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5DATA001C.2 Machine Learning & Data Mining

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Clustering Part

1. Data preprocessing tasks

This part consists of 2 tasks one is outlier removal and the other one is scaling. So here outlier removal will be done first because if we scale the data with outliers even if the output shows the values between 0 and 1(min-max normalization) still the range of these values will be affected by these outliers if some large or even small value is present in each feature. So removing the outliers before the scaling is always the best option.

1. Outlier removal

By plotting boxplots for all the features we can view the outliers present in the dataset.

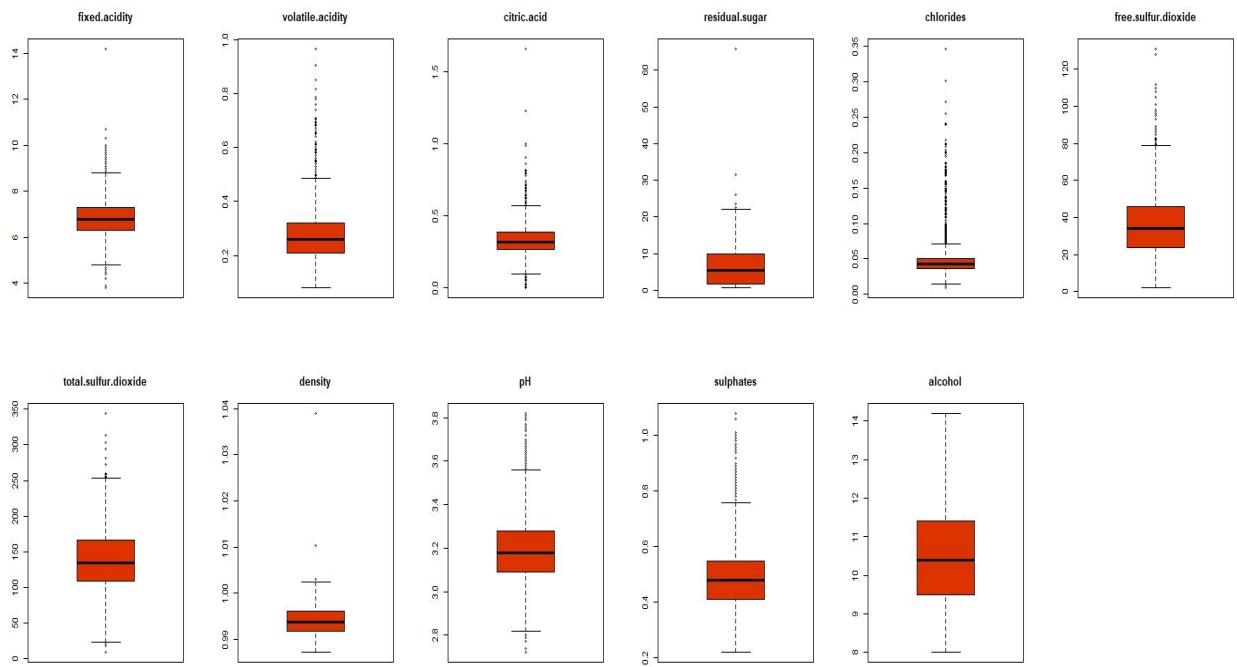


Figure 1: Viewing outliers

You can clearly see that all the features have outliers except alcohol. So they need to be removed from the dataset. In order to remove them we will use the extreme of the lower whisker ($1/4$ th quartile - $1.4 * \text{IQR}$) and the extreme of the upper whisker ($3/4$ th quartile + $1.4 * \text{IQR}$) values. Anything that is lower than the extreme of the lower whisker value and anything that is higher than the extreme

of the upper whisker values of each feature will be removed from the dataset. Initially in the dataset we had 4710 observations and after extreme outlier removal we now had 3747 observations. By plotting the boxplot again for all the features you can verify that most of the outliers have been removed.

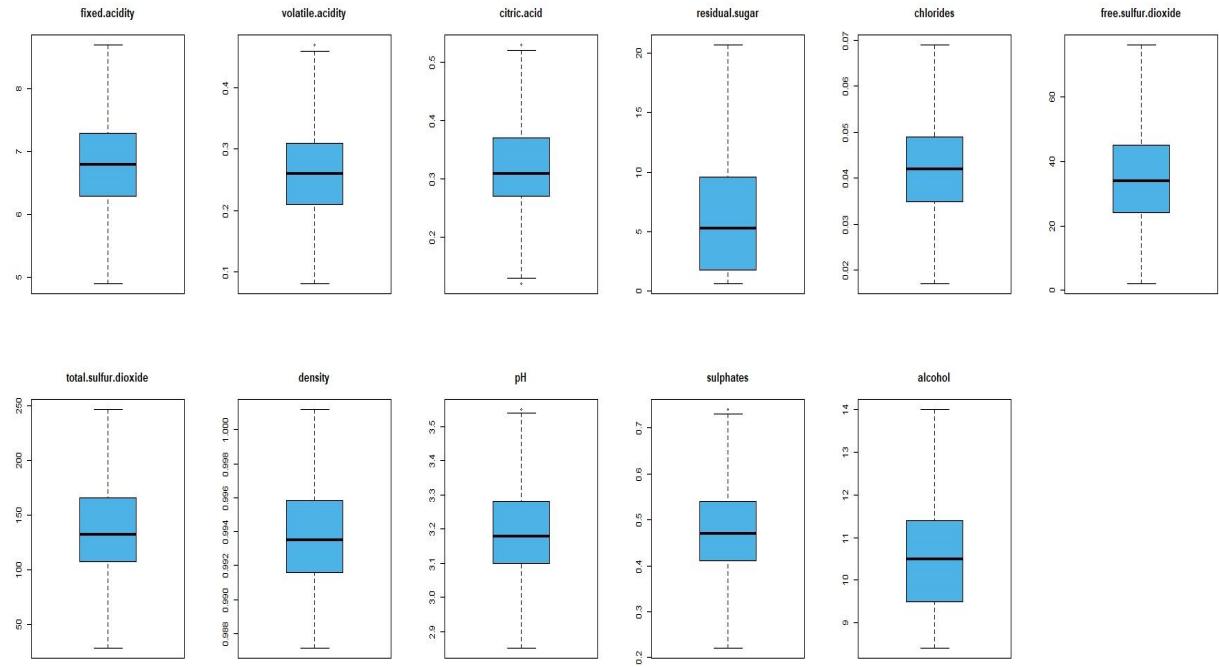


Figure 2: Viewing after removing outliers

And now you can see that most of the outliers have been removed from the dataset. And now you are good to go with data normalization with your dataset.

2. Scaling

The main goal of scaling is to make every feature in your dataset to have the same scale so each feature is equally important. To scale the data again we have 2 options. One is Normalization (min-max) and the other one is Standardization.

In order to select which scaling is best for the dataset, we will plot a histogram to see how our data is being distributed for each feature. The following picture of the histogram shows how the data in each feature is being distributed in the wine dataset.

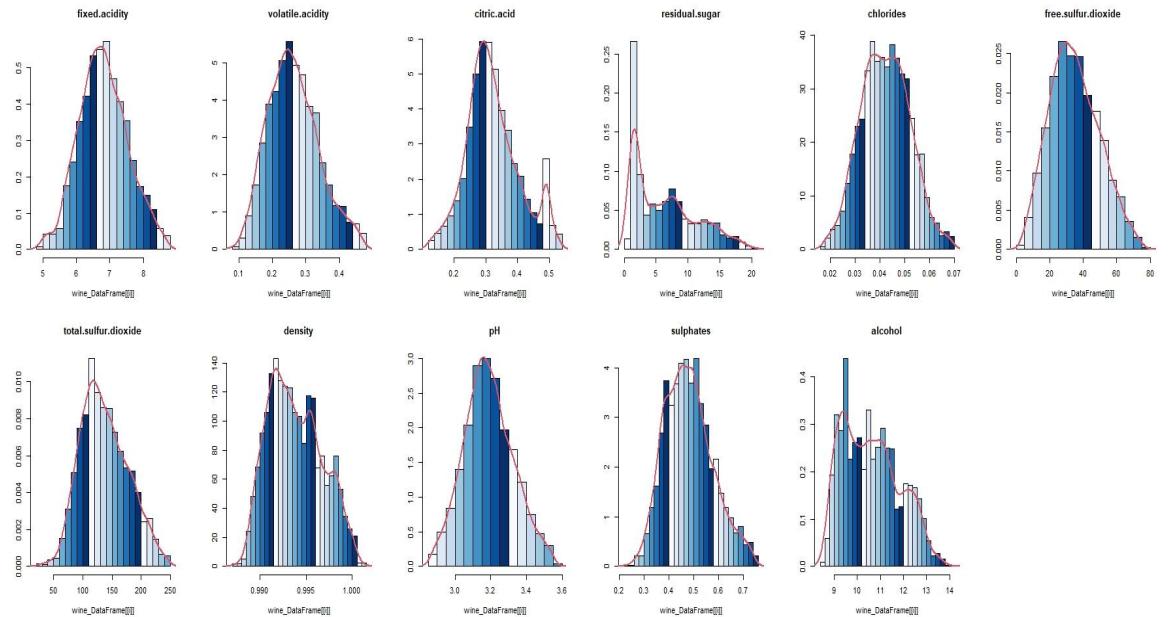


Figure 3: Histogram for distribution

As you can see here that the distribution of some features falls under Normal/Gaussian distribution and others falls under skewed distribution. Standardization is preferable if we have Gaussian distribution for all the features. But here we will be using Normalization (min-max) because some of the features fall under skewed distribution.

Min-max Normalization is basically rescaled each feature value so that feature values will be ended up in the ranging between 0 and 1.

```
> summary(wine_DataFrame_without_quality)
fixed.acidity  volatile.acidity  citric.acid  residual.sugar  chlorides  free.sulfur.dioxide
Min. :0.0000  Min. :0.0000  Min. :0.0000  Min. :0.0000  Min. :0.0000  Min. :0.0000
1st Qu.:0.3684 1st Qu.:0.3333  1st Qu.:0.3659  1st Qu.:0.0597  1st Qu.:0.3462  1st Qu.:0.2973
Median :0.5000  Median :0.4615  Median :0.4634  Median :0.2338  Median :0.4808  Median :0.4324
Mean   :0.5006  Mean   :0.4680  Mean   :0.4913  Mean   :0.2870  Mean   :0.4855  Mean   :0.4447
3rd Qu.:0.6316 3rd Qu.:0.5897  3rd Qu.:0.6098  3rd Qu.:0.4478  3rd Qu.:0.6154  3rd Qu.:0.5811
Max.   :1.0000  Max.   :1.0000  Max.   :1.0000  Max.   :1.0000  Max.   :1.0000  Max.   :1.0000
total.sulfur.dioxide  density  pH  sulphates  alcohol
Min. :0.0000  Min. :0.0000  Min. :0.0000  Min. :0.0000  Min. :0.0000
1st Qu.:0.3630  1st Qu.:0.3180  1st Qu.:0.3571  1st Qu.:0.3654  1st Qu.:0.1964
Median :0.4795  Median :0.4535  Median :0.4714  Median :0.4808  Median :0.3750
Mean   :0.4979  Mean   :0.4768  Mean   :0.4841  Mean   :0.4988  Mean   :0.3927
3rd Qu.:0.6301  3rd Qu.:0.6182  3rd Qu.:0.6143  3rd Qu.:0.6154  3rd Qu.:0.5357
Max.   :1.0000  Max.   :1.0000  Max.   :1.0000  Max.   :1.0000  Max.   :1.0000
> |
```

Figure 4: Summary of wine dataset

As you can see, the minimum and maximum value for all the features are set to 0 and 1. So now all the features will be treated equally important in your training phase.

2. Defining the number of cluster center

In order to define the number of clusters we will use some built-in methods like the Elbow method, Silhouette method, Gap statistic Method and NBclust method.

