FINAL ASSIGNMENT

May 13, 2020

0.0.1 Team Members:

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0.0.2 INTRODUCTION

The goal of this assignment is to predict the number of wine cases that are sold based on some chemical properties of the wine. This is done by exploring the various features in the dataset, cleaning the data and employing some analytical tools and techniques to develop models. The model that will best predict the wine sales is chosen.

0.0.3 The work is carried out in different stages.

1) Data Exploration - Data is cleaned, scaled and analyzed
2) Data Preparation - Analyzing correlation between wine properties & deciding the ones that contribute the most towards sales
3) Building Models - Developing different models to best predict the wine sales based on properties
4) Model Selection - Selecting the model with least error and low implementation cost

0.0.4 Initial observations:

- The categorical features, STARS and LabelAppeal seem to vary proportionally with TARGET over the entire range
- STARS : seems to be logically the most valuable variable for indicating desire for purchase. 4 Stars = Excellent, 1 Star = Poor A high number of STARS suggests high sales (TARGET).
- LabelAppeal : Marketing Score indicating the appeal of label design for consumers High numbers suggest customers like the label design Higher numbers suggest better sales

[56]:
```
# Import the required functionality
import numpy as np
import pandas as pd
import matplotlib.pylab as plt
from sklearn import preprocessing
from sklearn.model_selection import train_test_split
```

```
import seaborn as sns

%matplotlib inline

from sklearn.impute import KNNImputer
from sklearn.decomposition import PCA  #principal components Analysis
from sklearn.cluster import KMeans  # clustering
from sklearn.metrics import silhouette_score #evaluation metric for # of␣
 ↪clusters
from adjustText import adjust_text  #pip install adjustText
from sklearn.model_selection import cross_val_predict

from pandas.plotting import scatter_matrix
from sklearn.neural_network import MLPClassifier

from sklearn import neighbors
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error   #RMSE

from sklearn.neighbors import KNeighborsRegressor
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor

from sklearn.ensemble import AdaBoostRegressor
from sklearn.ensemble import BaggingRegressor

from sklearn.neural_network import MLPRegressor

from sklearn.linear_model import LinearRegression,Lasso, Ridge,RidgeCV, LassoCV
from sklearn.model_selection import GridSearchCV
from dmba import plotDecisionTree
import pydotplus
from sklearn import tree
import pydot
import graphviz
import math
import itertools

import warnings
warnings.filterwarnings('ignore')
```

1. DATA EXPLORATION

[57]:
```
df = pd.read_csv('WINE_.csv')
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 12795 entries, 0 to 12794
```

```
Data columns (total 16 columns):
 #   Column               Non-Null Count  Dtype
---  ------               --------------  -----
 0   INDEX                12795 non-null  int64
 1   TARGET               12795 non-null  int64
 2   FixedAcidity         12795 non-null  float64
 3   VolatileAcidity      12795 non-null  float64
 4   CitricAcid           12795 non-null  float64
 5   ResidualSugar        12179 non-null  float64
 6   Chlorides            12157 non-null  float64
 7   FreeSulfurDioxide    12148 non-null  float64
 8   TotalSulfurDioxide   12113 non-null  float64
 9   Density              12795 non-null  float64
 10  pH                   12400 non-null  float64
 11  Sulphates            11585 non-null  float64
 12  Alcohol              12142 non-null  float64
 13  LabelAppeal          12795 non-null  int64
 14  AcidIndex            12795 non-null  int64
 15  STARS                9436 non-null   float64
dtypes: float64(12), int64(4)
memory usage: 1.6 MB
```

A priliminary scan of the data indicates a lot of missing values for the features.

