**Informatics Institute of Technology**

**Department of Computing (BSc.) in Computer Science**

**Module: 5DATA001C.2**

**Machine Learning and Data Mining**

**Module Leader: Mr. Achala Aponso**

**Tutorial 1**

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# Clustering Part

With the given problem description, we will be able to perform all tasks whit in below steps.

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## EDA- Get High Level Idea about dataset

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From above figure we will be able to get an idea about the dataset and the data distribution with Min and Max Values and Some Statistical Measures of the Dataset.

There are 4710 total observations and 12 features in this dataset. There is a column called quality which is ordinal variable to represent quality of each red wine sample and it has four qualities such as 5,6,7,8 and in this project, I will map these values to 1,2,3,4 and it will be help in next stages.

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Missing Values!

Graphical user interface, text

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There are not any missing values that we have to deal with in this dataset.

Chart, scatter chart

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By using this figure, we can see alcohol level is the most correlated feature for the Quality.

## Outlier Removal and Feature Scaling - Preprocessing

**Outlier Removal**

Outlier is a silent killer, an observation that is numerically distant from the rest of the data or in a simple word it is the value which is out of the range.

Reasons for outliers,

\* Data Entry Errors: - Human errors such as errors caused during data collection, recording, or entry can cause outliers in data.

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\* Measurement Error: - It is the most common source of outliers. This is caused when the measurement instrument used turns out to be faulty.

\* Natural Outlier: - When an outlier is not artificial (due to error), it is a natural outlier. Most of real-world data belong to this category.

For detect outliers we can use different techniques such as Hypothesis Testing, Z-score methos, Isolation Forest and Visualizing the Data. In this Project We use Z-score Method.

**IQR method**

Diagram

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Figure 1 : IQR method

Any Value which is -1.5\*IQR > x or 1.5\*IQR > x treated as outliers.

\* Q1 represents the 1st quartile/25th percentile of the data.

\* Q2 represents the 2nd quartile/median/50th percentile of the data.

\* Q3 represents the 3rd quartile/75th percentile of the data.

\* (Q1–1.5\*IQR) represent the smallest value in the data set and (Q3+1.5\*IQR) represent the largest value in the data set.

**Z-Score Method**

Using this method, we will be able to find how many Slandered Deviations value away from the mean.

Chart, histogram

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Figure shows area under normal curve and how much area that standard deviation covers.

\* 68% of the data points lie between + or - 1 standard deviation.

\* 95% of the data points lie between + or - 2 standard deviation

\* 99.7% of the data points lie between + or - 3 standard deviation

By experimenting above mentioned IQR method I experienced most of the data points are eliminated with IQR method. Because of that reason we are using Z-score method to Scale and Remove Outliers in this Dataset.

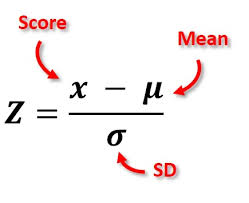


Figure : z-score formula

A screenshot of a computer screen

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Figure : applying z-score normalization

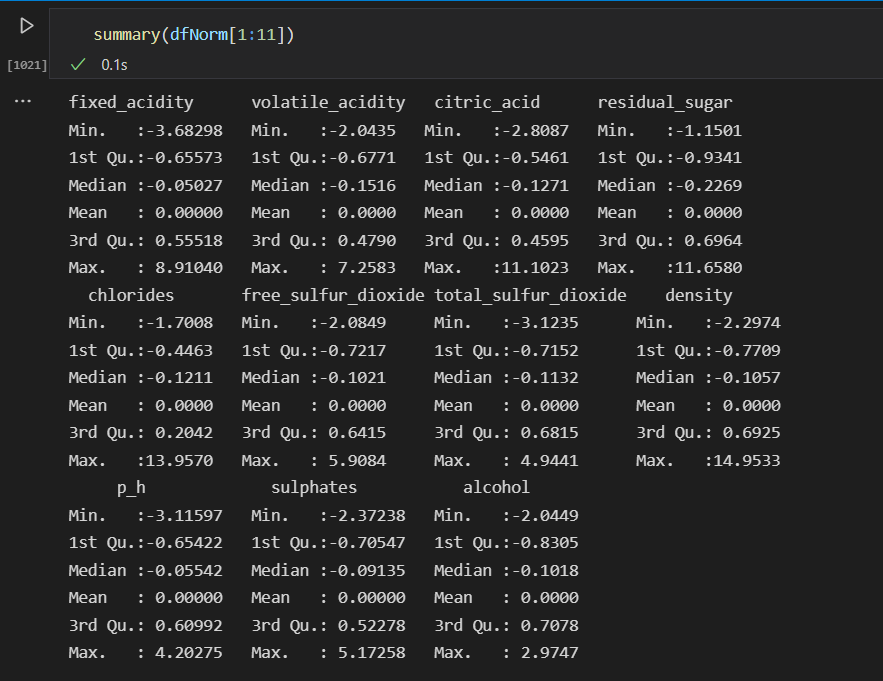


Figure : summary of normalized data frame

Eliminating all outliers using z-score,

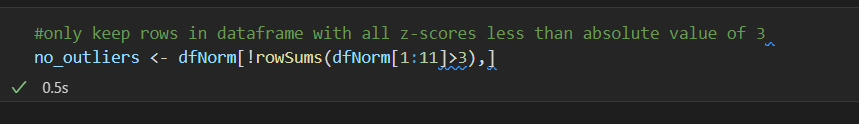


Figure : eliminating outliers

Below figure shows a summary of final dataset after scaling and outlier removal.

