model8 as they have lesser parameters.

Talking about efficiency of the models. The lower the parameters within the model – the better the higher the efficiency. In one hidden layer -> model1 has 10 params and model12 had 16 params – and in two hidden layer -> model2 and model5 has 34 params while model6 and model8 has 60

params -> meaning that the models will low count of params works efficiently. The lower the param count -> the simpler the model's structure. Meaning that only less time and computational power is required to run the model properly. Models will less params like model1 for one hidden layer and both model2 and model5 in two hidden layer works with higher efficiency and even performance as it will faster too. Also, models will lower parameters generalize to unseen data better!

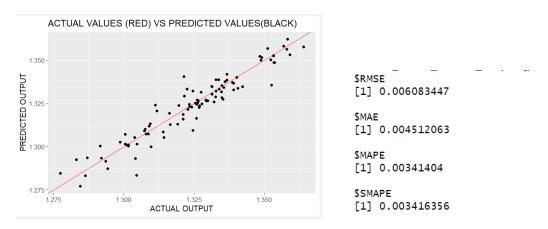
Time Series Plot for Predicted and Actual values



Model11 is taken as the best model due to having the lowest average error values compared to all the other models trained!

Above are the plots for both the predicted and actual values in one graph in a time series format. As you can see, both have similar shape and edges but not exactly as it is not a 100% accurate model. The above diagrams plot was done using **model11** as it was considered as the best model out of all the models set up during the code run. As the shape is almost the same in both the actual and predicted TS plot -> we can conclude that the model prediction is mostly accurate.

Plot for Predicted and Actual Values



Model11 is taken as the best model due to having the lowest average error values compared to all the other models trained!

The above diagram represents – prediction values vs actual values. The red line represents the actual values, and the dots represent the predicted values. The further the dot is from the red line – shows the error / how it has not predicted the values 100%. Fortunately, when inspecting, we could see that most of the dots are close to the red line – so we could conclude that the model has predicted to some extent a low loss rate as shown in the index matrices!