1. Elbow method

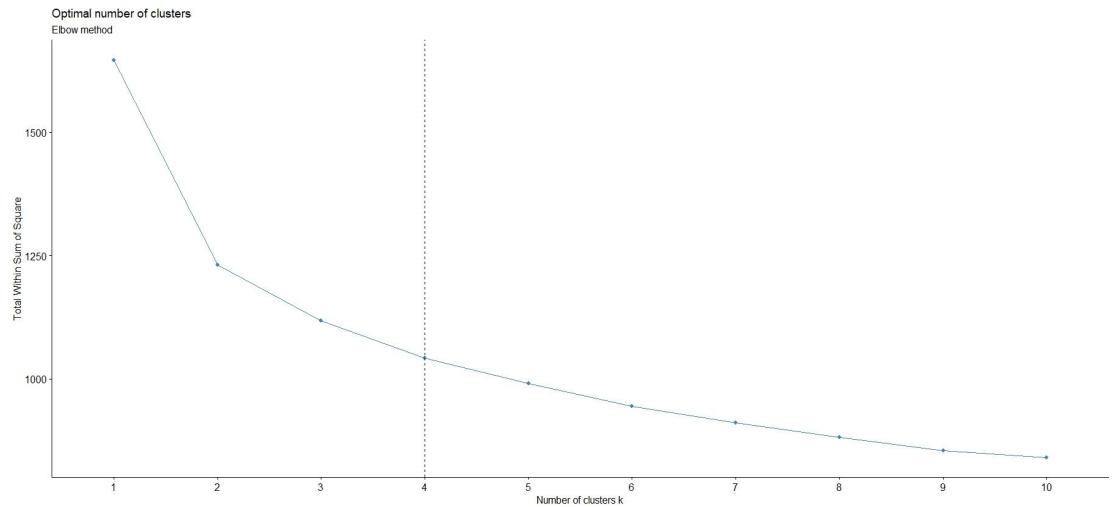


Figure 5: Elbow plot

As you can see here the elbow plot suggests that 4 as the best cluster.

2. Silhouette method

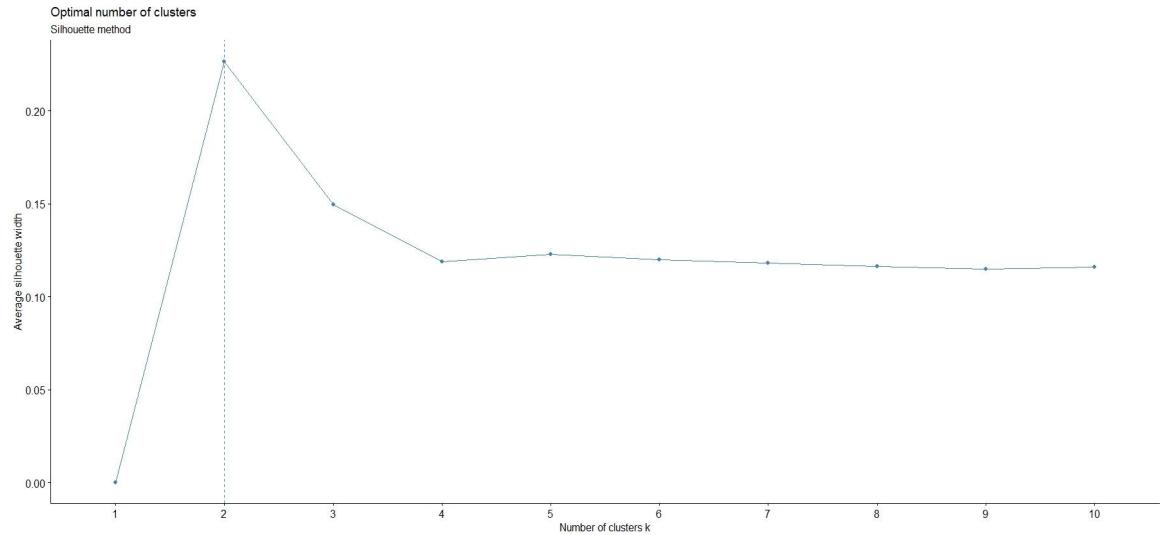


Figure 6: Silhouette plot

As you can see here the silhouette plot suggests that 2 as the best cluster.

3. Gap statistic method

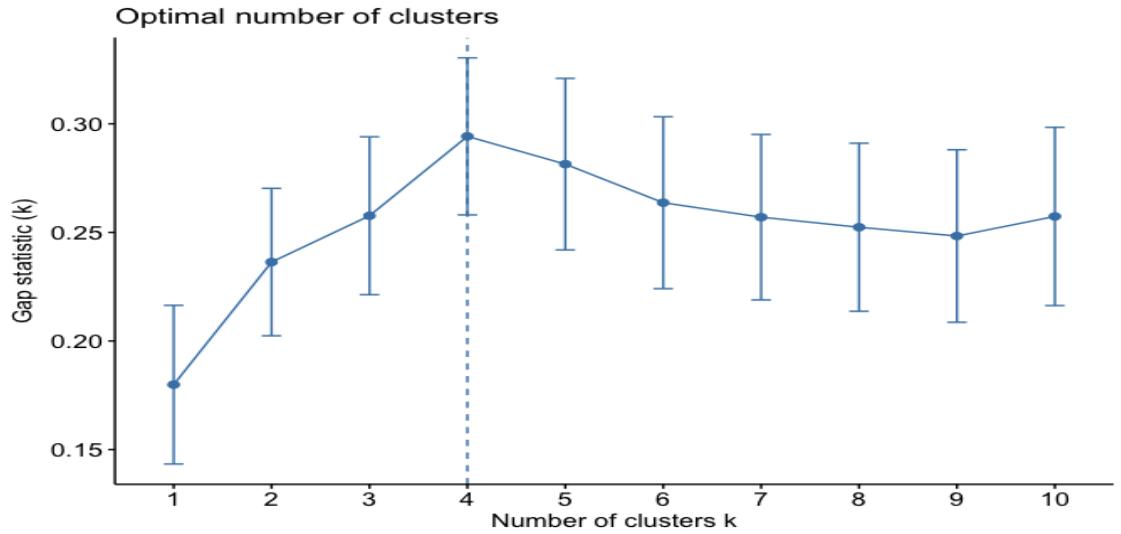


Figure 7: Gap statistic plot

As you can see here the Gap statistic method suggests that 4 as the best cluster.

4. NBclust method

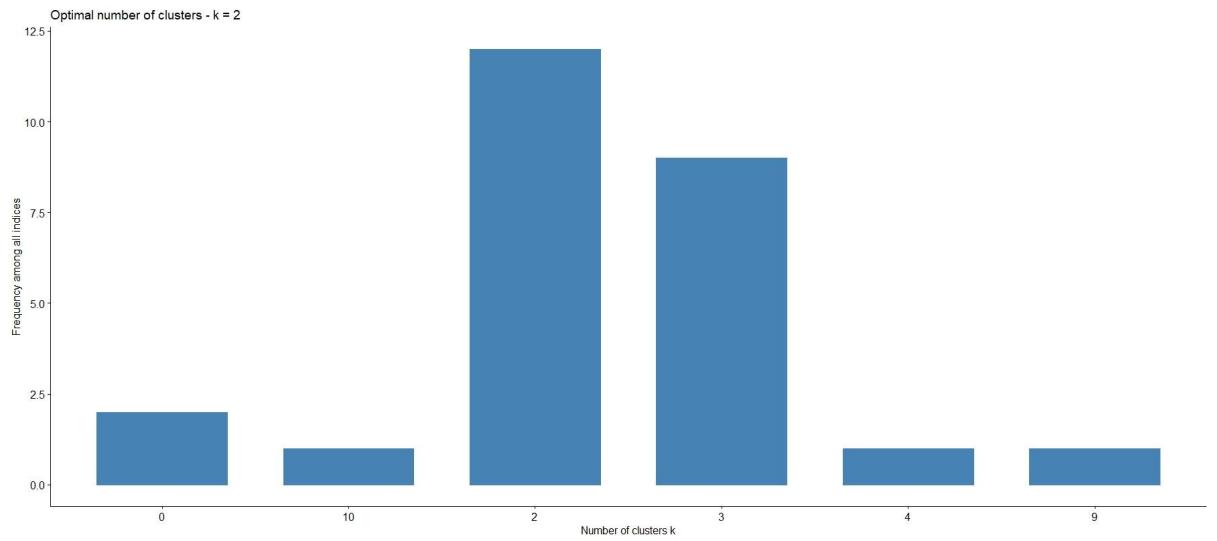


Figure 8: NBclust plot

```

> fviz_nbclust(nb)
Among all indices:
=====
* 2 proposed 0 as the best number of clusters
* 12 proposed 2 as the best number of clusters
* 9 proposed 3 as the best number of clusters
* 1 proposed 4 as the best number of clusters
* 1 proposed 9 as the best number of clusters
* 1 proposed 10 as the best number of clusters

conclusion
=====
* According to the majority rule, the best number of clusters is 2 .

```

Figure 9: NBclust results

As you can see clearly, the NBclust method suggests that 2 as the best cluster.

So here 2 of the methods (Elbow & Gap statistic) suggest 4 as the best cluster cluster and other 2 methods (Silhouette & NBclust) suggest 2 as the best cluster. Since we have four quality labels namely 5, 6, 7 & 8 as our output labels in our wine dataset it's obvious that we should have 4 clusters in our dataset. So k = 4 is the optimum number of clusters that we should have in our wine dataset.

3. K-means clustering analysis

Here we will perform k-means analysis for k = 2, k = 3 & k = 4 and then we will evaluate the produced cluster output against the 12th(quality) column for each k values by producing confusion matrices with actual quality labels and predicted cluster results. And with the confusion matrices we will calculate the accuracy, recall (sensitivity) and specificities.

- Accuracy = $(TP + TN) / (TP + FN + TN + FP)$
- Recall (sensitivity) = $TP / (TP + FN)$
- Specificity = $TN / (TN + FP)$

(TP - True Positive, TN - True Negative, FP - False Positive, FN - False Negative)

As you can see that the quality 5 is being described more by cluster 1 and the rest of the qualities (6, 7 & 8) are being described by cluster 2. So with this information we will make our Confusion Matrix including the accuracy, recall and precision for the clusters.

```
> confusion_Matrix
Confusion Matrix and Statistics

      Reference
Prediction   1     2
      1    600   850
      2   434  1863

          Accuracy : 0.6573
          95% CI  : (0.6419, 0.6725)
No Information Rate : 0.724
P-Value [Acc > NIR] : 1

          Kappa : 0.2374

McNemar's Test P-Value : <2e-16

          Sensitivity : 0.5803
          Specificity  : 0.6867
          Pos Pred Value : 0.4138
          Neg Pred Value : 0.8111
          Prevalence    : 0.2760
          Detection Rate : 0.1601
          Detection Prevalence : 0.3870
          Balanced Accuracy : 0.6335

'Positive' class : 1

> |
```

Figure 11: Confusion matrix ($k=2$)