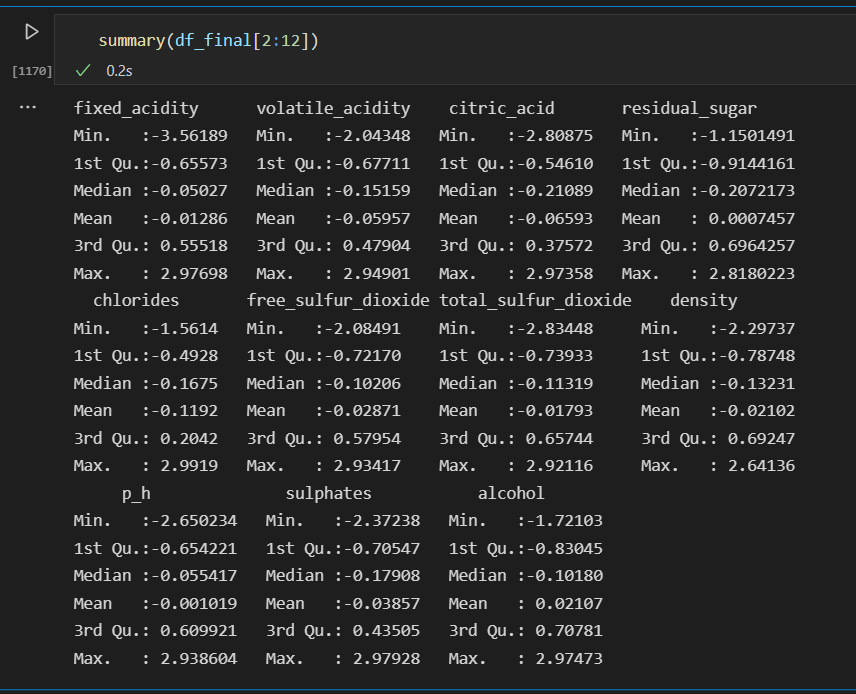
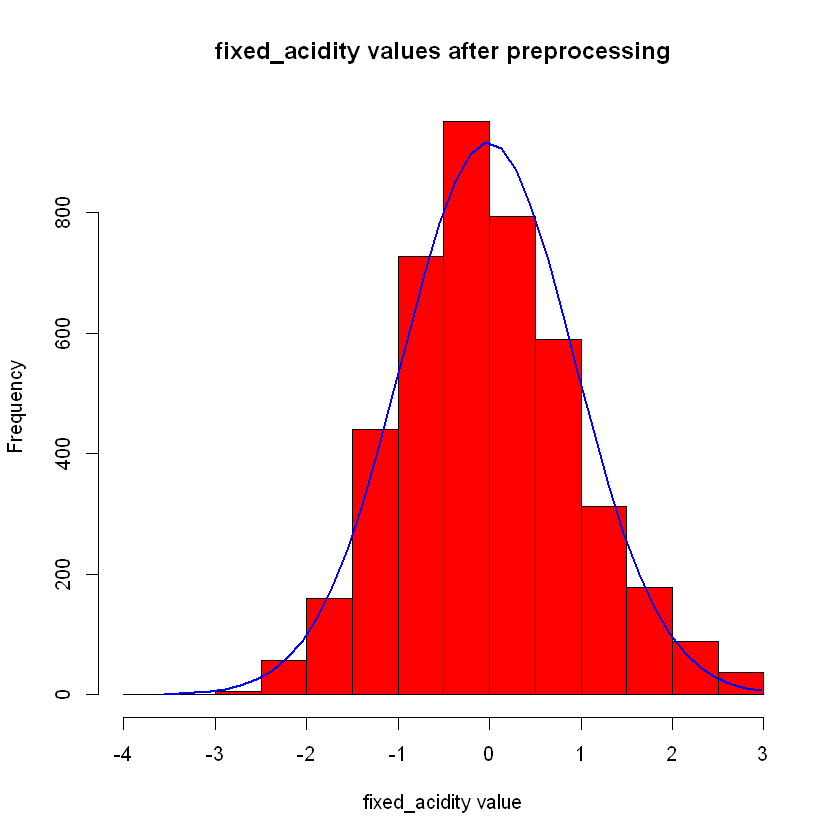
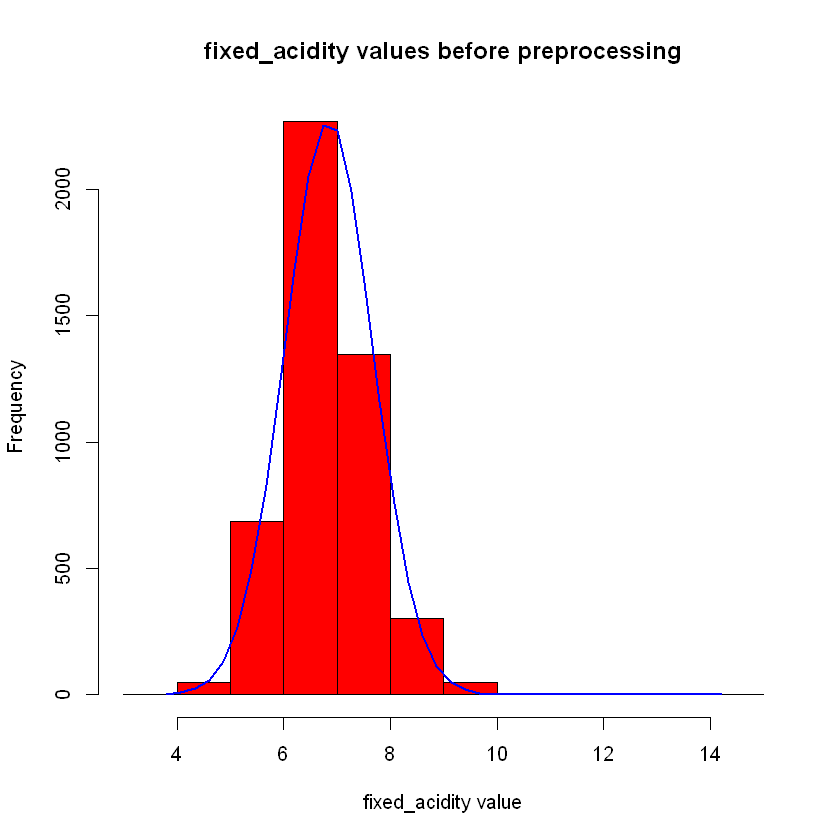
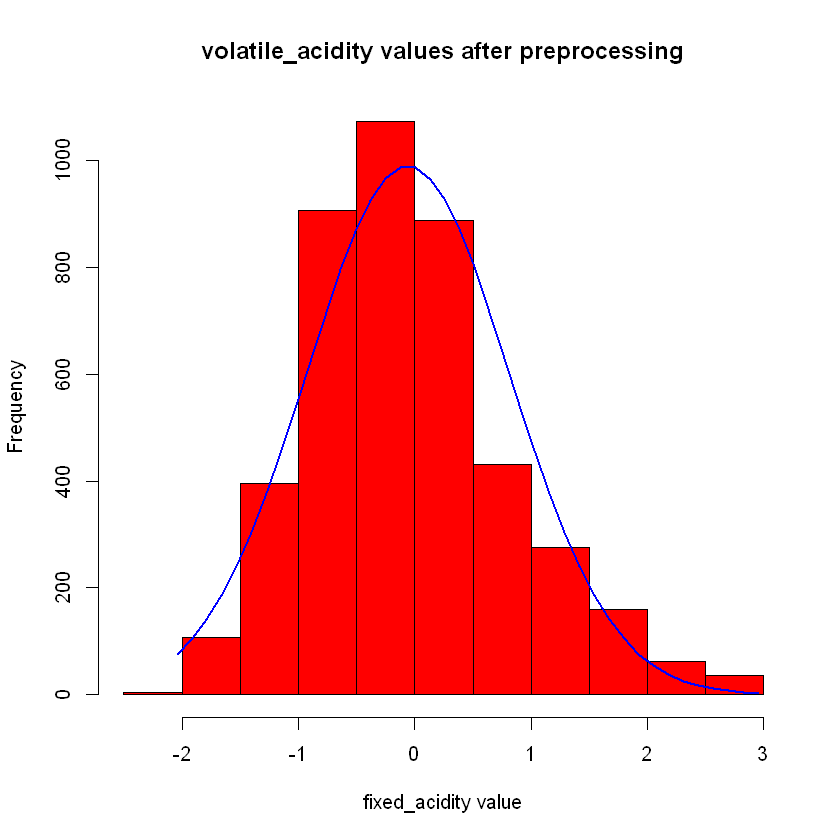
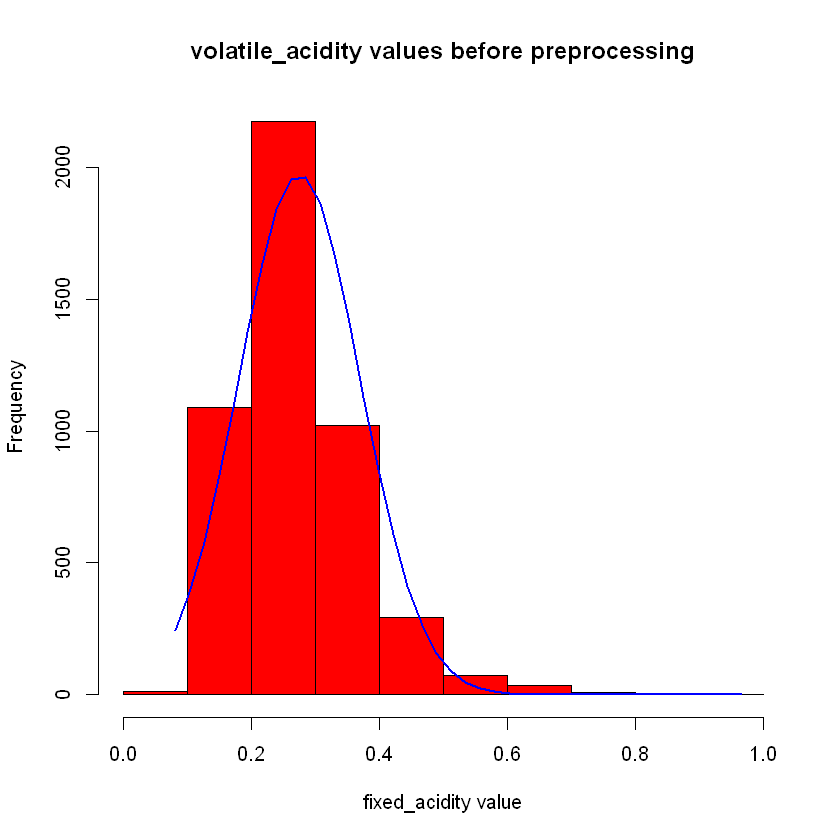