Appendix (Code)

```
##### K MEANS CLUSTERING #####
library(ggplot2) # FOR PLOTTING
library(factoextra)
library(NbClust) # FOR K VALUE FIINDING NB CLUST
library(cluster)
# READING DATASET
library(readxl)
Whitewine_v6 <- read_excel("C:/My Files/ml cw/Whitewine_v6.xlsx")
# CHECKING STRUCURE OF DATASET
str(Whitewine_v6)
# REMOVING IF ANY NULL VALUES PRESENT
df <- na.omit(Whitewine v6)
# CONVERTING DATASET TO DATAFRAME
dfNormZ <- as.data.frame((Whitewine_v6[1:11]))
### USING TUKEYS METHOD TO IDENTIFY OUTLIERS ###
# FUNCTION TO DETECT OUTLIERS
detect outliers tukey <- function(x) {
 qnt <- quantile(x, probs=c(0.25, 0.75), na.rm = TRUE)
 iqr < -IQR(x, na.rm = TRUE)
 fence low \leftarrow qnt[1] - 1.5 * igr
```

```
fence high \leftarrow qnt[2] + 1.5 * iqr
 outliers \leftarrow which(x < fence low | x > fence high)
return(outliers)
# APPLYING THE ABOVE FUNTCION TO EACH VARIABLE/FEATURE IN THE
DATASET
outliers tukey <- apply(dfNormZ, 2, detect outliers tukey)
# COMBINE OUTLEIRS DETECTED FOR ALL FEATURES
all outliers <- unique(unlist(outliers tukey))
# REMOVING THE DETECTED OUTLIERS FROM THE DATASET
dfNormZ no outliers <- dfNormZ[-all outliers, ]
# SCALING THE CLEANED DATASET
dfNormZ no outliers <- scale(dfNormZ no outliers)
# CONVERTING IT TO A DATA FRAME NOW
dfNormZ no outliers <- as.data.frame(dfNormZ no outliers)
# BOXPLOTING BOTH THE DATA FRAME WITH OUTLIERS AND WITHOUT
OUTLIERS
boxplot(dfNormZ, main = "With Outliers")
boxplot(dfNormZ no outliers, main = "Without Outliers")
# VISUALIZING USING GPLOT BOTH THE DATA FRAME WITH OUTLIERS AND
WITHOUT OUTLIERS
ggplot(data = dfNormZ, aes(x = dfNormZ[,9], y = dfNormZ[,9])) +
```

```
geom point() +
 labs(title = "With Outliers", x = "Variable 1", y = "Variable 2")
ggplot(data = dfNormZ_no_outliers, aes(x = dfNormZ_no_outliers[,9], y =
dfNormZ_no_outliers[,9])) +
 geom point() +
 labs(title = "Without Outliers", x = "Variable 1", y = "Variable 2")
## PERFORM NB CLUST ##
# EUCLIDEAN
set.seed(10)
nb <- NbClust(dfNormZ_no_outliers, distance = "euclidean", min.nc = 2, max.nc = 10,
        method = "kmeans", index="all")
# MANHATTAN
set.seed(8)
nb <- NbClust(dfNormZ_no_outliers, distance = "manhattan", min.nc = 2, max.nc = 10, method
         "kmeans", index="all")
# MAXIMUM
set.seed(6)
nb <- NbClust(dfNormZ no outliers, distance = "maximum", min.nc = 2, max.nc = 10, method
         "kmeans",
                    index="all")
# SILHOUTTE
set.seed(12)
```

```
silh nb <- fviz nbclust(dfNormZ no outliers, kmeans, method = "silhouette")
print(silh nb)
# GAP STATS
set.seed(14)
gap nb <- fviz nbclust(dfNormZ no outliers, kmeans, method = "gap stat")
print(gap nb)
# ELBOW
k = 2:10
set.seed(42)
WSS = sapply(k, function(k) {kmeans(dfNormZ no outliers, centers=k)$tot.withinss})
plot(k, WSS, type="b", xlab= "Number of k", ylab="Within sum of squares")
# ELBOW FOR OPTIMUM CLUSTERS
wss nb <- fviz nbclust(dfNormZ no outliers, kmeans, method = "wss")
print(wss nb)
### K MEANS CLUSTERING ###
# ASSINGING K VALUE
k \text{ value} = 2
# PASSING AND GETTING THE K MEANS
km <- kmeans(dfNormZ_no_outliers, centers= k_value, nstart= 20)
km
```

```
# CALCULATING CENTROIDS
centroids <- km$centers
# PLOTTING
# fviz_cluster(km,data=dfNormZ_no_outliers)
# PLOTTING
library(fpc)
plotcluster(dfNormZ_no_outliers, km$cluster)
# CALCULATING WSS AND BSS
wine wss = km$tot.withinss
wine_wss
wine bss = km$betweenss
wine_bss
# CALCULATING TSS -> SUM OF BOTH WSS AND BSS
wine tss= wine wss+wine bss
wine_tss
# RATIO BETWEEN WSS AND TSS
ratio wss bss <- wine wss / wine tss
ratio_wss_bss
# RATIO BETWEEN BSS AND TSS
ratio_wss_tss <- wine_bss / wine_tss
ratio_wss_tss
```

```
# SILHOUTTE PLOT
silh <- silhouette(km$cluster, dist(dfNormZ_no_outliers))</pre>
fviz silhouette(silh)
# AVERGAE WIDTH EXTRACTING AND PRINTING
avg_silh_width <- mean(silh[, "sil_width"])</pre>
print(paste("Average silhoette width score is ", avg_silh_width))
# CALCULATING EIGEN VALUES AND EIGEN VECTORS
pca <- dfNormZ no outliers
wine.cov <- cov(pca)
# VALUES
wine.eigen <- eigen(wine.cov)</pre>
str(wine.cov)
# VECTORS
vectors <- wine.eigen$vectors</pre>
phi
# CALCULATING SCORES FOR ALL PC -> PRINCIPAL COMPONENTS
PC <- as.matrix(dfNormZ no outliers) %*% phi
PC
```

```
eigenVal <- wine.eigen$values
cumulative scores <- cumsum(eigenVal) / sum(eigenVal)</pre>
cumulative scores
# CALCULATING SELECTED CUMULATIVE SCORE - ANYTHING BELOW 0.85 THE
THRESHOLD GIVEN
select cumula scores <- which(cumulative scores > 0.85)[1]
select cumula scores
# CREATE A DATASET WITH THE PCA PROCESSED DATA
transformed <- as.data.frame(PC[, 1:select_cumula_scores])
head(transformed)
head(dfNormZ no outliers)
## PERFORM NB CLUST ##
# EUCLIDEAN
set.seed(10)
nb <- NbClust(transformed, distance = "euclidean", min.nc = 2, max.nc = 10, method =
"kmeans", index="all")
# MANHATTAN
set.seed(8)
nb <- NbClust(transformed, distance = "manhattan", min.nc = 2, max.nc = 10, method =
"kmeans", index="all")
# MAXIMUM
```