2. K-means analysis when (k = 3)

```

> set.seed(5005)
> KM <- kmeans(wine_DataFrame_norm[,-12], centers = 3, nstart = 25)
> KM
K-means clustering with 3 clusters of sizes 1198, 1252, 1297

Cluster means:
  fixed.acidity volatile.acidity citric.acid residual.sugar chlorides free.sulfur.dioxide
1     0.4876329      0.5232332     0.4976994     0.1692975   0.3203898        0.3642163
2     0.5270094      0.4916134     0.5093899     0.5566656   0.5956470        0.5757815
3     0.4869436      0.3940751     0.4677962     0.1354427   0.5317152        0.3924389
  total.sulfur.dioxide density pH sulphates alcohol
1       0.3742348    0.2865380    0.4480444    0.4383749   0.6300655
2       0.6460658    0.7067857    0.4352008    0.5020890   0.2040307
3       0.4692089    0.4304020    0.5644785    0.5513166   0.3556325

Clustering vector:
 [1] 1 3 3 3 2 3 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 1 1 2 2 2 2 2 2 3 3 3 2 2 2 2 2 3 1 3 2 2 2 2 2
 [52] 2 2 2 1 2 2 1 2 2 2 1 1 2 2 2 1 3 2 1 2 2 1 2 2 2 2 2 3 1 1 2 1 3 2 2 2 2 2 3 1 1 2 1 2 2 2 3 1 1 2 1 2 2 2 2 3 1 2 2 2 3 2 2
[103] 3 3 3 2 2 2 2 2 2 2 2 2 3 3 3 1 1 3 3 1 2 2 3 2 3 3 2 3 2 2 2 2 2 3 1 2 2 2 2 2 3 1 2 2 2 2 3 3 3 2 2 2 3 3 3 2 2 3 1 2 2 2 3 2 2
[154] 2 3 3 2 2 2 2 2 1 2 3 2 2 2 2 3 3 3 3 2 2 2 2 2 2 2 3 2 2 2 2 3 1 3 3 1 2 3 1 3 3 1 2 3 2 2 2 3 3 1 2 2 2 2 3 2 2 2 3 3 3 2 2
[205] 2 2 2 1 2 3 1 3 3 3 3 1 1 3 2 3 3 2 3 2 3 2 1 3 3 1 2 3 1 1 2 1 1 3 3 2 2 3 2 3 1 3 1 2 1 1 3 2 3 3 2 2 3 3 3 2 2
[256] 2 2 3 1 1 3 2 3 3 3 3 2 2 2 2 2 3 3 1 3 3 2 2 1 1 3 2 3 3 3 3 1 1 3 3 3 3 3 3 2 2 2 2 3 3 3 3 2 2 3 3 1 1 2 2
[307] 3 3 3 3 3 3 3 2 3 3 1 2 3 3 3 2 3 3 2 2 2 3 2 2 2 2 2 3 2 2 2 2 1 3 3 3 3 2 3 3 2 2 2 2 3 3 1 3 2 3 1 2 3
[358] 2 3 1 2 3 2 3 2 3 2 2 1 2 2 2 2 3 2 2 2 2 2 2 2 1 3 3 2 2 2 2 3 1 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 2 2 3
[409] 3 3 3 2 3 2 1 3 3 1 3 1 2 2 2 2 2 2 3 2 3 3 3 3 2 2 2 3 2 3 2 3 2 2 2 3 2 2 2 3 2 2 2 2 3 2 2 2 3 2 2 2 3
[460] 3 2 2 3 2 2 2 2 2 2 2 3 3 3 3 2 3 3 3 2 2 2 3 3 2 1 1 3 3 2 2 2 2 2 2 2 3 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 3 2
[511] 3 1 2 2 2 3 2 2 3 2 2 3 2 2 3 2 3 2 2 3 2 2 3 2 2 2 3 2 3 2 2 2 3 2 3 2 2 2 3 2 3 2 2 2 3 2 3 2 2 2 2 3 2 2 2 3 2
[562] 3 2 2 2 1 1 3 3 3 2 2 2 3 2 3 3 2 2 2 2 1 2 2 2 2 3 2 3 2 2 2 3 2 3 2 2 2 2 2 3 2 3 2 2 2 2 2 2 2 1 3 3 3 3
[613] 1 1 2 2 2 2 2 2 2 2 3 1 3 2 3 2 2 2 3 1 2 3 1 1 2 1 3 1 1 2 2 2 2 1 2 2 2 2 2 3 3 2 1 2 3 3 3 2 1 2 3 3 3 1
[664] 3 1 1 3 3 2 3 3 3 2 1 3 2 1 3 3 2 1 2 3 2 3 3 1 2 3 2 3 3 2 3 2 2 3 3 2 3 2 3 2 3 2 3 1 3 3 1 1 2 1 3 3 2 3
[715] 2 1 2 2 2 2 1 3 2 3 1 3 3 2 2 2 2 1 2 2 2 2 3 3 2 3 2 2 3 2 3 2 2 2 2 3 2 2 2 2 2 1 3 2 2 2 1 1 1 1 3 1 2
[766] 2 2 1 2 2 3 3 3 3 2 1 2 3 3 3 3 3 3 3 1 2 2 2 2 1 2 2 2 2 2 3 3 2 3 3 3 3 3 3 2 1 2 3 2 2 1 2 3 2 3 2 3 2 2 3
[817] 2 2 2 2 2 3 2 3 3 3 3 2 2 2 1 1 2 2 2 2 2 3 3 2 3 2 2 3 1 2 2 2 3 1 3 2 3 3 2 3 1 2 2 3 3 3 2 2 2 1 2 2 3
[868] 2 3 3 3 2 2 3 2 3 3 2 2 2 2 2 3 2 3 2 3 1 3 3 2 2 3 2 2 2 2 2 3 2 2 2 2 3 3 3 1 2 2 3 2 2 3 2 2 2 3 2 3 1
[919] 2 2 2 2 3 2 2 2 3 3 2 3 2 2 2 2 3 3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 2 2 3 3 2 2 2 2 3 2 2 2 3 3 2 2 3 2 2 3 3
[970] 3 3 2 2 2 3 3 3 1 3 2 3 2 3 1 1 1 2 1 3 2 1 3 1 1 2 3 1 3 3 3 2  reached getoptoption("max.print") -- omitted 2747 entries ]

within cluster sum of squares by cluster:
[1] 349.2902 377.1902 391.4500
  (between_SS / total_SS =  32.1 %)

Available components:
[1] "cluster"      "centers"       "totss"         "withinss"      "tot.withinss" "betweenss"     "size"
[8] "iter"          "ifault"        >
  
```

Figure 12: k-means results (k=3)

- Each cluster sizes => 1198, 1252, 1297
- Total Within Cluster Sum of Squares (WSS) => 1117.93
- Between Cluster Sum of Squares (BSS) => 528.7978
- Total Sum of Squares (TSS) => 1646.728
- (BSS / TSS) => 32.1 %

The following code snippet and the related output shows which quality label is represented by which cluster.

```

> table(KM.clusters, wine_DataFrame_labels)
wine_DataFrame_labels
KM.clusters  5 6 7 8
1 127 556 431 84
2 535 575 122 20
3 372 672 219 34
  
```

As you can see that the quality 5 is being described more by cluster 2 and the quality 6 is being described more by cluster 3 the rest of the qualities (7 & 8) are being described by cluster 1. So with this information we will make our Confusion Matrix including the accuracy, recall and precision for the clusters.

```
> confusion_Matrix
Confusion Matrix and Statistics

          Reference
Prediction   1   2   3
      1 515 127 556
      2 142 535 575
      3 253 372 672

Overall Statistics

    Accuracy : 0.4596
    95% CI   : (0.4435, 0.4757)
    No Information Rate : 0.4812
    P-Value [Acc > NIR] : 0.9962

    Kappa : 0.1856

McNemar's Test P-value : <2e-16
```

```
Statistics by Class:

           class: 1 class: 2 class: 3
Sensitivity       0.5659   0.5174   0.3727
Specificity        0.7593   0.7357   0.6785
Pos Pred Value     0.4299   0.4273   0.5181
Neg Pred Value     0.8450   0.8000   0.5384
Prevalence         0.2429   0.2760   0.4812
Detection Rate     0.1374   0.1428   0.1793
Detection Prevalence 0.3197   0.3341   0.3461
Balanced Accuracy   0.6626   0.6266   0.5256
```

Figure 13: Confusion matrix (k=3)

As you can see that the quality 5 is being described more by cluster 1, quality 6 is being described more by cluster 3, quality 7 is being described more by cluster 2 and the quality 8 being described more by cluster 4. So with this information we will make our Confusion Matrix including the accuracy, recall and precision for the clusters.

```
> confusion_Matrix
Confusion Matrix and statistics

      Reference
Prediction   1   2   3   4
      1 520 117 549 21
      2  51 326 348 62
      3 253 168 502 26
      4 210 161 404 29

Overall Statistics

  Accuracy : 0.3675
  95% CI  : (0.352, 0.3832)
  No Information Rate : 0.4812
  P-value [Acc > NIR] : 1

  Kappa : 0.143

  McNemar's Test P-value : <2e-16

Statistics by class:

          class: 1 class: 2 class: 3 class: 4
Sensitivity      0.5029  0.4223  0.2784  0.21014
Specificity       0.7468  0.8450  0.7701  0.78526
Pos Pred Value    0.4308  0.4142  0.5290  0.03607
Neg Pred Value    0.7976  0.8493  0.5350  0.96296
Prevalence        0.2760  0.2060  0.4812  0.03683
Detection Rate    0.1388  0.0870  0.1340  0.00774
Detection Prevalence 0.3221  0.2100  0.2533  0.21457
Balanced Accuracy  0.6248  0.6337  0.5242  0.49770
> |
```

Figure 15: Confusion matrix ($k=4$)

(Cluster Plots when k = 2, k = 3 & k=4)

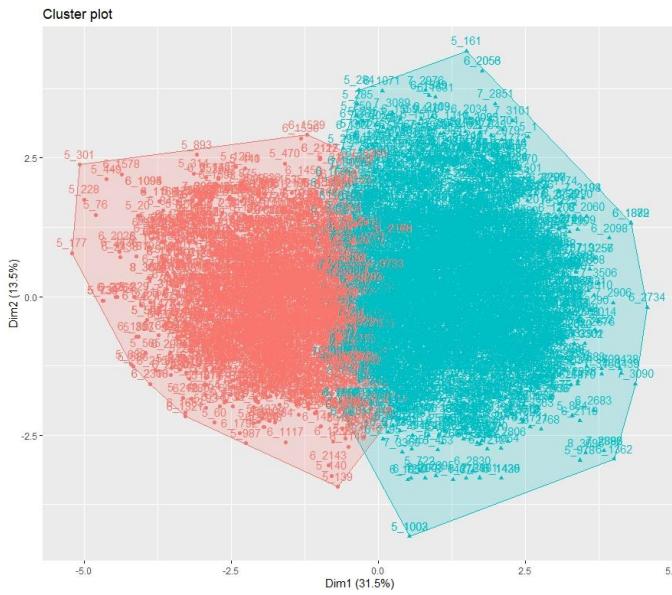


Figure 16: Cluster plot (k=2)

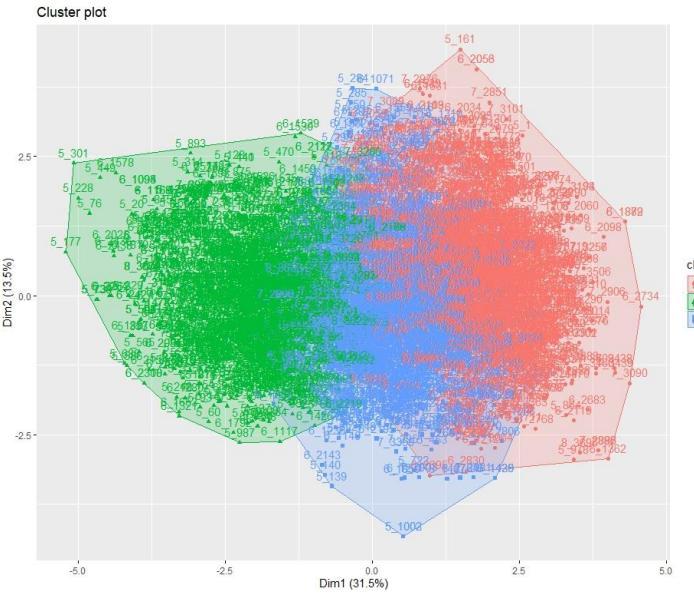


Figure 17: Cluster plot (k=3)