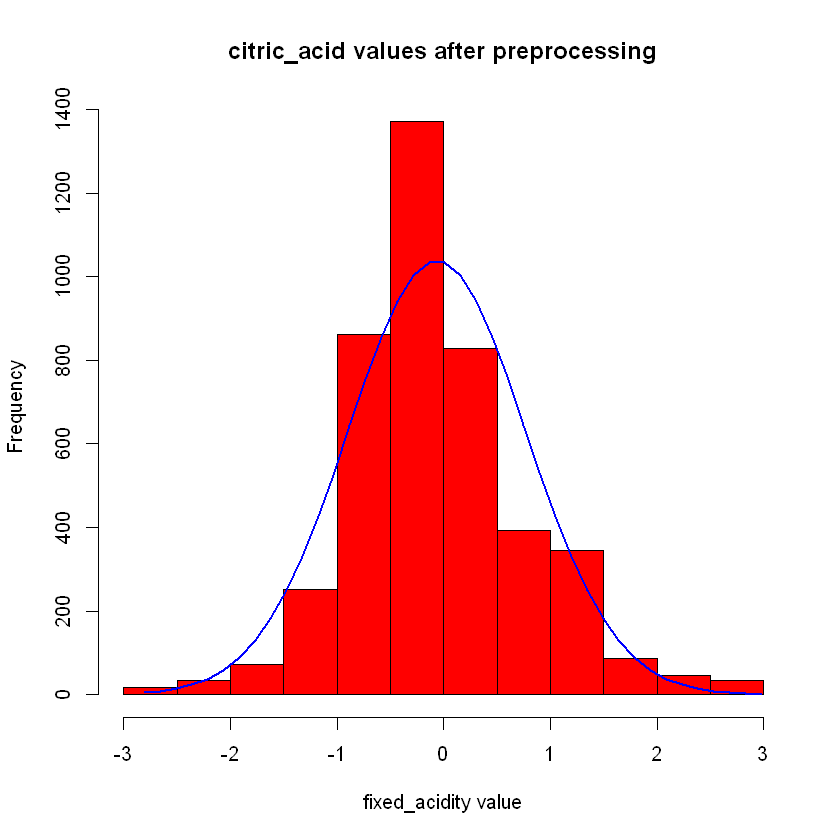
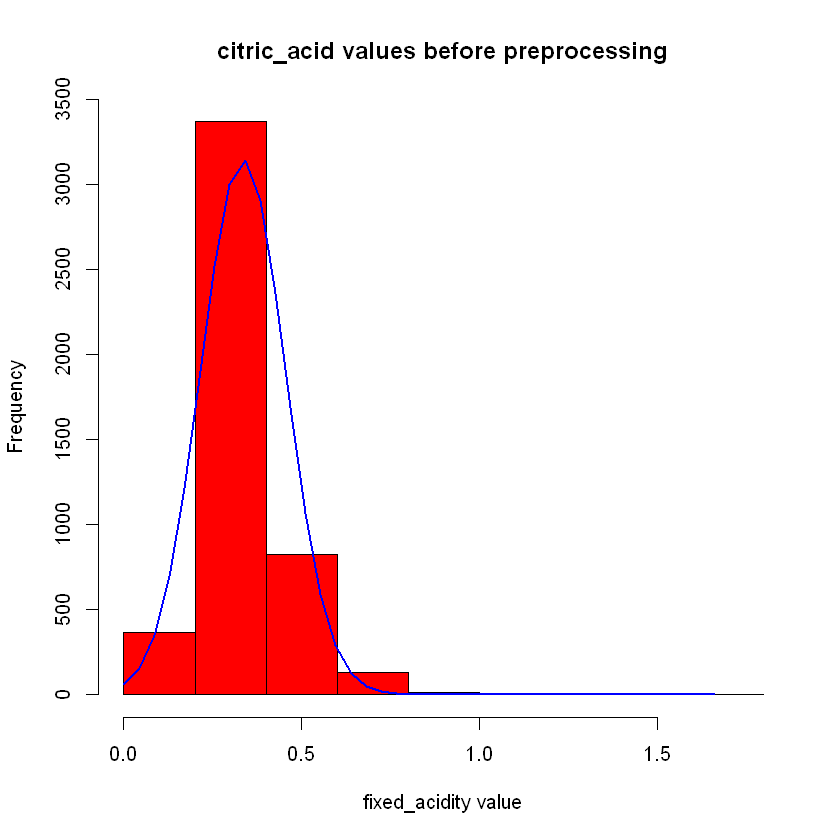
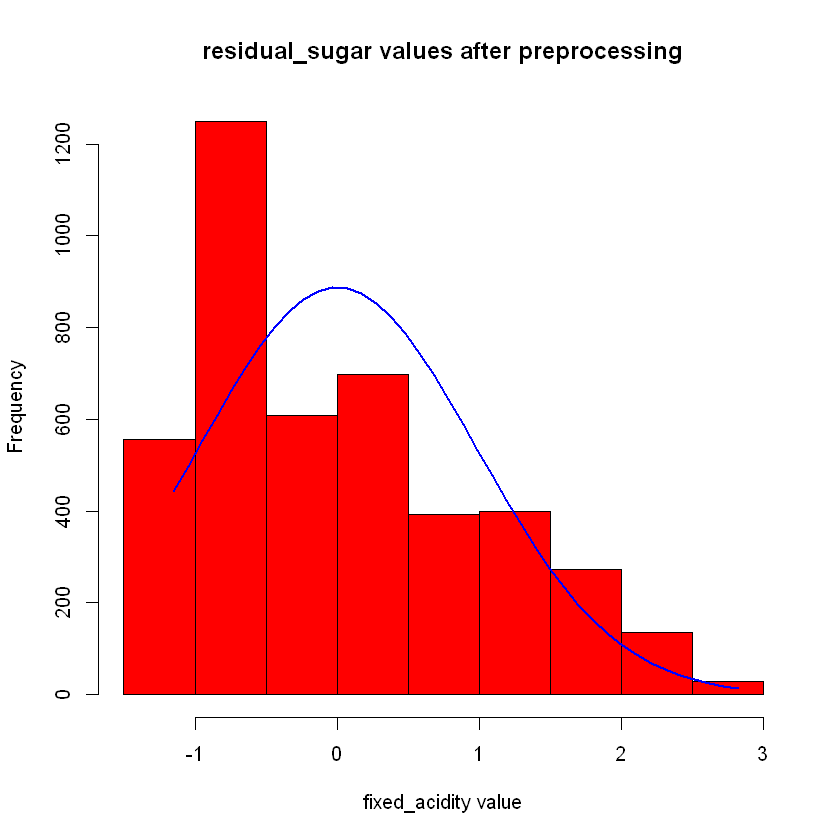
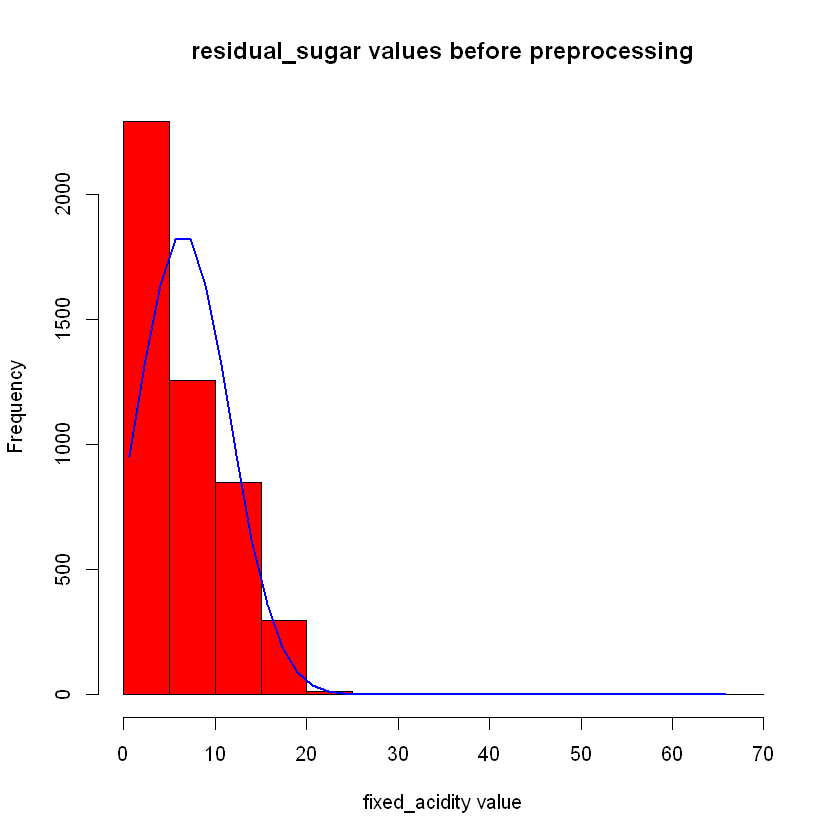