The STARS feature in particular has 26.25% of data missing

[4]:
```
for x in ['TARGET','LabelAppeal','STARS']:
    print(df[x].value_counts().shape)
```

```
(9,)
(5,)
(4,)
```

5 different types of Label Appeal values and 4 types of STAR ratings for the data

Lower STAR rating results in lesser number of wine TARGETS being sampled. Hence, the missing values can be imputed as 0 for STAR

[5]:
```
# Mean, SD and Min-MAx of all the features

df.describe()
```

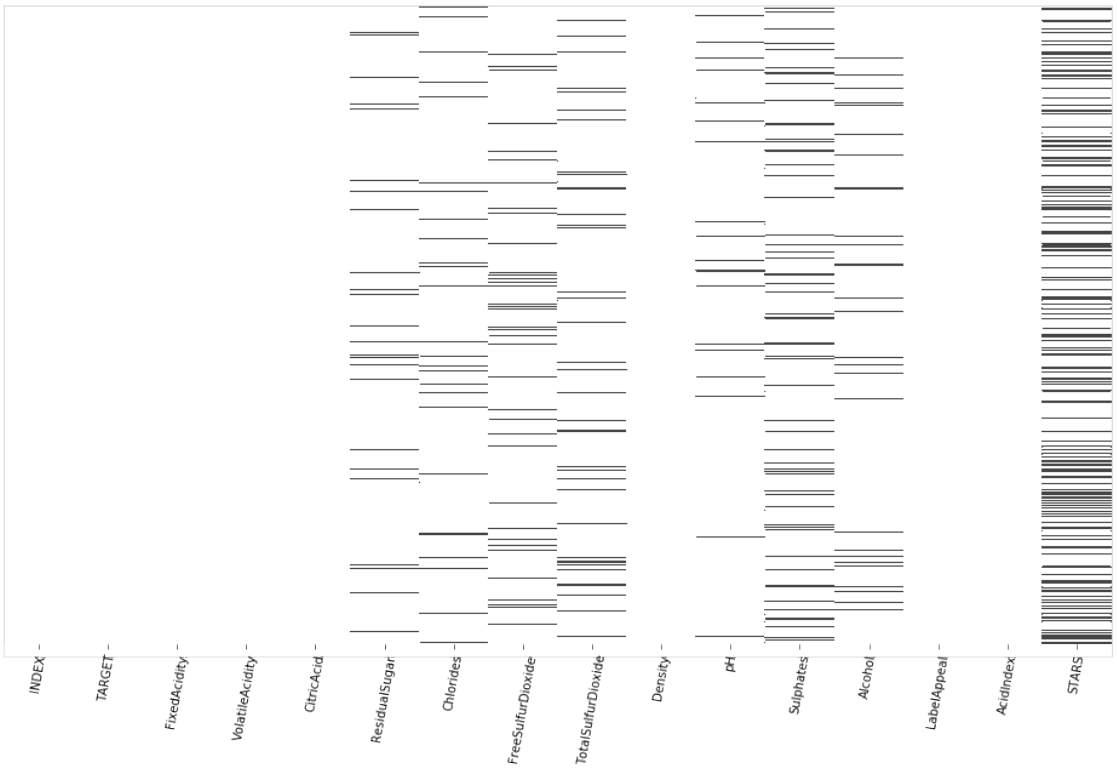
[5]:

	INDEX	TARGET	FixedAcidity	VolatileAcidity	\
count	12795.000000	12795.000000	12795.000000	12795.000000	
mean	8069.980305	3.029074	7.075717	0.324104	
std	4656.905107	1.926368	6.317643	0.784014	
min	1.000000	0.000000	-18.100000	-2.790000	
25%	4037.500000	2.000000	5.200000	0.130000	
50%	8110.000000	3.000000	6.900000	0.280000	
75%	12106.500000	4.000000	9.500000	0.640000	

```
max    16129.000000      8.000000     34.400000         3.680000

         CitricAcid  ResidualSugar     Chlorides  FreeSulfurDioxide  \
count  12795.000000   12179.000000  12157.000000       12148.000000
mean       0.308413       5.418733      0.054822          30.845571
std        0.862080      33.749379      0.318467         148.714558
min       -3.240000    -127.800000     -1.171000        -555.000000
25%        0.030000      -2.000000     -0.031000           0.000000
50%        0.310000       3.900000      0.046000          30.000000
75%        0.580000      15.900000      0.153000          70.000000
max        3.860000     141.150000      1.351000         623.000000

       TotalSulfurDioxide       Density            pH     Sulphates  \
count        12113.000000  12795.000000  12400.000000  11585.000000
mean           120.714233      0.994203      3.207628      0.527112
std            231.913211      0.026538      0.679687      0.932129
min           -823.000000      0.888090      0.480000     -3.130000
25%             27.000000      0.987720      2.960000      0.280000
50%            123.000000      0.994490      3.200000      0.500000
75%            208.000000      1.000515      3.470000      0.860000
max           1057.000000      1.099240      6.130000      4.240000

            Alcohol   LabelAppeal     AcidIndex        STARS
count  12142.000000  12795.000000  12795.000000  9436.000000
mean      10.489236     -0.009066      7.772724     2.041755
std        3.727819      0.891089      1.323926     0.902540
min       -4.700000     -2.000000      4.000000     1.000000
25%        9.000000     -1.000000      7.000000     1.000000
50%       10.400000      0.000000      8.000000     2.000000
75%       12.400000      1.000000      8.000000     3.000000
max       26.500000      2.000000     17.000000     4.000000
```

[6]:
```
# Exploring data for missing values using HeatMap

naInfo = np.zeros(df.shape)
naInfo[df.isna().values] = 1
naInfo = pd.DataFrame(naInfo, columns=df.columns)

fig, ax = plt.subplots()
fig.set_size_inches(13, 9)
ax = sns.heatmap(naInfo, vmin=0, vmax=1, cmap=["white", "#444444"], cbar=False,␣
 ↪ax=ax)
ax.set_yticks([])

rect = plt.Rectangle((0, 0), naInfo.shape[1], naInfo.shape[0], linewidth=1,
                     edgecolor='lightgrey',facecolor='none')
rect = ax.add_patch(rect)
```

```
rect.set_clip_on(False)

plt.xticks(rotation=80)
plt.tight_layout()
plt.show()
```



The above heatmap indicates missing values in every column/feature with a '_____'

[7]:
```
# Counting the missing values in the data

print(df.isnull().sum())
```

```
INDEX                 0
TARGET                0
FixedAcidity          0
VolatileAcidity       0
CitricAcid            0
ResidualSugar       616
Chlorides           638
FreeSulfurDioxide   647
TotalSulfurDioxide  682
Density               0
pH                  395
```

```
Sulphates             1210
Alcohol                653
LabelAppeal              0
AcidIndex                0
STARS                 3359
dtype: int64
```

[8]:
```
# Imputing missing values in STAR column with 0s

df['STARS'] = df['STARS'].fillna(0)
```

[88]:
```
# Scaling the data using MinMax scaler

scaler = preprocessing.MinMaxScaler()
scaled_data = pd.DataFrame(scaler.fit_transform(df), index=df.index, columns=df.
 ↪columns)
scaled_data.head()
```