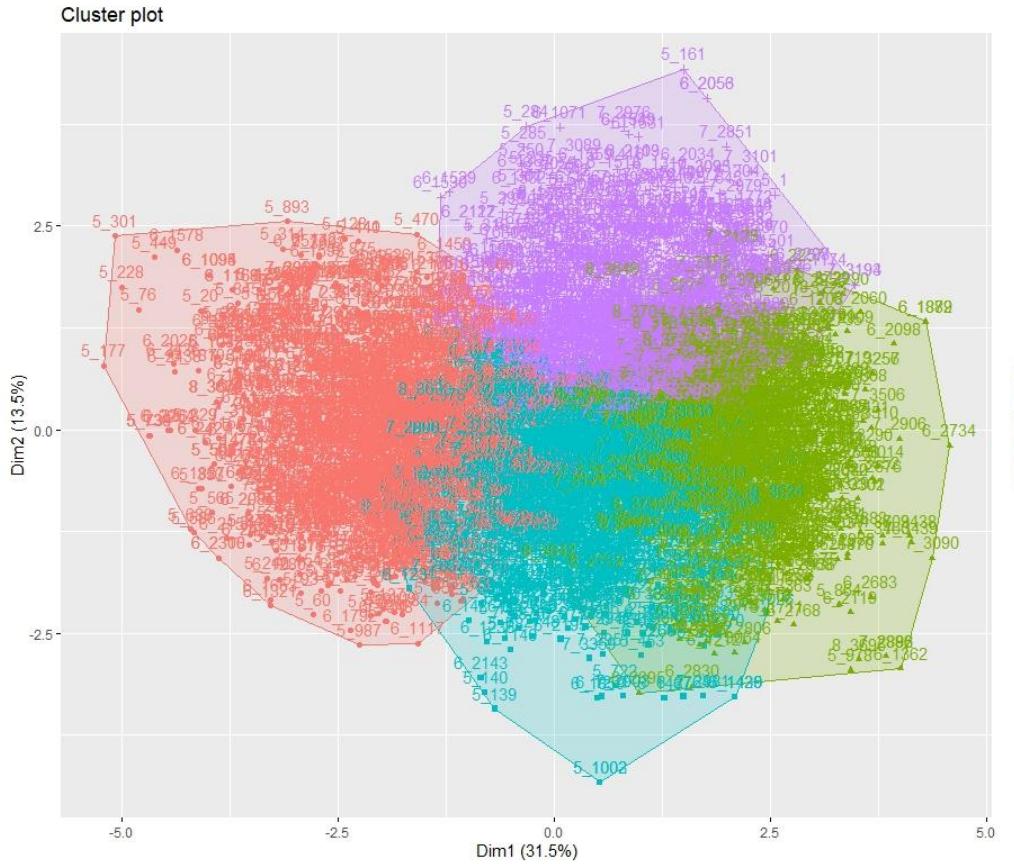


Figure 18: Cluster plot (k=4)

4. Defining the winner cluster.

In order to define the best cluster out of the 3 clusters mentioned above we will consider the total within sums of square (WSS) and the between sums of square (BSS) values.

Within sums of square (WSS) values will show us how well the separation is being done in each cluster. The lower the within sums of square value the higher the separation. So we should get the k value which gives the lower value for the within sums of squares.

Between sums of square (BSS) values will show us how well the cohesion is being done within the clusters. The higher the between sums of square value the higher the cohesion. So we should get the k value which gives the higher value for between sums of squares.

And we should calculate $((\text{Between sums of square} / \text{Total sums of square}) * 100)$ for all the k values and we should choose the k value which gives the higher value for $((\text{BSS}) / (\text{TSS}) * 100)$. And the Total sums of squares will be calculated by adding Total within sums of square value with the Between sums of square value ($\text{TSS} = \text{WSS} + \text{BSS}$).

The following table shows the summary for all the values of each cluster ($k = 2$, $k = 3$ & $k = 4$).

Value for k (no of cluster centers)	Total within sums of square (WSS)	Between sums of square (BSS)	Total sums of square (TSS)	$(\text{BSS}) / (\text{TSS})$
$k = 2$	1230.926	415.8025	1646.728	25.3 %
$k = 3$	1117.93	528.7978	1646.728	32.1 %
$k = 4$	1042.585	604.1429	1646.728	36.7 %

Tabel 1: Summary of clustering results ($k = 2, 3, 4$)

As you see when $k = 4$ only it gives lower value for WSS (1042.585) and higher value for BSS (604.1429) and also it gives higher percentage for $((\text{BSS}) / (\text{TSS}) * 100)$. So it's obvious that the optimum value for k is 4. So the winner cluster value for the wine dataset is 4.

The following picture is the cluster plot for the winner cluster which is $k = 4$ in our case.

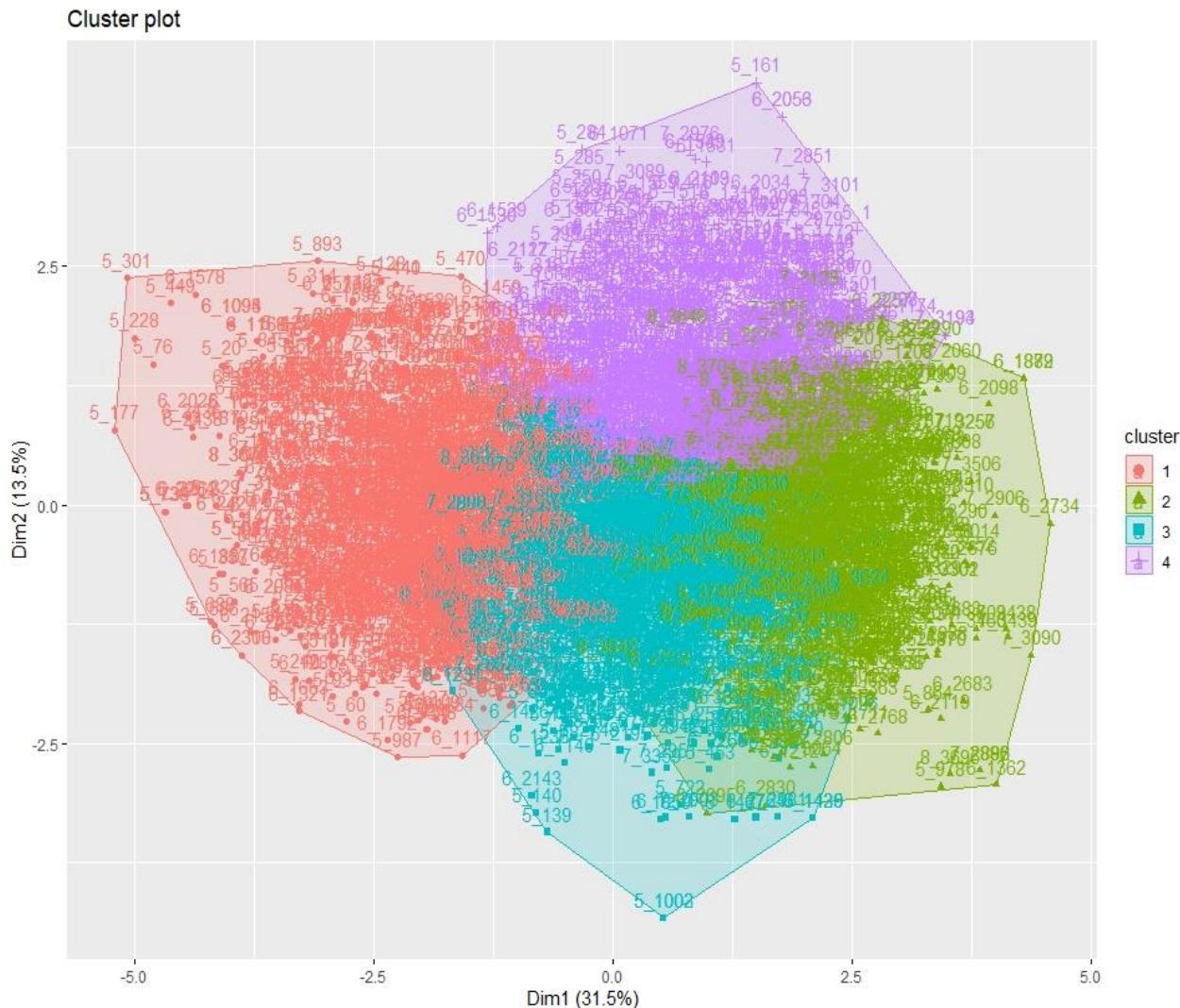


Figure 19: Winner Cluster plot ($k=4$)

5. Applying Principal Component Analysis (PCA)

Principal component analysis (PCA) is a method of obtaining important variables (in the form of components) from a large set of variables available in a data set. It extracts a low dimensional set of features by taking a projection of irrelevant dimensions from a high dimensional data set with a motive to capture as much information as possible.

With the use of Principal component analysis (PCA) we can reduce the dimensionality of the dataset. In order to apply the PCA to a dataset it is a must to scale the data first. We can get the maximum use of PCA only if we apply PCA for a scaled dataset.

The following is the code snippet and the related summary output for applying PCA to our normalized wine dataset.

```
> #PCA APPLYING.....
> PCA_components <- prcomp(~fixed.acidity + volatile.acidity + citric.acid
+ residual.sugar + chlorides + free.sulfur.dioxide
+ total.sulfur.dioxide + density + pH + sulphates +
alcohol, data = wine_DataFrame_norm,
scale. = T)
> summary(PCA_components)
Importance of components:
PC1    PC2    PC3    PC4    PC5    PC6    PC7    PC8    PC9    PC10   PC11
Standard deviation 1.8627 1.2208 1.0917 1.0505 0.99697 0.87666 0.85730 0.76251 0.6170 0.52192 0.11276
Proportion of variance 0.3154 0.1355 0.1084 0.1003 0.09036 0.06987 0.06681 0.05286 0.0346 0.02476 0.00116
Cumulative Proportion 0.3154 0.4509 0.5593 0.6596 0.74994 0.81980 0.88662 0.93948 0.9741 0.99884 1.00000
>
```

Figure 20: PCA application

As you can see the summary of the principal components it shows that the first 8 principal components achieve the cumulative score > 96%. So now we will transform our dataset into which we have only the first 8 principal components. The following code snippet shows the code and the output of the transformed dataset.

```
> trnfrm_PCA_components <- as.data.frame(PCA_components$x[,1:8])
> head(trnfrm_PCA_components)
   PC1      PC2      PC3      PC4      PC5      PC6      PC7      PC8
1 2.54585895 2.8826716 -0.4357777 0.007385251 1.5053353 0.41091506 0.4484454 0.008014836
2 0.18688467 2.4153025 -0.9567648 0.605963803 1.0671895 0.01806569 0.4802707 -1.309010536
3 1.61494065 1.5545729 -1.8854779 0.937242107 1.3056175 0.61628142 0.1278765 -0.513822030
4 -0.62594099 -1.4782284 1.2154589 0.962230833 0.7514572 0.79021212 -0.4605018 -0.464103249
5 -1.09005515 -2.0978627 1.4801774 1.253275981 -0.5629674 -0.62552601 0.6883195 -0.541439942
6 -0.09345576 -0.9366681 1.8242048 0.463288700 0.5480815 -1.38161454 -1.0542516 0.003285588
>
```

Figure 21: Viewing principal components

As you can see, the transformed dataset only has the first 8 principal components. And Now we need to provide this transformed dataset for our k-means algorithm.