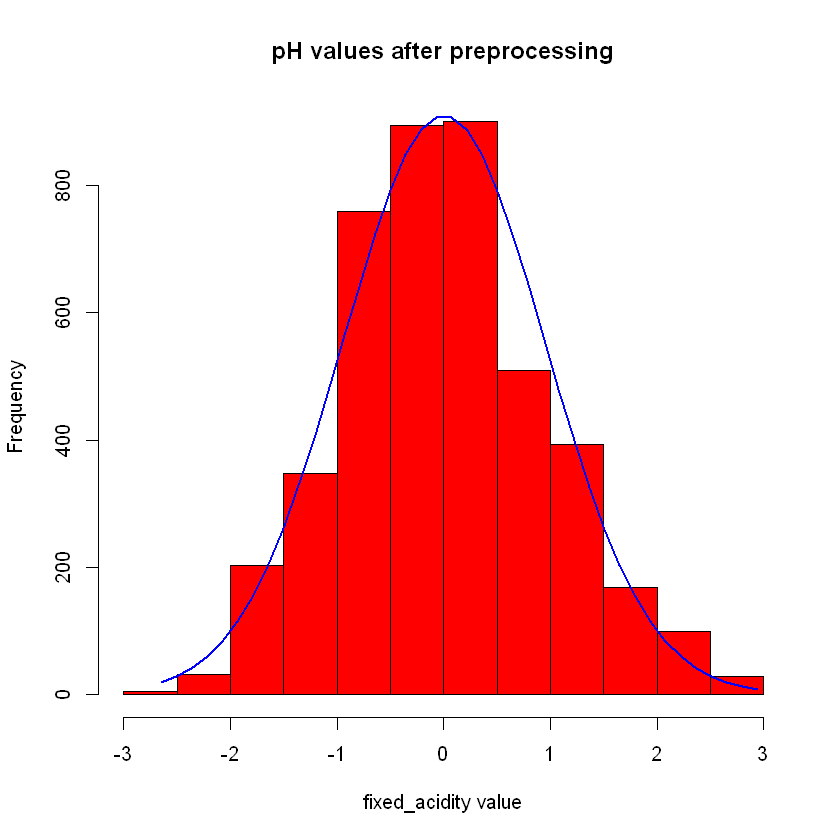
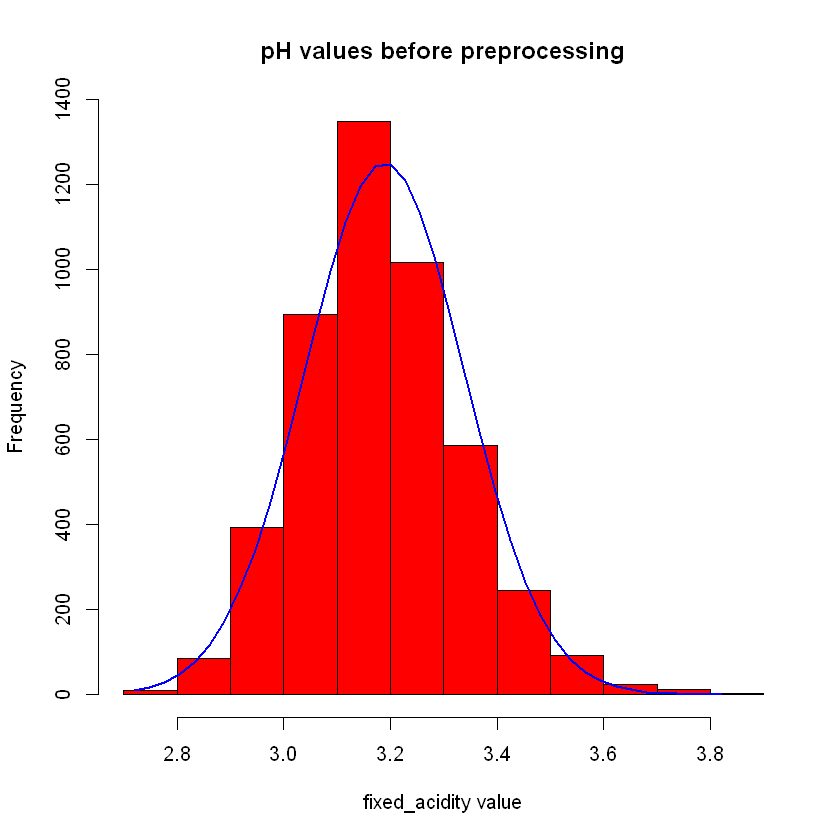
Figure : summary of scaled and outlier removed data frame