CALCULATING SCORE PER PC

```
set.seed(6)
nb <- NbClust(transformed, distance = "maximum", min.nc = 2, max.nc = 10, method =
"kmeans", index="all")
# ELBOW METHOD
k = 2:10
set.seed(42)
WSS = sapply(k, function(k) {kmeans(transformed, centers=k)$tot.withinss})
plot(k, WSS, type="b", xlab= "Number of k", ylab="Within sum of squares")
# ELBOW FOR OPTIMAL CLUSTER
wss_nb <- fviz_nbclust(transformed, kmeans, method = "wss")
print(wss nb)
# SILHOUETTE
set.seed(12)
silh nb <- fviz nbclust(transformed, kmeans, method = "silhouette")
print(silh nb)
# GAP STATS
set.seed(14)
gap nb <- fviz nbclust(transformed, kmeans, method = "gap stat")
print(gap_nb)
### K MEANS CLUSTERING ###
# K VALUE
k value = 2
#KMEANS
```

```
pca_km <- kmeans(transformed, centers= k_value, nstart= 20)
pca km
# CALCULATE CENTROIDS
centroid pca <- pca km$centers
# PLOTTING
# fviz cluster(pca km,data=transformed)
plotcluster(transformed, pca_km\cluster)
# CALCULATE WSS AND BSS
wine_pca_wss = pca_km$tot.withinss
wine_pca_wss
wine pca bss = pca km\$betweenss
wine_pca_bss
# CALCULATING TSS -> SUM OF BOTH WSS AND BSS
wine_pca_tss= wine_pca_wss+wine_pca_bss
wine_pca_tss
# RATIO BETWEEN WSS AND TSS
ratio_wss_tss <- wine_pca_wss / wine_pca_tss
ratio wss tss
# RATIO BETWEEN BSS AND TSS
ratio_bss_tss <- wine_pca_bss / wine_pca_tss
```

```
ratio_bss_tss
# SILHOUTTE PLOT
silh <- silhouette(pca km$cluster, dist(transformed))
fviz silhouette(silh)
# AVERGAE WIDTH EXTRACTING AND PRINTING
avg silh width <- mean(silh[, "sil width"])</pre>
print(paste("Average silhoette width score is ", avg_silh_width))
# CONVERTING DATASET INTO A FORMAT FOR CALINSKI HARABASZ
transformed <- dist(transformed)</pre>
str(transformed)
# CALINSKI HARABASZ INDEX CALCULATION
library(fpc)
calin Harab index <- cluster.stats(transformed, pca km$cluster)$ch
print(calin Harab index)
##### NEURAL NETWORK #####
library(neuralnet) # NEURAL NETWORK
library(MLmetrics) # ERROR VALUES
library(readxl) # READ DATASET
```