6. K-means clustering analysis for PCA

Now we will perform k-means clustering for this newly transformed dataset with the winner k value, which is 4 that we got previously.

```
> set.seed(1600) #Setting seed
> KM.PCA <- kmeans(trnfrm_PCA_components, centers = 4, nstart = 25)
> KM.PCA
K-means clustering with 4 clusters of sizes 1179, 867, 782, 919

Cluster means:
          PC1        PC2        PC3        PC4        PC5        PC6        PC7        PC8
1 -2.2656845 -0.06476213  0.1863376 -0.08491831 -0.05872567  0.02637979  0.1818482  0.07578242
2  0.7321132  1.37716526 -0.0158793  0.08707282  0.07971244 -0.01026658 -0.2148729 -0.14313497
3  2.1911789 -0.37809047  0.5464889 -0.42683563 -0.09677130 -0.04241151  0.2898052  0.10074141
4  0.3514669 -0.89442980 -0.6890957  0.39000219  0.08248318  0.01193161 -0.2771837 -0.04790995

Clustering vector:
   1   2   3   4   5   6   7   8   9   10  11  12  13  14  15  16  17  18  19  20  21  22
  2   2   2   4   1   4   1   1   1   4   2   1   2   1   1   1   1   1   1   1   1   1
 23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41  42  43  44
  4   1   1   1   1   1   1   1   1   4   2   3   1   1   1   1   4   2   3   1   1   1
 45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60  61  62  63  64  65  66
  1   3   4   1   1   1   1   1   1   1   1   1   1   1   1   1   1   2   1   1   1   1
 67  68  69  70  71  72  73  74  75  76  77  78  79  80  81  82  83  84  85  86  87  88
  4   1   2   1   1   2   1   1   1   1   1   1   1   4   2   2   2   2   1   3   4   1
 89  90  91  92  93  94  95  96  97  98  99  100 101 102 103 104 105 106 107 108 109 110
  2   3   1   2   1   1   2   2   2   1   1   2   1   1   1   4   4   4   4   1   1
 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132
  1   1   1   1   4   4   4   2   2   2   3   1   1   4   1   4   4   1   1
 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154
  1   2   1   1   1   1   4   4   1   1   1   4   4   4   2   2   4   1   1
 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176
  4   4   1   1   1   1   2   1   3   1   1   1   4   3   2   4   1   1
 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198
  1   1   1   1   2   1   1   1   1   4   2   4   2   1   1   1   1   2   1

```

Figure 22: k-means results PCA 1

```
 1   1   1   2   4   4   3   1   1   1   1   1   1   2   1   2   1   1   1   1   1   4   1
925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946
 1   1   2   4   1   2   1   1   1   4   4   4   4   2   4   1   1   1   1   1   1   1   1
947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968
 1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1
969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990
 4   4   3   1   1   1   1   4   2   4   3   4   1   4   1   2   2   2   1   1   2   4   1
991 992 993 994 995 996 997 998 999 1000
 3   4   2   3   4   4   2   1   2   1
[ reached getoption("max.print") -- omitted 2747 entries ]

within cluster sum of squares by cluster:
[1] 8009.623 5863.153 4599.807 6074.283
  (between_SS / total_SS =  36.6 %)

Available components:
[1] "cluster"      "centers"       "totss"         "withinss"      "tot.withinss" "betweenss"     "size"
[8] "iter"          "ifault"
>
```

Figure 23: k-means results PCA 2

- Each cluster sizes => 1179, 867, 782, 919
- Total Within Cluster Sum of Squares (WSS) => 24546.87
- Between Cluster Sum of Squares (BSS) => 14165.18
- Total Sum of Squares (TSS) => 38712.05
- (BSS / TSS) => 36.6 %

The following picture is the cluster plot for the k-means clustering with the first 8 principal components.

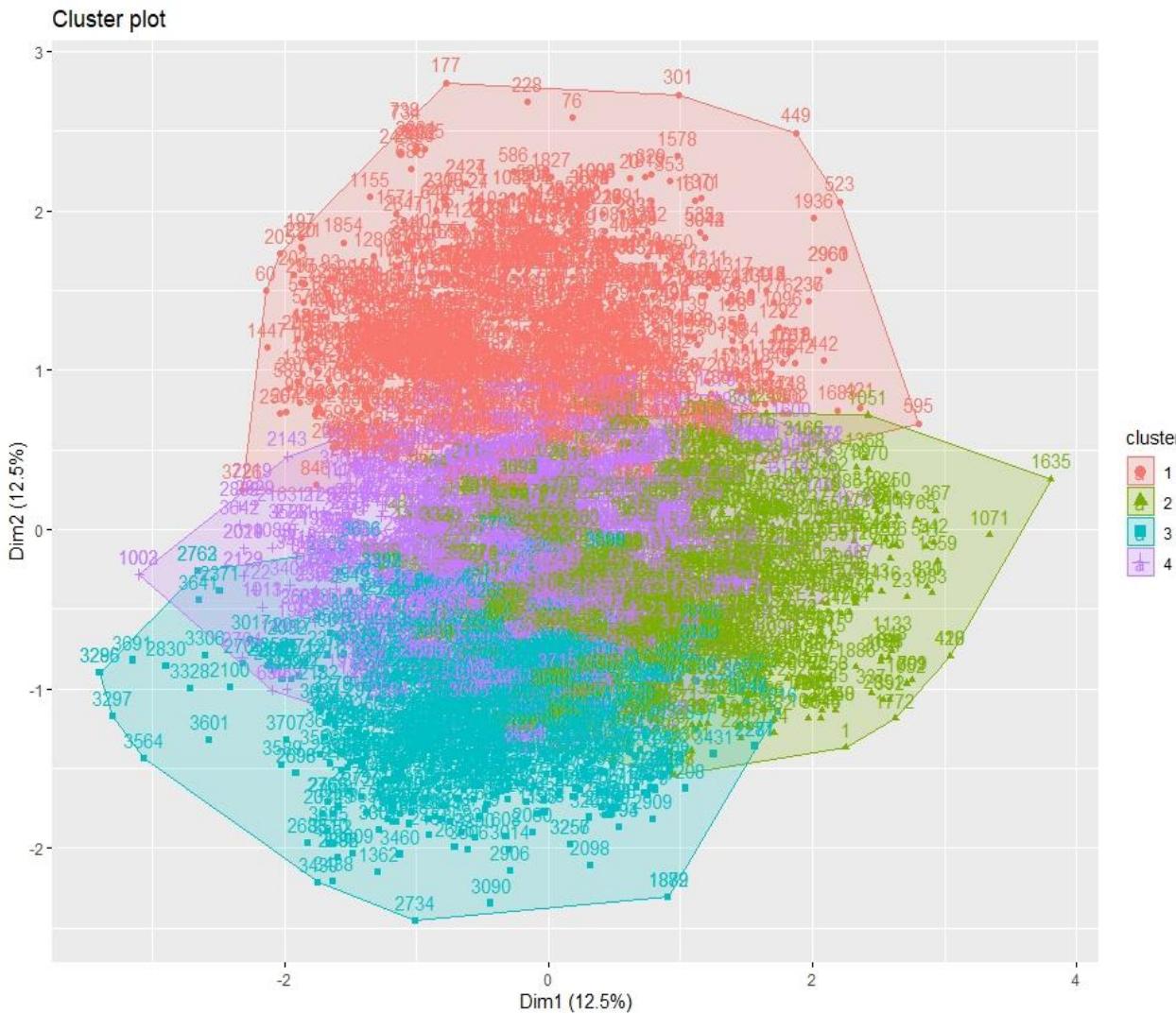


Figure 24: Cluster plot (PCA)

7. K-means clustering with PCA and without PCA results analysis and comparison

Winner cluster value (k = 4)	Total within sums of square (WSS)	Between sums of square (BSS)	Total sums of square (TSS)	(BSS)/ (TSS)
K-means without PCA	1042.585	604.1429	1646.728	36.7 %
K-means with PCA	24546.87	14165.18	38712.05	36.6 %

Tabel 2: Summary of clustering with PCA and without PCA

As you can see even though we reduced the dimensions by applying PCA to our dataset the percentage of $((BSS) / (TSS) * 100)$ still it gives approximately the same percentage (36.6%) as the percentage we got from the k-means clustering without applying PCA (36.7%).

It shows that applying PCA is a good way to reduce the dimension of your dataset. Which leads to faster computing for your clustering analysis.

Energy Forecasting Part

1. Preparing various input vectors for both (AR) and (NARX) approaches.

For the AR approach we have constructed 4 datasets using various time-delayed input vectors of the 11th hour attribute with the help of R programming language. The following is the code snippet that has been used to create the 4 datasets for the AR approach.

```
library(readxl)

#Loading the data set and creating the data Frame.
dataFrame <- read_excel("C:\\\\Users\\\\SEAN\\\\Desktop\\\\MachineLearningandDataMining\\\\MLCW\\\\Uow_Load.xlsx")
str(dataFrame)

columns= c("Day1", "Day2", "Day3", "Day4", "NextDay")

# pass this vector length to ncol parameter
# and now with 0
DataFrame_days = data.frame(matrix(nrow = 0, ncol = length(columns)))

# assign column names
colnames(DataFrame_days) = columns

i <- 1
while(i<497){
  values <- data.frame(dataFrame$Time11[i], dataFrame$Time11[i+1], dataFrame$Time11[i+2], dataFrame$Time11[i+3], dataFrame$Time11[i+4])
  #naming the Data Frame - Step 2
  names(values) <- c("Day1", "Day2", "Day3", "Day4", "NextDay")
  DataFrame_days <- rbind(DataFrame_days, values)
  i = i + 1
}

str(DataFrame_days)
write.csv(DataFrame_days, "C:\\\\Users\\\\SEAN\\\\Desktop\\\\MachineLearningandDataMining\\\\MLCW\\\\test_DataFrame_AR(4).csv")
```

Figure 25: For producing AR input vectors

The names of the constructed dataset files and the details of those 4 dataset files is as follows.

- DataFrame_AR(1) => Dataset which is responsible for predicting the next day's (t) electricity consumption based on the (t-1) day electricity consumption data.
- DataFrame_AR(2) => Dataset which is responsible for predicting the next day's (t) electricity consumption based on the (t-1) and (t-2) days electricity consumption data.
- DataFrame_AR(3) => Dataset which is responsible for predicting the next day's (t) electricity consumption based on the (t-1), (t-2) and (t-3) days electricity consumption data.
- DataFrame_AR(4) => Dataset which is responsible for predicting the next day's (t) electricity consumption based on the (t-1), (t-2), (t-3) and (t-4) days electricity consumption data.

A	B	C	D	E	F	G
1	Day1	NextDay				
2	1	88.6	106			
3	2	106	114.8			
4	3	114.8	109			
5	4	109	102.4			
6	5	102.4	87.2			
7	6	87.2	67.6			
8	7	67.6	116.2			
9	8	116.2	116			
10	9	116	114.2			
11	10	114.2	113.4			
12	11	113.4	120.4			
13	12	120.4	84.8			
14	13	84.8	66.8			
15	14	66.8	121.2			
16	15	121.2	124.6			
17	16	124.6	118.6			
18	17	118.6	133.8			

Figure 26: Dataframe_AR(1)

A	B	C	D	E	F	G
1	Day1	Day2	NextDay			
2	1	88.6	106	114.8		
3	2	106	114.8	109	102.4	
4	3	114.8	109	102.4	87.2	
5	4	109	102.4	87.2	67.6	
6	5	102.4	87.2	67.6	116.2	
7	6	87.2	67.6	116.2	116	
8	7	67.6	116.2	116	114.2	
9	8	116.2	116	114.2	113.4	
10	9	116	114.2	113.4	120.4	
11	10	114.2	113.4	120.4	84.8	
12	11	113.4	120.4	84.8	66.8	
13	12	120.4	84.8	66.8	121.2	
14	13	84.8	66.8	121.2	124.6	
15	14	66.8	121.2	124.6	118.6	
16	15	121.2	124.6	118.6	133.8	
17	16	124.6	118.6	133.8	126.8	
18	17	118.6	133.8	126.8	100.8	

Figure 27: Dataframe_AR(2)

A	B	C	D	E	F	G
1	Day1	Day2	Day3	NextDay		
2	1	88.6	106	114.8	109	
3	2	106	114.8	109	102.4	
4	3	114.8	109	102.4	87.2	
5	4	109	102.4	87.2	67.6	
6	5	102.4	87.2	67.6	116.2	
7	6	87.2	67.6	116.2	116	
8	7	67.6	116.2	116	114.2	
9	8	116.2	116	114.2	113.4	
10	9	116	114.2	113.4	120.4	
11	10	114.2	113.4	120.4	84.8	
12	11	113.4	120.4	84.8	66.8	
13	12	120.4	84.8	66.8	121.2	
14	13	84.8	66.8	121.2	124.6	
15	14	66.8	121.2	124.6	118.6	
16	15	121.2	124.6	118.6	133.8	
17	16	124.6	118.6	133.8	126.8	
18	17	118.6	133.8	126.8	100.8	

Figure 28: Dataframe_AR(3)