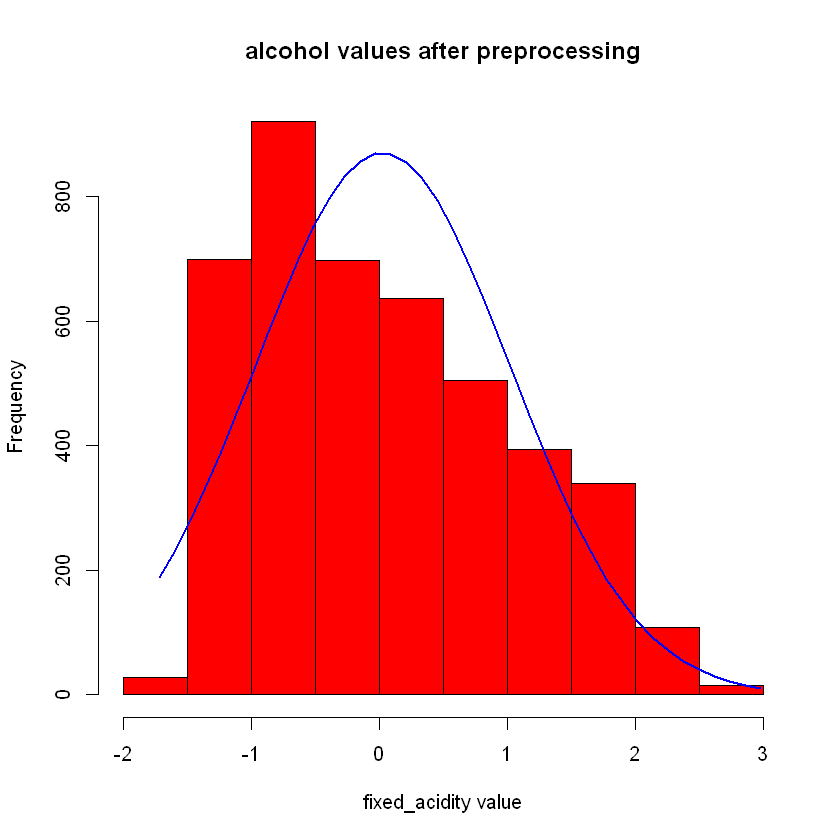
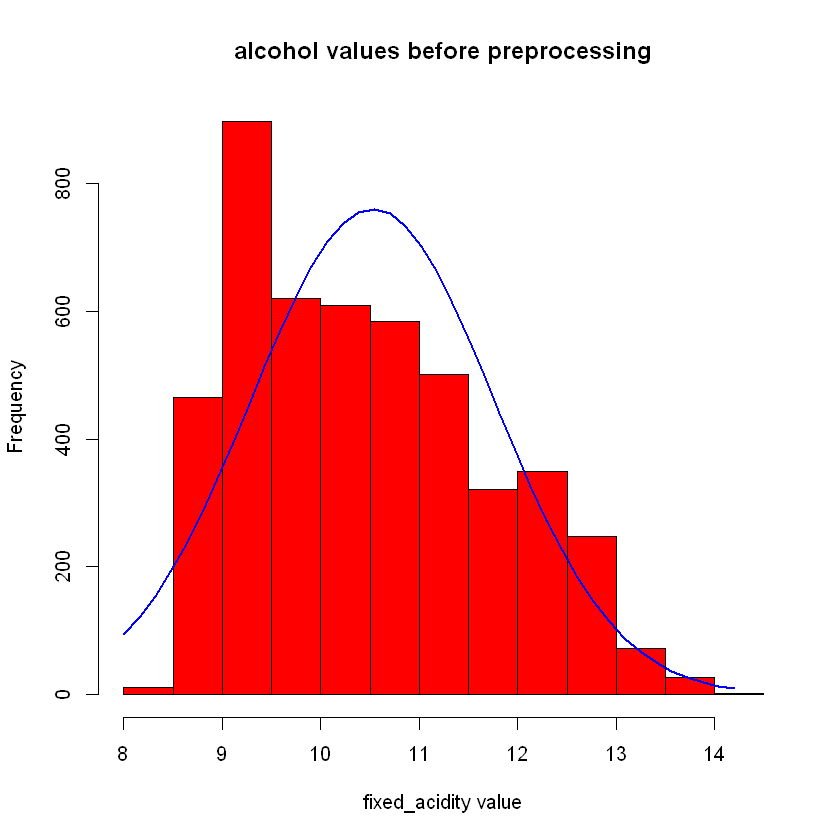