library(ggplot2) # FOR PLOT

```
# SMAPE INBUILT FUNCTION DID NOT WORK SO HAD TO SET IT UP
smape <- function(actual values, predictions) {
return (mean(2 * abs(actual values - predictions) / (abs(actual values) + abs(predictions))))
}
# DEFINING NORMALIZATION AND DENORMALIZATION
normalize \leq- function(x) {return((x - min(x)) / (max(x) - min(x)))}
unnormalize <- function(x, min, max) {return( (max - min)*x + min )}
# READING DATASET
ExchangeUSD <- read excel("C:/My Files/ml cw/ExchangeUSD.xlsx")
# ADDING APRROPRIATE COL NAMES
colnames(ExchangeUSD) <- c("Input 1", "Input 2", "Output")
output col og dataset <- ExchangeUSD[3]
head(output col og dataset)
# GETTING LAGGED VALUES FOR FIRST FOUR OF THE THRID COL OF DATASET
lagged output 1 <- lag(output col og dataset, 1)
lagged output 2 <- lag(output col og dataset, 2)
lagged output 3 <- lag(output col og dataset, 3)
lagged output 4 <- lag(output col og dataset, 4)
# CREATING IO MATRICES WITH VARYING COMBINATIONS OF LAGGED VALUES
IO matrix 1 <- cbind(lagged output 1, lagged output 2, lagged output 3, lagged output 4,
output col og dataset)
IO matrix 2 <- cbind(lagged output 2, lagged output 1, lagged output 3, lagged output 4,
output col og dataset)
```

```
IO matrix 3 <- cbind(lagged output 4, lagged output 3, lagged output 2, lagged output 1,
output col og dataset)
IO matrix 4 <- cbind(lagged output 3, lagged output 4, lagged output 2, lagged output 1,
output col og dataset)
# PRITNING THE FIRST FEW TO INSPECT
head(IO matrix 1)
head(IO matrix 2)
head(IO matrix 3)
head(IO matrix 4)
# REMOVING NA VALUES OF THE IO MATRICES
IO matrix 1 <- IO matrix 1[complete.cases(IO matrix 1),]
IO matrix 2 <- IO matrix 2[complete.cases(IO matrix 2),]
IO matrix 3 <- IO matrix 3[complete.cases(IO matrix 3),]
IO matrix 4 <- IO matrix 4[complete.cases(IO matrix 4),]
# PRINTING THE FIRST FEW TO INSPECT
head(IO matrix 1)
head(IO matrix 2)
head(IO matrix 3)
head(IO matrix 4)
# NORMALIZING THE DATA USING MIN MAX
IO matrix 1 normz <- normalize(IO matrix 1)
IO matrix 2 normz <- normalize(IO matrix 2)
IO matrix 3 normz <- normalize(IO matrix 3)
IO matrix 4 normz <- normalize(IO matrix 4)
```

```
# PRINTING THE FIRST FEW TO INSPECT
head(IO matrix 1 normz)
head(IO matrix 2 normz)
head(IO matrix 3 normz)
head(IO matrix 4 normz)
str(IO matrix 4_normz)
IO matrix 4 normz
# RENAMING COL NAMES
colnames(IO matrix 1 normz) <- c("lagged1", "lagged2", "lagged3", "lagged4", "actualOutput")
colnames(IO matrix 2 normz) <- c("lagged1", "lagged2", "lagged3", "lagged4", "actualOutput")
colnames(IO matrix 3 normz) <- c("lagged1", "lagged2", "lagged3", "lagged4", "actualOutput")
colnames(IO matrix 4 normz) <- c("lagged1", "lagged2", "lagged3", "lagged4", "actualOutput")
# INSPECTING JUST ONE TO CHECK WHETHER COLUMN NAME CHANGED
head(IO matrix 1 normz)
### DATASPLIT -> TRAINING 400 - REST FOR TESTING & CCONVERT TO
DATAFRAMES TO BE USED IN NN
# TRAINING PART
training_set_1 <- as.data.frame(IO matrix 1 normz[1:400,])
training set 2 <- as.data.frame(IO matrix 2 normz[1:400,])
training set 3 <- as.data.frame(IO matrix 3 normz[1:400,])
training set 4 <- as.data.frame(IO matrix 4 normz[1:400,])
# TESTING PART
testing set 1 <- as.data.frame(IO matrix 1 normz[401:nrow(IO matrix 1 normz),])
```

```
testing set 2 <- as.data.frame(IO matrix 2 normz[401:nrow(IO matrix 2 normz),])
testing set 3 <- as.data.frame(IO matrix 3 normz[401:nrow(IO matrix 3 normz),])
testing set 4 <- as.data.frame(IO matrix 4 normz[401:nrow(IO matrix 4 normz),])
# PRINT FIRST FEW JUST TO CHECK WHETHER PROPERLY SPLITTED
nrow(training set 1)
nrow(training set 2)
nrow(training set 3)
nrow(training set 4)
nrow(testing set 1)
nrow(testing set 2)
nrow(testing set 3)
nrow(testing set 4)
##### CREATING MLP MODELS ####
# FUNCTION TO SET UP MODELS EASILY
train mlp model <- function(seed, input, train data, hidden layers, activation) {
 set.seed(seed)
 input formula <- as.formula(paste("actualOutput ~", paste(input, collapse = " + ")))
 model <- neuralnet(input formula, data = train data, hidden = hidden layers,
            act.fct = activation, linear.output = TRUE)
 return(model)
}
```

```
# FUNCTION TO SET UP MODELS EASILY WWITHOUT FUNCTION
train mlp model no func <- function(seed, input, train data, hidden layers) {
 set.seed(seed)
 input formula <- as.formula(paste("actualOutput ~", paste(input, collapse = " + ")))
 model <- neuralnet(input formula, data = train data, hidden = hidden layers, linear.output =
TRUE)
 return(model)
}
# MODEL1
mlp model1 <- train mlp model no func(12, c("lagged1", "lagged2", "lagged3", "lagged4"),
                   training set 1, c(5)
# MODEL2
mlp model2 <- train mlp model(14, c("lagged1", "lagged2", "lagged3", "lagged4"),
                   training set 1, c(4, 6), "logistic"
# MODEL3
mlp model3<- train mlp model no func(16, c("lagged1", "lagged3", "lagged4", "lagged2"),
                   training set 1, c(6, 8)
# MODEL4
mlp model4<- train mlp model(18, c("lagged1", "lagged3", "lagged2", "lagged4"),
                   training set 1, c(4, 6, 8), "logistic"
# MODEL5
mlp model5<- train mlp model(20, c("lagged1", "lagged4", "lagged3", "lagged2"),
              training set 1, c(8, 6), "tanh"
```

```
# MODEL6
mlp model6<- train mlp model(22, c("lagged1", "lagged4", "lagged3", "lagged2"),
              training set 1, c(6, 8), "logistic"
# MODEL7
mlp model7<- train mlp model(24, c("lagged2", "lagged1", "lagged3", "lagged4"),
              training set 2, c(4, 8, 4), "logistic")
# MODEL8
mlp model8<- train mlp model(26, c("lagged2", "lagged3", "lagged4", "lagged1"),
                 training set 2, c(6, 4), "tanh")
# MODEL9
mlp model9<- train mlp model(28, c("lagged2", "lagged4", "lagged1", "lagged3"),
                 training set 2, c(4, 6, 8), "tanh")
# MODEL10
mlp model10<- train mlp model(30, c("lagged4", "lagged3", "lagged2", "lagged1"),
                 training set 3, c(6, 6, 9), "tanh")
# MODEL11
mlp model11<- train mlp model(32, c("lagged4", "lagged1", "lagged3", "lagged2"),
                 training set 3, c(6, 4, 8), "logistic")
# MODEL12
mlp model12<- train mlp model(34, c("lagged3", "lagged4", "lagged2", "lagged1"),
                 training set 4, c(8), "tanh")
```

```
# MODEL13
mlp_model13<- train_mlp_model_no_func(36, c("lagged3", "lagged1", "lagged4", "lagged2"),
                training set 4, c(8, 4, 6)
# MODEL14
mlp model14<- train mlp model(38, c("lagged3", "lagged2", "lagged1", "lagged4"),
                     training set 4, c(10, 6, 8), "tanh")
# PLOTTING FOR INPECTION
plot(mlp model1)
plot(mlp_model2)
plot(mlp model3)
plot(mlp model4)
plot(mlp_model5)
plot(mlp model6)
plot(mlp model7)
plot(mlp model8)
plot(mlp_model9)
plot(mlp_model10)
plot(mlp_model11)
plot(mlp model12)
plot(mlp_model13)
plot(mlp model14)
```