A	B	C	D	E	F	G
1	Day1	Day2	Day3	Day4	NextDay	
2	1	88.6	106	114.8	109	102.4
3	2	106	114.8	109	102.4	87.2
4	3	114.8	109	102.4	87.2	67.6
5	4	109	102.4	87.2	67.6	116.2
6	5	102.4	87.2	67.6	116.2	116
7	6	87.2	67.6	116.2	116	114.2
8	7	67.6	116.2	116	114.2	113.4
9	8	116.2	116	114.2	113.4	120.4
10	9	116	114.2	113.4	120.4	84.8
11	10	114.2	113.4	120.4	84.8	66.8
12	11	113.4	120.4	84.8	66.8	121.2
13	12	120.4	84.8	66.8	121.2	124.6
14	13	84.8	66.8	121.2	124.6	118.6
15	14	66.8	121.2	124.6	118.6	133.8
16	15	121.2	124.6	118.6	133.8	126.8
17	16	124.6	118.6	133.8	126.8	100.8
18	17	118.6	133.8	126.8	100.8	69.6

Figure 29: Dataframe_AR(4)

For the NARX approach we have constructed 4 datasets using various time-delayed input vectors of the 9th, 10th, and 11th hour attributes with the help of R programming language. The following is the code snippet that has been used to create the 4 datasets for the NARX approach.

```

library(readxl)

#Loading the data set and creating the data Frame.
dataFrame <- read_excel("C:\\\\Users\\\\SEAN\\\\Desktop\\\\MachineLearningandDataMining\\\\MLCW\\\\UOW_Load.xlsx")
str(dataFrame)
|
#"Day2_9", "Day2_10", "Day2_11", "Day3_9", "Day3_10", "Day3_11", "Day4_9", "Day4_10", "Day4_11",
columns= c("Day1_9", "Day1_10", "Day1_11", "NextDay_9", "NextDay_10", "NextDay_11")

# pass this vector length to ncol parameter
# and nrow with 0
dataFrame_days = data.frame(matrix(nrow = 0, ncol = length(columns)))

# assign column names
colnames(DataFrame_days) = columns

#, dataFrame$Time9[i+2], dataFrame$Time10[i+2], dataFrame$Time11[i+2], dataFrame$Time9[i+3], dataFrame$Time10[i+3], dataFrame$Time11[i+3])
i < 1
while(i<500){
  values <- data.frame(dataFrame$Time9[i], dataFrame$Time10[i], dataFrame$Time11[i], dataFrame$Time9[i+1], dataFrame$Time10[i+1], dataFrame$Time11[i+1])
  #Naming the Data Frame - Step 2
  names(values) <- c("Day1_9", "Day1_10", "Day1_11", "NextDay_9", "NextDay_10", "NextDay_11")
  DataFrame_days <- rbind(DataFrame_days, values)
  i = i +1
}

str(DataFrame_days)
write.csv(DataFrame_days, "C:\\\\Users\\\\SEAN\\\\Desktop\\\\MachineLearningandDataMining\\\\MLCW\\\\test_DataFrame_NARX(1).csv")

```

Figure 30: For producing NARX input vectors

The names of the constructed dataset files and the details of those 4 dataset files is as follows.

- DataFrame_NARX(1) => Dataset which is responsible for predicting the next day's (t) 11th hour electricity consumption based on the (t-1) day's 9th, 10th, and 11th hour electricity consumption data and with (t) day's 9th, 10th hour electricity consumption data.
- DataFrame_NARX(2) => Dataset which is responsible for predicting the next day's (t) 11th hour electricity consumption based on the (t-1) and (t-2) day's 9th, 10th, and 11th hour electricity consumption data and with (t) day's 9th, 10th hour electricity consumption data.
- DataFrame_NARX(3) => Dataset which is responsible for predicting the next day's (t) 11th hour electricity consumption based on the (t-1), (t-2) and (t-3) day's 9th, 10th, and 11th hour electricity consumption data and with (t) day's 9th, 10th hour electricity consumption data.
- DataFrame_NARX(4) => Dataset which is responsible for predicting the next day's (t) 11th hour electricity consumption based on the (t-1), (t-2), (t-3) and (t-4) day's 9th, 10th, and 11th hour electricity consumption data and with (t) day's 9th, 10th hour electricity consumption data.

A	B	C	D	E	F	G	H
1	Day1_9	Day1_10	Day1_11	NextDay_9	NextDay_10	NextDay_11	
2	1	89.4	90.6	88.6	108.2	104.6	106
3	2	108.2	104.6	106	110	111.6	114.8
4	3	110	111.6	114.8	106.4	104.4	109
5	4	106.4	104.4	109	97.8	100.4	102.4
6	5	97.8	100.4	102.4	87	90.8	87.2
7	6	87	90.8	87.2	68.8	67	67.6
8	7	68.8	67	67.6	110.2	113	116.2
9	8	110.2	113	116.2	111.2	114.6	116
10	9	111.2	119.2	116	109	114.6	114.2
11	10	109	114.6	114.2	99.8	109	113.4
12	11	99.8	109	113.4	111	114.8	120.4
13	12	111	114.8	120.4	88.4	89.6	84.8
14	13	88.4	89.6	84.8	63.4	63.6	66.8
15	14	63.4	63.6	63.6	66.8	114.4	116.2
16	15	114.4	116.2	121.2	112.2	114.6	124.6
17	16	111.2	114.6	124.6	124.6	119.6	117.4
18	17	119.6	117.4	118.6	117.6	123.6	133.8
19	18	117.6	123.6	133.8	120.4	130.4	120.4
20	19	120.4	130.4	126.8	105	101.4	100.8
21	20	105	101.4	100.8	67.6	68	67.6
22	21	67.6	68	69.6	133.8	132.4	138.4
23	22	133.8	132.4	138.4	126	129	138.4
24	23	126	129	138.4	119.2	129.4	133.8
25	24	119.2	129.4	133.8	126.4	130.4	124.6

Figure 31: Dataframe_NARX(1)

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Day1_9	Day1_10	Day1_11	Day2_9	Day2_10	Day2_11	Day3_9	Day3_10	Day3_11	Day4_9	Day4_10	Day4_11	Day5_9	Day5_10	Day5_11	
2	1	89.4	90.6	88.6	108.2	104.6	106	110	111.6	114.8	106.4	104.4	109	97.8	100.4	
3	2	108.2	104.6	106	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4	87.2	84.8	
4	3	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4	87	90.8	87.2	67	67.6	
5	4	106.4	104.4	109	97.8	100.4	102.4	87	90.8	87.2	68.8	67	67.6	113	116.2	
6	5	97.8	100.4	102.4	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2	119.2	116	
7	6	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2	111.2	116	109	114.6	114.2	
8	7	68.8	67	67.6	110.2	113	116.2	111.2	116.2	114.2	114.6	112.2	111.2	99.8	109	
9	8	110.2	113	116.2	111.2	119.2	116	109	114.6	114.2	99.8	109	113.4	111	114.8	
10	9	111.2	119.2	116	109	114.6	114.2	99.8	109	113.4	111	114.8	120.4	88.4	84.8	

Figure 32: Dataframe_NARX(2)

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Day1_9	Day1_10	Day1_11	Day2_9	Day2_10	Day2_11	Day3_9	Day3_10	Day3_11	Day4_9	Day4_10	Day4_11	Day5_9	Day5_10	Day5_11	
2	1	89.4	90.6	88.6	108.2	104.6	106	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4
3	2	108.2	104.6	106	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4	87.2	84.8	84.8
4	3	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4	87	90.8	87.2	67	67.6	113
5	4	106.4	104.4	109	97.8	100.4	102.4	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2
6	5	97.8	100.4	102.4	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2	119.2	116	116
7	6	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2	111.2	116	109	114.6	114.2	114.2
8	7	68.8	67	67.6	110.2	113	116.2	111.2	119.2	116	109	114.6	112.2	99.8	109	113.4
9	8	110.2	113	116.2	111.2	119.2	116	109	114.6	114.2	99.8	109	113.4	111	114.8	120.4
10	9	111.2	119.2	116	109	114.6	114.2	99.8	109	113.4	111	114.8	120.4	88.4	84.8	84.8

Figure 33 Dataframe_NARX(3)

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Day1_9	Day1_10	Day1_11	Day2_9	Day2_10	Day2_11	Day3_9	Day3_10	Day3_11	Day4_9	Day4_10	Day4_11	Day5_9	Day5_10	Day5_11	
2	1	89.4	90.6	88.6	108.2	104.6	106	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4
3	2	108.2	104.6	106	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4	87.2	84.8	84.8
4	3	110	111.6	114.8	106.4	104.4	109	97.8	100.4	102.4	87	90.8	87.2	67	67.6	113
5	4	106.4	104.4	109	97.8	100.4	102.4	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2
6	5	97.8	100.4	102.4	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2	119.2	116	116
7	6	87	90.8	87.2	68.8	67	67.6	110.2	113	116.2	111.2	116	109	114.6	114.2	114.2
8	7	68.8	67	67.6	110.2	113	116.2	111.2	119.2	116	109	114.6	112.2	99.8	109	113.4
9	8	110.2	113	116.2	111.2	119.2	116	109	114.6	114.2	99.8	109	113.4	111	114.8	120.4
10	9	111.2	119.2	116	109	114.6	114.2	99.8	109	113.4	111	114.8	120.4	88.4	84.8	84.8

Figure 34: Dataframe_NARX(4)

2. Data Normalization

Since we know that there are 2 possible ways that we can use to scale our data. One way is Normalization and the other way is Standardization. If the dataset does not have a normal or more or less normal distribution for some feature, Standardization may not be the most suitable method. So it's always best to Normalize the dataset for neural network problems. So here we will use the min-max Normalization to scale each feature in the range between 0 and 1.

The following code snippets shows how we normalize our given dataset in order to build neural networks for both AR and NARX approaches.

```
> #Normalizing the Data
> normalization <- function(x) {
+   (x - min(x))/(max(x) - min(x))
+ }
>
> #apply Min-Max normalization.
> DataFrame_days_scale <- data.frame(lapply(DataFrame_days[1:columnNumbers], normalization))
> head(DataFrame_days_scale)
  Day1     Day2     Day3     Day4    NextDay
1 0.3733826 0.5341959 0.6155268 0.5619224 0.5009242
2 0.5341959 0.6155268 0.5619224 0.5009242 0.3604436
3 0.6155268 0.5619224 0.5009242 0.3604436 0.1792976
4 0.5619224 0.5009242 0.3604436 0.1792976 0.6284658
5 0.5009242 0.3604436 0.1792976 0.6284658 0.6266174
6 0.3604436 0.1792976 0.6284658 0.6266174 0.6099815
> |
```

Figure 35: min-max normalization for `dataFrame_AR(4)`

```
> #Normalizing the Data
> normalization <- function(x) {
+   (x - min(x))/(max(x) - min(x))
+ }
>
> #apply Min-Max normalization.
> DataFrame_days_scale <- data.frame(lapply(DataFrame_days[1:columnNumbers], normalization))
> head(DataFrame_days_scale)
  Day1_9  Day1_10 Day1_11 Day2_9  Day2_10 Day2_11 Day3_9  Day3_10 Day3_11 Day4_9  Day4_10 Day4_11 NextDay_9 NextDay_10 NextDay_11
1 0.4295154 0.4156627 0.3733826 0.6365639 0.5562249 0.5341959 0.6563877 0.6265060 0.6155268 0.6167401 0.5542169 0.5619224 0.5220264 0.5140562 0.5009242
2 0.6365639 0.5562249 0.5341959 0.6563877 0.6265060 0.6155268 0.6167401 0.5542169 0.5619224 0.5220264 0.5140562 0.5009242 0.4030837 0.4176707 0.3604436
3 0.6563877 0.6265060 0.6155268 0.6167401 0.5542169 0.5619224 0.5220264 0.5140562 0.5009242 0.4030837 0.4176707 0.3604436 0.2026432 0.1787149 0.1792976
4 0.6167401 0.5542169 0.5619224 0.5220264 0.5140562 0.5009242 0.4030837 0.4176707 0.3604436 0.2026432 0.1787149 0.1792976 0.6585903 0.6405622 0.6284658
5 0.5220264 0.5140562 0.5009242 0.4030837 0.4176707 0.3604436 0.2026432 0.1787149 0.1792976 0.6585903 0.6405622 0.6284658 0.6696035 0.7028112 0.6266174
6 0.4030837 0.4176707 0.3604436 0.2026432 0.1787149 0.1792976 0.6585903 0.6405622 0.6284658 0.6696035 0.7028112 0.6266174 0.6453744 0.6566265 0.6099815
> |
```

Figure 36: min-max normalization for `dataFrame_NARX(4)`

Normalization/scaling is typically recommended and sometimes very important. Especially for neural networks, normalization can be very crucial because when you input unnormalised inputs to activation functions, you can get stuck in a very flat region in the domain and may not learn at all. Or worse, you can end up with numerical issues.