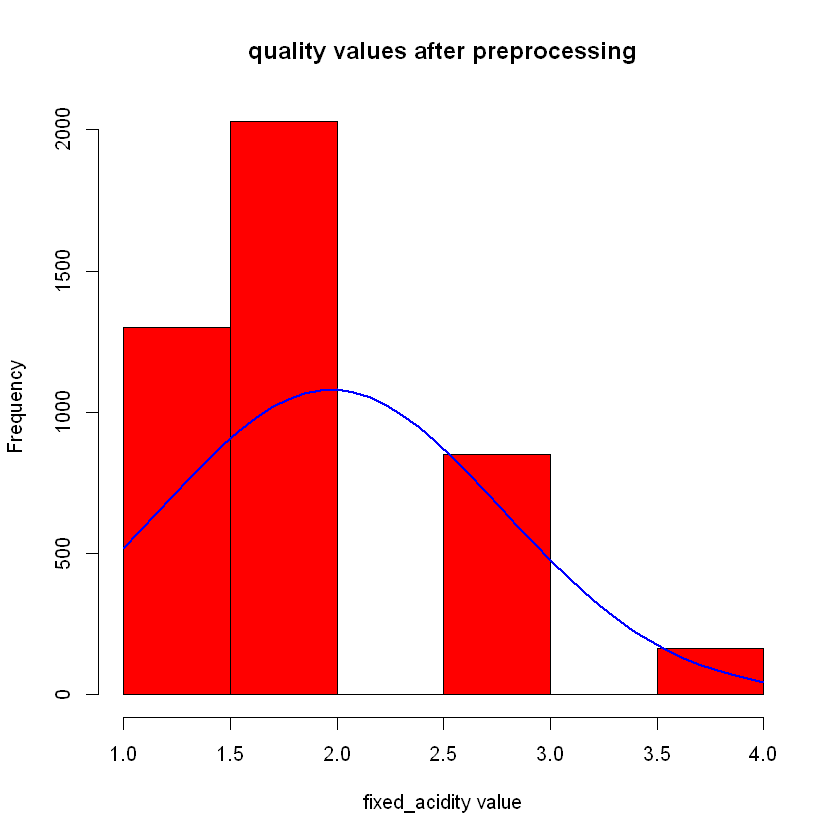
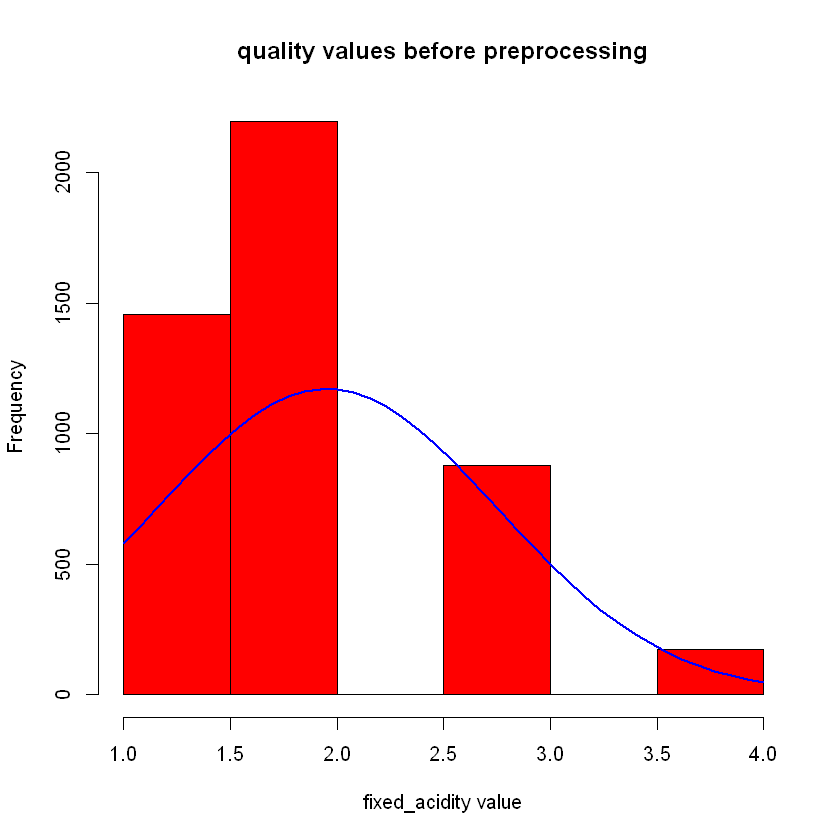