MAKING PREDICTIONS

```
## DENORMALIZING THE PREDICTED VALUES AND ACTUAL VALUES ##
training original data <- output col og dataset[1:400,]
nrow(training original data)
# GETTING THE MIN AND MAX VALUE OF THE OUTPUT COL TO BE PASSED TO THE
DENORMALIZING FUNCTION
min output <- min(training original data$Output)
max output <- max(training original data$Output)
paste("min output: " ,min output)
paste("maz output: " ,max_output)
# CREATED THIS AS THE SAME CODE WILL BE USED TWICE IN THE LATTER PART
OF THE CODE
calc error values helper <- function(predicted, actual) {
 ### CALCULATING ERROR VALUES ####
# CALC RMSE
 rmse <- RMSE(predicted, actual)
 # CALC MAE
 mae <- MAE(predicted, actual)
 # CALC MAPE
 mape <- MAPE(predicted, actual)
 # CALC SMAPE
 smape <- smape(predicted, actual)</pre>
 # RETURN LIST OF ALL THE ERROR STATS
```

```
return(list(RMSE = rmse, MAE = mae, MAPE = mape, SMAPE = smape))
}
calc error stats <- function(model, testing set) {</pre>
 # GENERATING THE PREDICTIONS USING THE MODEL AND THE TEST DATASET
 predictions <- predict(model, testing set)</pre>
# EXTRACTING PREDICTED VALUES
 predicted values <- as.vector(predictions)</pre>
 actual values <- testing set$actualOutput
 # DDENORMALIZING THE PREDICTED VALUES
 predicted values denorm <- unnormalize(predicted values, min output, max output)
 # DENORMALIZING THE ACTUAL VALUES
 actual values denorm <- unnormalize(actual values, min output, max output)
 return (calc error values helper(predicted values denorm, actual values denorm))
}
error stats <- list()
is.na(testing set 1)
# PASSING IN THE MODEL AND ITS RELEVANT TESTING SET
```

```
error stats[[2]] <- calc error stats(mlp model2, testing set 1)
error stats[[3]] <- calc error stats(mlp model3, testing set 1)
error stats[[4]] <- calc error stats(mlp model4, testing set 1)
error stats[[5]] <- calc error stats(mlp model5, testing set 1)
error stats[[6]] <- calc error stats(mlp model6, testing set 1)
error stats[[7]] <- calc error stats(mlp model7, testing set 2)
error_stats[[8]] <- calc_error_stats(mlp_model8, testing_set_2)
error stats[[9]] <- calc error stats(mlp model9, testing set 2)
error stats[[10]] <- calc error stats(mlp model10, testing set 3)
error stats[[11]] <- calc error stats(mlp model11, testing set 3)
error stats[[12]] <- calc error stats(mlp model12, testing set 4)
error stats[[13]] <- calc error stats(mlp model13, testing set 4)
error stats[[14]] <- calc error stats(mlp model14, testing set 4)
# DISPLAYIN IT AS A DATA FRAME FOR BETTER COMPARISON
error stats df <- data.frame(MLP MODEL=paste("model -", 1:14),
                   RMSE = sapply(error stats, function(x) x\$RMSE),
                   MAE = sapply(error stats, function(x) x$MAE),
                   MAPE = sapply(error stats, function(x) x$MAPE),
                   SMAPE = sapply(error stats, function(x) x\$SMAPE))
```