3. MLP Neural Network Analysis

1. MLP Neural Network Analysis for AR approach

Dataset Name (contains input vectors)	No of hidden layers and nodes in each layer	Learning rate	Activation Function	Testing Performance Analysis		
				RMSE	MAE	MAPE
DataFrame_AR(1)	1 (5)	0.001	logistic	19.69127	16.9423	0.179792
DataFrame_AR(1)	2 (8, 5)	0.001	tanh	19.63556	16.62699	0.1755653
DataFrame_AR(2)	1 (5)	0.001	tanh	16.54231	13.74638	0.1431922
DataFrame_AR(2)	2 (9, 6)	0.0001	logistic	15.98554	13.40043	0.1409552
DataFrame_AR(3)	1 (6)	0.0001	tanh	14.77517	12.44712	0.1304804
DataFrame_AR(3)	2 (8, 4)	0.001	logistic	14.77917	12.53184	0.128366
DataFrame_AR(4)	1 (7)	0.0005	logistic	14.48904	11.89507	0.1256197
DataFrame_AR(4)	2 (9, 5)	0.0001	logistic	14.06588	11.33218	0.119508

Tabel 3: MLP Neural Network Analysis for AR approach

2. MLP Neural Network Analysis for NARX approach

Dataset Name (contains input vectors)	No of hidden layers and nodes in each layer	Learning rate	Activation Function	Testing Performance Analysis		
				RMSE	MAE	MAPE
DataFrame_NARX(1)	1 (5)	0.001	logistic	9.251488	7.632887	0.06884571
DataFrame_NARX(1)	2 (8, 5)	0.001	tanh	9.137165	7.529608	0.06885017
DataFrame_NARX(2)	1 (10)	0.001	tanh	9.188893	7.633953	0.06958234
DataFrame_NARX(2)	2 (9, 6)	0.0001	logistic	8.961525	7.341603	0.06627507
DataFrame_NARX(3)	1 (6)	0.0001	tanh	8.97989	7.390405	0.06751549
DataFrame_NARX(3)	2 (9, 5)	0.001	logistic	8.681214	7.128098	0.0646964
DataFrame_NARX(4)	1 (13)	0.0005	logistic	8.802666	7.330058	0.0671484
DataFrame_NARX(4)	2 (14, 8)	0.0001	logistic	8.135052	6.666759	0.06102992

Tabel 4: MLP Neural Network Analysis for NARX approach

In the above tables there are three standard statistical indices,

RMSE - Root Mean Square Error (RMSE) is the standard deviation of the residuals (prediction errors). Residuals are a measure of how far from the regression line data points are; RMSE is a measure of how spread out these residuals are. In other words, it tells you how concentrated the data is around the line of best fit.

MAE - Mean Absolute Error of your model refers to the mean of the absolute values of each prediction error on all instances of the test dataset. Prediction error is the difference between the actual value and the predicted value for that instance. Statistically, Mean Absolute Error (MAE) refers to the results of measuring the difference between two continuous variables. Let us assume variables M and N represent the same phenomenon but have recorded different observations.

MAPE - Mean Absolute Percentage Error (MAPE) is a statistical measure to define the accuracy of a machine learning algorithm on a particular dataset. MAPE can be considered as a loss function to define the error termed by the model evaluation. Using MAPE, we can estimate the accuracy in terms of the differences in the actual v/s estimated values.(MAPE - Mean Absolute Percentage Error in Python - AskPython, no date)

4. Choosing the best MLP Network

As you can see from both “AR” and “NARX” MLP Neural Network comparison tables the green color highlighted ones are the best 1 hidden layer MLP networks and the red color highlighted ones are the best 2 hidden layer MLP networks.

As you can see, that NARX approach gives relatively low values for the RMSE, MAE and MAPE. It means that the NARX approach is performing really well when compared to AR approach for this specific time series problem.

And the above-mentioned 2 hidden layer best MLP network from the NARX Network Network comparison table gives relatively small values for the RMSE, MAE and MAPE. which means that this MLP Neural Network was the best MLP Neural Network out of all the networks from both tables.

The following picture shows the best MLP Neural Network.

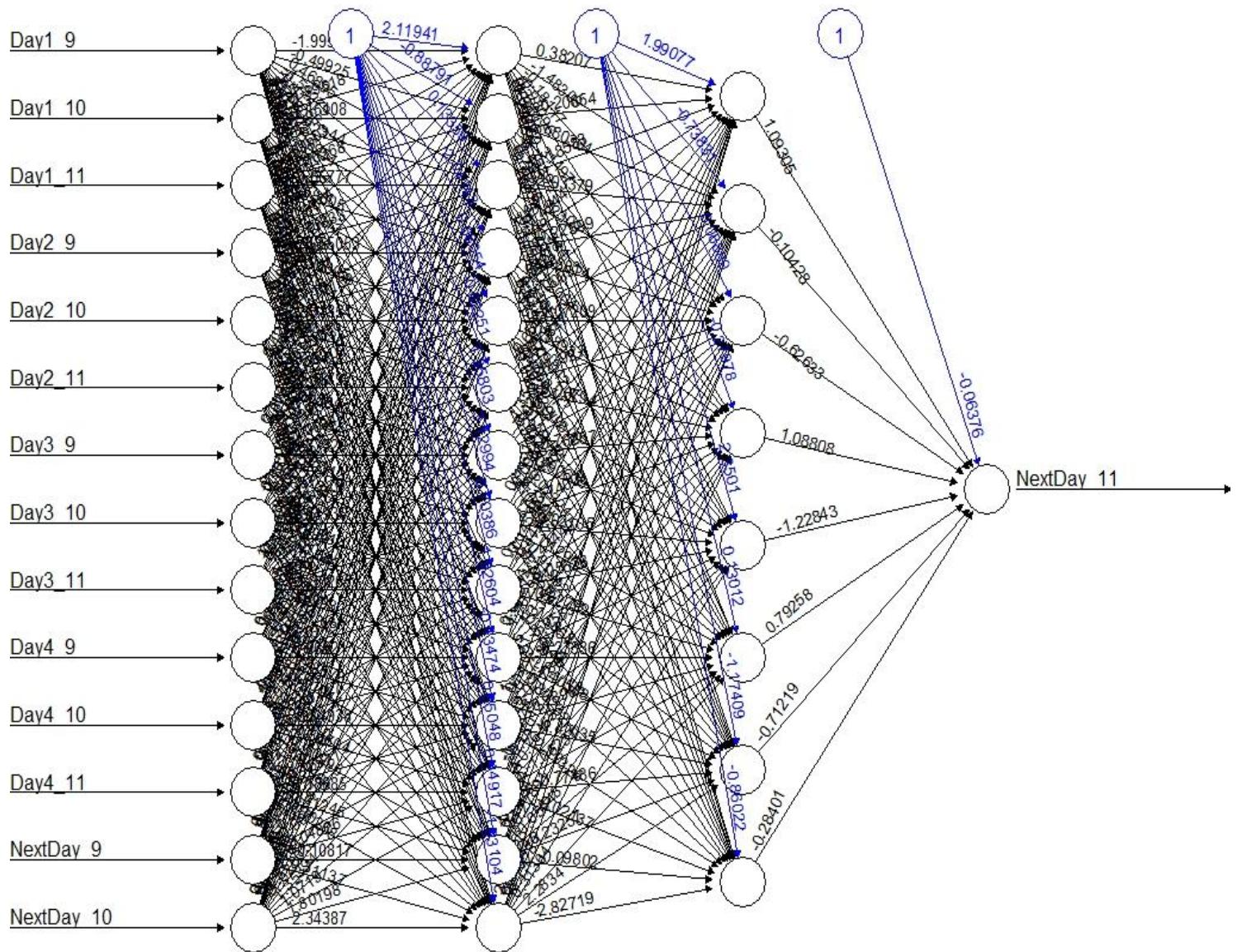


Figure 37: Best MLP Neural Network

Best MLP Neural Network Analysis

- RMSE => 8.135052
- MAE => 6.666759
- MAPE => 0.06102992

And the following picture shows the details about the (desired output vs predicted output) from the testing dataset.

	desired_Output	predicted_Output
1	113.6	105.78411
2	100.8	103.99796
3	124.0	116.31028
4	124.8	116.92487
5	119.0	108.96205
6	89.4	83.36382
7	58.2	55.30111
8	133.8	121.51773
9	124.0	116.03632
10	126.2	124.01003
11	121.8	115.70094
12	123.8	109.16038
13	95.6	83.92985
14	54.2	53.24203
15	125.8	118.54160
16	128.2	118.74230
17	116.2	118.74050
18	123.8	112.92986
19	112.8	104.89179
20	106.4	96.02626
21	51.4	48.64689
22	129.4	116.39928
23	137.0	118.40428
24	132.4	132.14659
25	140.8	115.04468
26	125.2	116.57004
27	94.0	87.87206
28	55.4	55.56579
29	137.8	125.50484
30	127.2	121.26555
31	131.0	127.77405
32	132.0	123.68893
33	127.8	117.33286
34	100.2	91.69613
35	53.6	59.26443
36	108.4	109.66037
37	120.0	108.75235
38	106.8	98.87220
39	103.0	102.02377
40	89.6	85.29034
41	88.4	83.06310
42	48.2	50.21511
43	103.4	97.03598
44	125.6	114.60018
45	100.0	104.23727
46	98.2	93.26594
47	92.4	85.81420
48	80.8	74.41106

Figure 38: Desired Output vs Predicted Output

Appendix - Clustering Part Code

```

1 library(MASS)
2 library(NbClust)
3 library(factoextra)
4 library(ClusterR)
5 library(cluster)
6 library(caret)
7 library(dplyr)
8 library(psych)
9 library(readxl)
10
11 ######Loading the Data set#####
12 wine_DataFrame <- read_excel("C:\\Users\\SEAN\\Desktop\\MachineLearningandDataMining\\MLCW\\Whitewine_v2.xlsx")
13 wine_DataFrame <- data.frame(wine_DataFrame)
14 str(wine_DataFrame)
15
16 #####Visualization of Outliers in each features of the data set#####
17 columnNames <- names(wine_DataFrame)
18 oldpar <- par(mfrow = c(2,6))
19 for (i in 1:11){
20   boxplot(wine_DataFrame[i], main = columnNames[i], col = "#DD3300")
21 }
22 par(oldpar)
23
24 #####visualizing how the distribution is looks like#####
25 oldpar <- par(mfrow = c(2,6))
26 for (i in 1:12){
27   truehist(wine_DataFrame[[i]], main = columnNames[i], col = blues9)
28   lines(density(wine_DataFrame[[i]]), col= 2, lwd=2)
29 }
30 par(oldpar)
31
32 #####Removal of Outliers#####
33 # The returned stats variable is a vector of length 5, containing the extreme of the lower whisker, the lower 'hinge', the median,
34 # and the upper 'hinge', the upper whisker.
35 for (i in 1:11){
36   stats <- boxplot.stats(wine_DataFrame[[i]], coef = 1.4)$stats
37   lower_boundry <- stats[1]
38   #print(lower_boundry)
39   upper_boundry <- stats[5]
40   #print(upper_boundry)
41   wine_DataFrame <- wine_DataFrame[!(wine_DataFrame[i] < lower_boundry | wine_DataFrame[i] > upper_boundry),]
42   #str(dataFrame1)
43 }
44
45 #####Visualization of each feature after outlier removal of the data set#####
46 oldpar <- par(mfrow = c(2,6))
47 for (i in 1:11){
48   boxplot(wine_DataFrame[i], main = columnNames[i], col = "#4DB3E6")
49 }
50 par(oldpar)
51
52 #####visualizing how the distribution is looks like after Outlier Removal#####
53 oldpar <- par(mfrow = c(2,6))
54 for (i in 1:11){
55   truehist(wine_DataFrame[[i]], main = columnNames[i], col = blues9)
56   lines(density(wine_DataFrame[[i]]), col= 2, lwd=2)
57 }
58 par(oldpar)
59
60 str(tail(wine_DataFrame))
61
62 ####Normalizing the Data#####
63
64 #define Min-Max normalization function
65 normalization <- function(x) {
66   (x - min(x)) / (max(x) - min(x))
67 }
68
69 #apply Min-Max normalization to first eleven columns in wine data-set.
70 wine_DataFrame_without_quality <- data.frame(lapply(wine_DataFrame[1:11], normalization))
71 str(wine_DataFrame_without_quality)
72 summary(wine_DataFrame_without_quality)
73
74 #combining the quality with the normalized data.
75 quality <- wine_DataFrame$quality
76 wine_DataFrame_norm <- cbind(wine_DataFrame_without_quality, quality)
77 str(wine_DataFrame_norm)
78
79
80 #####Visualization of each feature after Normalization of the data set#####
81 oldpar <- par(mfrow = c(2,6))
82 for (i in 1:11){
83   boxplot(wine_DataFrame_norm[i], main = columnNames[i], col = "#4DC6E6")
84 }
85 par(oldpar)