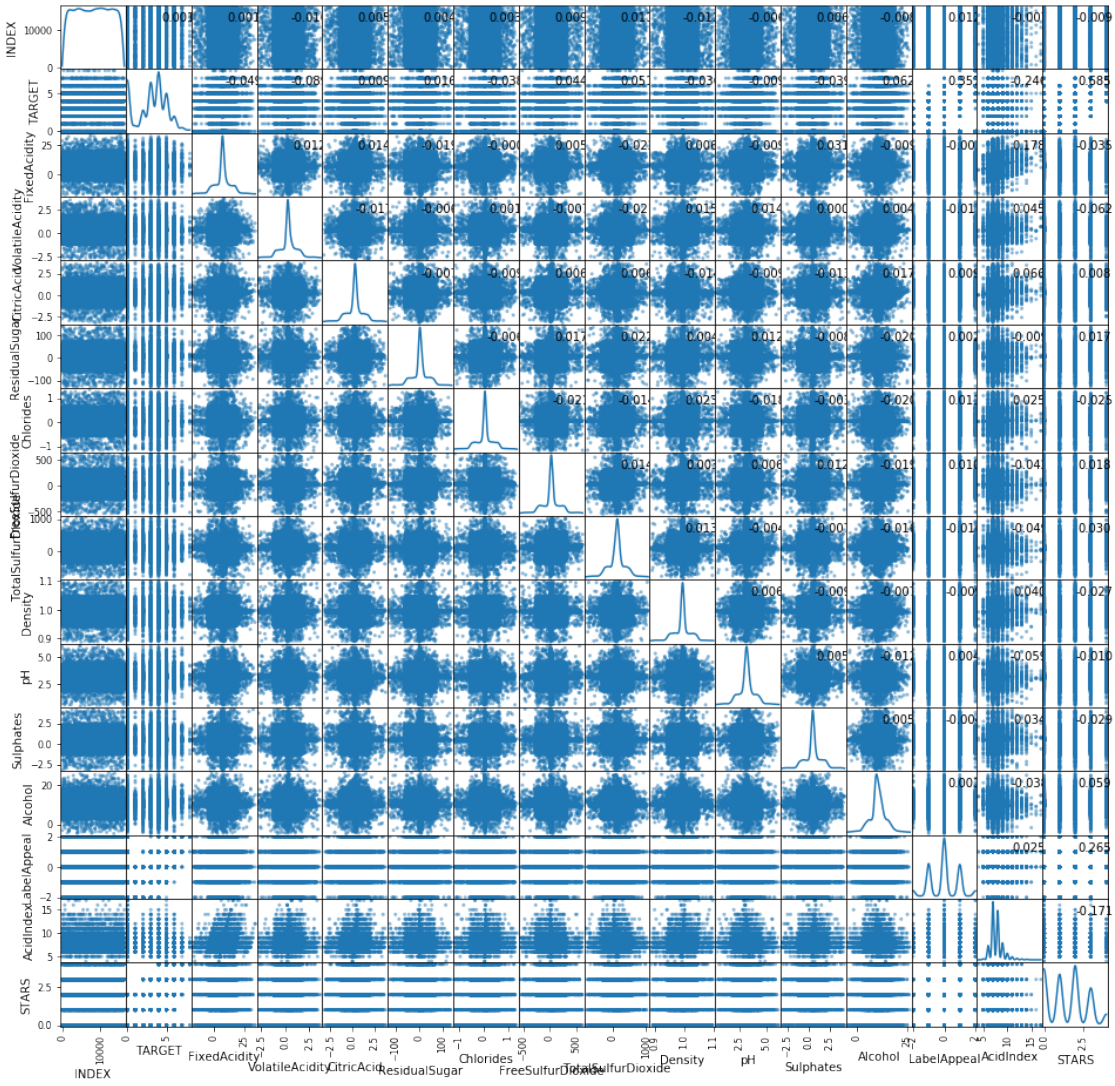
[88]:

	INDEX	TARGET	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	\
0	0.000000	0.375	0.405714	0.610510	0.318310	0.676706	
1	0.000062	0.375	0.430476	0.455951	0.342254	0.572225	
2	0.000186	0.625	0.480000	0.839258	0.332394	0.530210	
3	0.000248	0.375	0.453333	0.490726	0.461972	0.545083	
4	0.000310	0.500	0.497143	0.482226	0.278873	0.510132	

	Chlorides	FreeSulfurDioxide	TotalSulfurDioxide	Density	pH	\
0	0.239492	NaN	0.580319	0.495903	0.504425	
1	0.295797	0.483871	0.263830	0.662231	0.513274	
2	0.478985	0.652801	0.513298	0.507175	0.467257	
3	0.295797	0.489813	0.498936	0.512953	0.311504	
4	NaN	0.329372	0.495213	0.504286	0.467257	