From below figure we will be able to figure it out it doesn’t affect to Quality feature distribution to Scale and the Outlier removal task.



Scaling and outlier removal is very important task when doing ML use case, it will be helpful to increase performance and the accuracy of the Machine Learning Model.

## Define the number of cluster centers

**Manual Method**

This red wine dataset originally consisted with 1-10 range qualities but in this dataset, we will be able to detect 4 qualities which are 5,6,7 and 8. So there will be four clusters in this data frame and further clarification we must process with different methods and techniques to evaluate number of clusters in this red wine dataset.

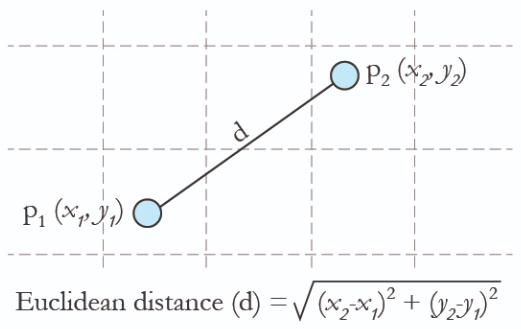
**Automated Methods**

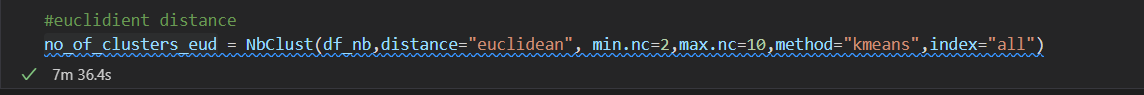
**1.NBclust**

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**i. Euclidian Distance**





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Chart, line chart, histogram

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**ii. Manhattan Distance**

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**2.Elbow Method**

**A screenshot of a computer

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In below figure k value is initializing 1 to 10 and it will calculate the “WSS” (With in cluster Sum of Square) and return. We need to plot this output to get a better idea about that. This elbow point is the optimal cluster value of k. in below figure it is k=4

Chart, line chart, histogram

Description automatically generated

**3.Silhouette Method**

This will calculate average Silhouette with each k value and display the optimal solution.