```

```

94 # Elbow method
95 fviz_nbclust(wine_DataFrame_norm[,-12], kmeans, method = "wss") +
96   geom_vline(xintercept = 4, linetype = 2) +
97   labs(subtitle = "Elbow method")
98
99 # Silhouette method
100 dataFrame3 <- sample_frac(wine_DataFrame_norm, 0.65)
101 str(dataFrame3)
102
103 fviz_nbclust(dataFrame3[,-12], kmeans, method = "silhouette") +
104   labs(subtitle = "Silhouette method")
105
106 # Gap statistic
107 # nboot = 50 to keep the function speedy.
108 # recommended value: nboot= 500 for your analysis.
109 # Use verbose = FALSE to hide computing progression.
110 fviz_nbclust(wine_DataFrame_norm[,-12], kmeans, nstart = 25, method = "gap_stat", nboot = 500) +
111   labs(subtitle = "Gap statistic method")
112
113 # NbClust Method
114 nb <- NbClust(wine_DataFrame_norm[,-12], distance = "euclidean", min.nc = 2,
115   max.nc = 10, method = "kmeans")
116 fviz_nbclust(nb)
117
118 #####K-Means clustering Model#####
119 str(wine_DataFrame_norm)
120 set.seed(5005)
121 KM <- kmeans(wine_DataFrame_norm[,-12], centers = 4, nstart = 25)
122 KM
123 KM$tot.withinss
124 KM$betweenss
125 KM$totss
126
127 #####Visualizing the clustering algorithm results#####
128 str(wine_DataFrame_norm)
129 temp_dataFrame <- wine_DataFrame_norm[,-12]
130 str(temp_dataFrame)
131
132 KM.clusters <- KM$cluster
133 rownames(temp_dataFrame) <- paste(wine_DataFrame_norm$quality, 1:dim(wine_DataFrame_norm)[1], sep = "_")
134 str(temp_dataFrame)
135 tail(temp_dataFrame)
136
137 fviz_cluster(list(data = temp_dataFrame, cluster = KM.clusters))
138
139 #####setting the labels#####
140 wine_dataFrame_labels <- wine_DataFrame_norm$quality
141 table(wine_dataFrame_labels)
142 tail(wine_dataFrame_labels)
143
144 #####to find which cluster is more describing the labels#####
145 table(KM.clusters, wine_dataFrame_labels)
146
147
148
149 #####Confusion matrix #####
150 cluster_wine_DataFrame_norm <- wine_DataFrame_norm
151 str(cluster_wine_DataFrame_norm)
152
153
154 cluster_wine_DataFrame_norm['quality'][cluster_wine_DataFrame_norm['quality'] == 5] <- 1
155 cluster_wine_DataFrame_norm['quality'][cluster_wine_DataFrame_norm['quality'] == 6] <- 3
156 cluster_wine_DataFrame_norm['quality'][cluster_wine_DataFrame_norm['quality'] == 7] <- 2
157 cluster_wine_DataFrame_norm['quality'][cluster_wine_DataFrame_norm['quality'] == 8] <- 4
158
159 head(cluster_wine_DataFrame_norm)
160
161 #add cluster assignment to original data.
162 final_data <- cbind(cluster_wine_DataFrame_norm, cluster = KM$cluster)
163
164 #view final data
165 head(final_data)
166 tail(final_data)
167
168
169 #Creates vectors having data points
170 expected_value <- factor(final_data$quality)
171 predicted_value <- factor(final_data$cluster)
172
173 #Creating confusion matrix
174 confusion_Matrix <- confusionMatrix(predicted_value, expected_value)
175 confusion_Matrix
176
177 ##### PCA #####
178 str(wine_DataFrame)
179 dataFrame1_scale <- as.data.frame(scale(wine_DataFrame[1 : 11]))
180 str(dataFrame1_scale)
181
182 str(wine_DataFrame_norm)

```

```

184 #PCA APPLYING.....
185 PCA_components <- prcomp(~fixed.acidity + volatile.acidity + citric.acid
186                         + residual.sugar + chlorides + free.sulfur.dioxide
187                         + total.sulfur.dioxide + density + pH + sulphates +
188                         alcohol, data = wine_DataFrame_norm,
189                         scale. = T)
190 summary(PCA_components)
191
192 PCA_components$sdev
193
194 VE <- PCA_components$sdev^2
195 PVE <- VE / sum(VE)
196 round(PVE, 2)
197
198 screeplot(PCA_components, type='l', main="Screeplot for principle components")
199
200
201 trnfrm_PCA_components <- as.data.frame(PCA_components$x[,1:8])
202 head(trnfrm_PCA_components)
203
204 #Setting seed
205 set.seed(1600)
206 KM.PCA <- kmeans(trnfrm_PCA_components, centers = 4, nstart = 25)
207 KM.PCA
208 KM.PCA$tot.withinss
209 KM.PCA$betweenss
210 KM.PCA$totss
211
212 ######
213 #visualizing the clustering algorithm results
214 KM.PCA.clusters <- KM.PCA$cluster
215 fviz_cluster(list(data = trnfrm_PCA_components, cluster = KM.PCA.clusters))
216
217 #####

```

Appendix - Energy Forecasting Part Code

(AR) approach

```
1 library(readxl)
2 library(neuralnet)
3 library(Metrics)
4 library(MLmetrics)
5
6
7 DataFrame_days <- read.csv("C:\\\\Users\\\\SEAN\\\\Desktop\\\\MachineLearningandDataMining\\\\MLCW\\\\DataFrame_AR(4).csv")
8 DataFrame_days <- DataFrame_days[-(1)]
9 str(DataFrame_days)
10
11 length_DataFrame_days <- nrow(DataFrame_days)
12 length_DataFrame_days
13
14 columnNumbers <- length(DataFrame_days)
15 columnNumbers
16
17 #Testing Data set with No scale.
18 Data_test_NoScale = DataFrame_days[431:length_DataFrame_days,]
19 str(Data_test_NoScale)
20 head(Data_test_NoScale)
21
22 #Normalizing the Data
23 normalization <- function(x) {
24   (x - min(x))/(max(x) - min(x))
25 }
26
27 #apply Min-Max normalization.
28 DataFrame_days_scale <- data.frame(lapply(DataFrame_days[1:columnNumbers], normalization))
29 head(DataFrame_days_scale)
30
31 #Training Data set
32 Data_train_scale = DataFrame_days_scale[1:430,]
33 str(Data_train_scale)
34
35 #Testing Data set
36 Data_test_scale = DataFrame_days_scale[431:length_DataFrame_days,]
37 str(Data_test_scale)
38 head(Data_test_scale)
39
40
41 #Building the MLP neural network
42 set.seed(4444)
43 nn <- neuralnet(NextDay ~., data = Data_train_scale, hidden = c(9,5),
44   learningrate = 0.0001, act.fct = "logistic",
45   linear.output = TRUE)
46 plot(nn)
47 nn$result.matrix
48
49 #Test the resulting output
50 temp_Data_test_scale <- Data_test_scale[1:columnNumbers-1]
51 head(temp_Data_test_scale)
52 str(temp_Data_test_scale)
53
54 #Prediction using our model
55 nn.results <- compute(nn, temp_Data_test_scale)
56 nn.results$net.result
57
58 #validation
59 results <- data.frame(actual = Data_test_scale$NextDay, prediction = nn.results$net.result)
60 results
61
62 actual = Data_test_NoScale$NextDay
63 head(actual)
64
65 predicted = (results$prediction * (max(Data_test_NoScale$NextDay) - min(Data_test_NoScale$NextDay))) + min(Data_test_NoScale$NextDay)
66 head(predicted)
67 head(Data_test_NoScale$NextDay)
68
69 class(actual)
70 class(predicted)
71
72 #calculate RMSE (Root Mean Square Error)
73 rmse(actual, predicted)
74
75 #calculate MAE (Mean Absolute Error)
76 mae(actual, predicted)
77
78 #calculate MAPE (Mean Absolute Percentage Error)
79 MAPE(predicted, actual)
80
```

(NARX) approach

```
1 library(readxl)
2 library(neuralnet)
3 library(Metrics)
4 library(MLmetrics)
5
6 DataFrame_days <- read.csv("C:\\\\Users\\\\SEAN\\\\Desktop\\\\MachineLearningandDataMining\\\\MLCW\\\\DataFrame_NARX(4).csv")
7 DataFrame_days <- DataFrame_days[-(1)]
8 str(DataFrame_days)
9
10 length_DataFrame_days <- nrow(DataFrame_days)
11 length_DataFrame_days
12
13 columnNumbers <- length(DataFrame_days)
14 columnNumbers
15
16 #Testing Data set with No scale.
17 Data_test_NoScale = DataFrame_days[431:length_DataFrame_days,]
18 str(Data_test_NoScale)
19 head(Data_test_NoScale)
20
21 #Normalizing the Data
22 normalization <- function(x) {
23   (x - min(x))/(max(x) - min(x))
24 }
25
26 #apply Min-Max normalization.
27 DataFrame_days_scale <- data.frame(lapply(DataFrame_days[1:columnNumbers], normalization))
28 head(DataFrame_days_scale)
29
30 #Training Data set
31 Data_train_scale = DataFrame_days_scale[1:430,]
32 str(Data_train_scale)
33
34 #Testing Data set
35 Data_test_scale = DataFrame_days_scale[431:length_DataFrame_days,]
36 str(Data_test_scale)
37 head(Data_test_scale)
38
39
40
41
42
46 #Building the MLP neural network
47 set.seed(4444)
48 nn <- neuralnet(NextDay_11 ~ ., data = Data_train_scale, hidden = c(14,8),
49   learningrate = 0.0001, act.fct = "logistic",
50   linear.output = TRUE)
51 plot(nn)
52 nn$result.matrix
53
54 #Test the resulting output
55 temp_Data_test_scale <- Data_test_scale[1:columnNumbers-1]
56 head(temp_Data_test_scale)
57 str(temp_Data_test_scale)
58
59 #Prediction using our model
60 nn.results <- compute(nn, temp_Data_test_scale)
61 nn.results$net.result
62
63 #validation
64 results <- data.frame(actual = Data_test_scale$NextDay_11, prediction = nn.results$net.result)
65 results
66
67 actual = Data_test_NoScale$NextDay_11
68 head(actual)
69
70 predicted = (results$prediction * (max(Data_test_NoScale$NextDay_11) - min(Data_test_NoScale$NextDay_11))) + min(Data_test_NoScale$NextDay_11)
71 head(predicted)
72 head(Data_test_NoScale$NextDay_11)
73
74 class(actual)
75 class(predicted)
76
77 #validation
78 results <- data.frame(desired_output = actual, predicted_output = predicted)
79 results
80
81 #calculate RMSE (Root Mean Square Error)
82 rmse(actual, predicted)
83
84 #calculate MAE (Mean Absolute Error)
85 mae(actual, predicted)
86
87 #calculate MAPE (Mean Absolute Percentage Error)
88 MAPE(predicted, actual)
89
```