	Sulphates	Alcohol	LabelAppeal	AcidIndex	STARS
0	0.344640	0.467949	0.50	0.307692	0.333333
1	0.519674	NaN	0.25	0.230769	0.666667
2	0.489824	0.855769	0.25	0.307692	0.666667
3	0.672999	0.349359	0.25	0.153846	0.000000
4	0.664858	0.589744	0.50	0.384615	0.333333

[10]:
```
# Scatter Plot

axes = scatter_matrix(df, alpha=0.5, diagonal='kde',figsize=(16, 16))
corr = scaled_data.corr().values
for i, j in zip(*plt.np.triu_indices_from(axes, k=1)):
    axes[i, j].annotate("%.3f" %corr[i,j], (0.8, 0.8), xycoords='axes␣
 ↪fraction', ha='center', va='center')
plt.show()
```



The Scatter plots indicate that lower Label Appeal implies lesser number of TARGET samples.

The plot of TARGEt vs STARS show greater the STAR rating, higher the number of TARGET samples sold

The scatter plots also indicate that there is no correlation between features like Ciric Acid, Acid content, Fixed Acidity etc.

The plots do not show any outlier for the features

[11]:
```
scaled_data.corr()
```

[11]:

	INDEX	TARGET	FixedAcidity	VolatileAcidity	\
INDEX	1.000000	0.001256	0.001133	-0.010224	
TARGET	0.001256	1.000000	-0.049011	-0.088793	
FixedAcidity	0.001133	-0.049011	1.000000	0.012375	