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Chart, line chart

Description automatically generated

Above figure silhouette method returned optimal number of clusters as 2.

As above mentioned, automated tools most of the tools suggested k=2 for optimal clustering and elbow method suggest k=4, from this idea and as form the instructions given in the problem we will perform k-means clustering from k=2, k=3 and k=4 in next chapter and evaluate each clusters using BSS/TSS and confusion matrix.

## K-means Clustering

From above chapter we discussed some automated and manual methods to select optimal cluster amount for k-means algorithm, in this chapter we will experimenting k=2, k=3 and k=4 as number of clusters and evaluate which is the “winning” clustering approach.

To evaluate this process, we use WSS (Between cluster Sums of Square) over TSS (Total cluster Sums of Square) and Confusion Metrix calculations such as accuracy/precision and recall.



Figure : confusion matrix

**K=2**

A picture containing graphical user interface

Description automatically generated

For further analysis we will divide data frame into x and y, x: all numerical features / y: quality.

Graphical user interface, application

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Above figure shows executing k-means inbuilt function in r with data and number of clusters. Then we will see the results.

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Then we will be able to create confusion matrix, below figure shows the confusion matrix,

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Then we visualize this result with the help of visualization libraries.

Chart, scatter chart

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**K=3**

Graphical user interface, application

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Graphical user interface, text

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Chart, scatter chart

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**K=4**

Graphical user interface, application

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Chart

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Visualizing all together,

Scatter chart

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**Compression Table**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Cluster amount | BSS/TSS | Accuracy | Recall/Sensitivity | Specificity |
| k=2 | 24.9% | 45.69% | class1:56.04% class2:61.86% | class1:68.68% class2:39.23% |
| k=3 | 32.0% | 40.53% | class1:53.12% class2:31.38% class3:50.88% | class1:70.85% class2:70.11% class3:71.24% |
| k=4 | 36.7% | 34.59% | class1:48.65% class2:24.04% class3:41.12%  class4:19.75% | class1:74.95% class2:77.16% class3:84.96%  class4:75.45% |

**Define “winning” cluster**

From above automated tools form previous chapter gives most optimal cluster is k=2 and after experimenting with different k values form this chapter, we will be able to see accuracy was changing time to time when executing the code with different times, but BSS/TSS percentage didn’t changed. For considering about BSS/TSS percentage reflect good fit of the clusters. The highest BSS/TSS percentage is k=4 and good to have as 4 clusters because we are dealing with some quality factor and if we consider as k=2 there are lots of different variations of wine samples may be together as same cluster. Because of those reasons I will consider k=4 is the “winning” cluster for this dataset and clustering is subjective and it can be use as different purposes.

**Evaluation Metrics,**

After we are doing Machine Learning Task, we must evaluate our results, so for that reason we use some evaluation metrics,



When we have labeled dataset to perform our task after the prediction, we will be able to define above matrix this is call confusion matrix,

**True Positives**: these values correctly predicted positive by model and actual class of predicted value is also yes

**True Negatives**: these values correctly predicted negative by model and actual class of predicted value is also no

**False Positives**: when actual class is no, and predicted class is yes

**False Negative**: when actual class in yes, and predicted class is no

Accuracy:

Accuracy is the most common performance measure, and it is simply a ratio of correctly predicted values vs total observations.

Table

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Precision:

Ratio of correctly predicted positive values to the total predicted positive observations

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Recall (Sensitivity):

Ratio of correctly predicted positive observations to all observation in actual class.

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## Dimensionality Reduction (PCA)

In this chapter we will reduce the intentionality of our dataset and evaluate which features are mostly affect to the quality of the wine sample and perform k-means “winning” clustering number for new dataset which is reduced dimensionality by using PCA.

Graphical user interface, text

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Above figure shows the dataset used for PCA analysis and the PCA function with numerical features.

Graphical user interface, text

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Graphical user interface, text

Description automatically generated with medium confidence

Below figure shows summary details of principle components in our data frame

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Chart, line chart

Description automatically generatedChart, histogram

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We can pot PCA’s to get some idea about it, but it’s difficult to get exact idea about that because we are plotting 2d graph and this PCA’s in various 12 dimensions.

Chart, scatter chart

Description automatically generated

Changing the Scale,

Chart, scatter chart

Description automatically generated

Merging new columns with data frame,

A screenshot of a computer screen

Description automatically generated with medium confidence

Plotting cumulative score > 96% features (PC9, PC10,PC11),

Chart, scatter chart

Description automatically generated

**K-means Clustering**

Graphical user interface, application

Description automatically generated

Above figure shows getting data and labels to do clustering and perform clustering with k=4

A picture containing background pattern

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We can see BSS/TSS is improved than previous chapter and it tells this clusters are fitted well.

Chart, scatter chart

Description automatically generated

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Description automatically generated with medium confidence

Text

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In previous chapter we perform k-means clustering with the original features of the dataset and at ‘winning” cluster value we got BSS/TSS as 36.7% then after we performed PCA to reduce the dimensionality of the dataset and we was able to reduce the dimension of the dataset. Them after we performed k-means clustering and got BSS/TSS=60.6% so we can see in 2nd stage we got more fitted clusters with the new dataset after clustering, while k-means is an unsupervised machine learning algorithm and reduce the dimensionality of the dataset affected to the improvement of the machine learning algorithm’s performance.

**Conclusion**

When we are dealing with Machine Learning first, we must clean the dataset and must do some preprocessing before dealing with machine learning. Then it will be very important to increase the performance of the Machine Learning model and after the machine learning stage we need to evaluate our outputs with some methods. Following these steps in sequency help to smooth the machine learning journey.

# Time Series Forecasting