error stats[[1]] <- calc error stats(mlp model1, testing set 1)

PRINTING THE DATA FRAME FOR A TABLE FORMAT - EASY TO DO COMPARISON error_stats_df

GENERATING THE PREDICTIONS USING THE MODEL AND THE TEST DATASET predictions <- predict(mlp_model11, testing_set_3)

```
# EXTRACTING PREDICTED VALUES
predicted values <- as.vector(predictions)</pre>
actual values <- testing set 2$actualOutput
nrow(testing set 2)
# DDENORMALIZING THE PREDICTED VALUES
predicted values denorm <- unnormalize(predicted values, min output, max output)
# DENORMALIZING THE ACTUAL VALUES
actual values denorm <- unnormalize(actual values, min output, max output)
# PRIINTING TO COMPARE
predicted values denorm
actual values denorm
nrow(as.data.frame(predicted values denorm))
nrow(as.data.frame(actual values denorm))
# PLOT USING G PLOT FOR PREDICTION OUTPUT VS DESIRED OUTPUT
plot data <- data.frame(Actual = actual values denorm, Predicted = predicted values denorm)
ggplot(plot data, aes(x = Actual, y = Predicted)) +
 geom point() +
 geom abline(intercept = 0, slope = 1, color = "red") +
 labs(x = "ACTUAL OUTPUT", y = "PREDICTED OUTPUT", title = "ACTUAL VALUES
(RED) VS PREDICTED VALUES(BLACK)")
```

```
# DATAFRAME CREATION FOR THE TIME SERIES PLOT
time series data <- data.frame(
 Index = 1:nrow(testing set 2),
Actual = actual values denorm,
 Predicted = predicted values denorm
)
# TIME SERIES OF BOTH IN ONE PLOT
ggplot(time\_series\_data, aes(x = Index)) +
 geom line(aes(y = Actual, color = "ACTUAL OUTPUT")) +
 geom line(aes(y = Predicted, color = "PREDICTED OUTPUT")) +
 labs(x = "TIME", y = "EXCHANGE RATE", title = "ACTUAL VALUES(BLUE) VS
PREDICTED VALUES(RED)") +
 scale color manual(values = c("ACTUAL OUTPUT" = "blue", "PREDICTED OUTPUT" =
"red")) +
 theme minimal()
# GETTING THE ERROR VALUES INDIVIDUALLY AGAIN AS REQUIRED
calc error values helper(predicted values denorm, actual values denorm)
```

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