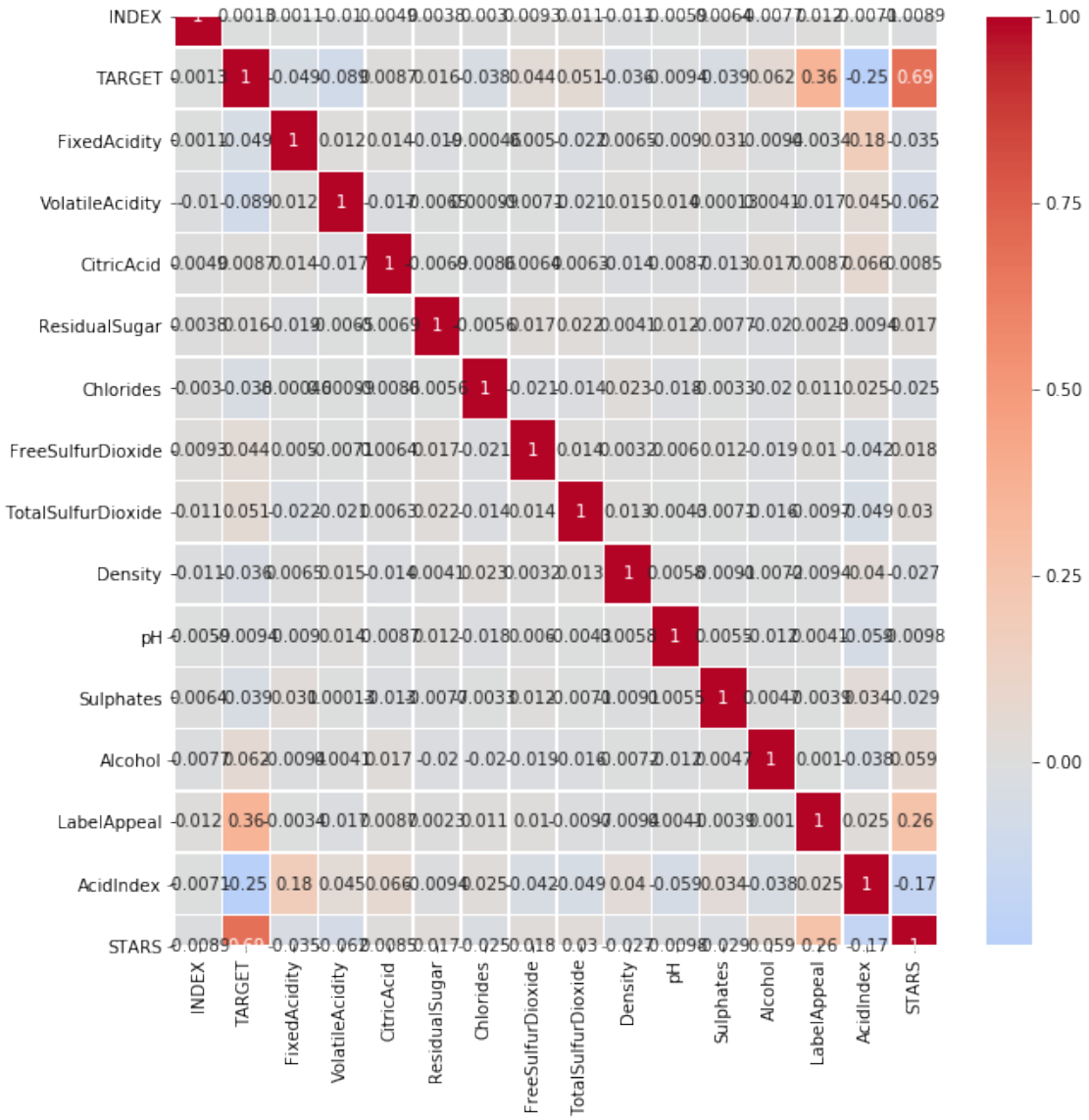
```
VolatileAcidity    -0.010224 -0.088793      0.012375         1.000000
CitricAcid          0.004922  0.008685      0.014240        -0.016953
ResidualSugar       0.003846  0.016491     -0.018855        -0.006483
Chlorides           0.002966 -0.038263     -0.000457         0.000987
FreeSulfurDioxide   0.009257  0.043824      0.004972        -0.007077
TotalSulfurDioxide  0.010756  0.051478     -0.022498        -0.021080
Density            -0.010779 -0.035518      0.006477         0.014735
pH                 -0.005853 -0.009445     -0.008983         0.013592
Sulphates           0.006413 -0.038850      0.030783         0.000129
Alcohol            -0.007677  0.062062     -0.009371         0.004073
LabelAppeal         0.011553  0.356500     -0.003366        -0.016987
AcidIndex          -0.007097 -0.246049      0.178437         0.044642
STARS              -0.008883  0.685381     -0.035416        -0.062276

                    CitricAcid  ResidualSugar  Chlorides  FreeSulfurDioxide  \
INDEX                 0.004922       0.003846   0.002966           0.009257
TARGET                0.008685       0.016491  -0.038263           0.043824
FixedAcidity          0.014240      -0.018855  -0.000457           0.004972
VolatileAcidity      -0.016953      -0.006483   0.000987          -0.007077
CitricAcid            1.000000      -0.006940  -0.008567           0.006428
ResidualSugar        -0.006940       1.000000  -0.005594           0.017493
Chlorides            -0.008567      -0.005594   1.000000          -0.020661
FreeSulfurDioxide     0.006428       0.017493  -0.020661           1.000000
TotalSulfurDioxide    0.006320       0.022479  -0.013994           0.013720
Density              -0.013952       0.004101   0.022657           0.003176
pH                   -0.008709       0.012118  -0.017605           0.006049
Sulphates            -0.012989      -0.007723  -0.003290           0.011593
Alcohol               0.017046      -0.019998  -0.019695          -0.018588
LabelAppeal           0.008650       0.002320   0.010509           0.010294
AcidIndex             0.065697      -0.009414   0.025238          -0.041717
STARS                 0.008485       0.017203  -0.024547           0.018171

                    TotalSulfurDioxide   Density        pH  Sulphates  \
INDEX                         0.010756 -0.010779 -0.005853   0.006413
TARGET                        0.051478 -0.035518 -0.009445  -0.038850
FixedAcidity                 -0.022498  0.006477 -0.008983   0.030783
VolatileAcidity              -0.021080  0.014735  0.013592   0.000129
CitricAcid                    0.006320 -0.013952 -0.008709  -0.012989
ResidualSugar                 0.022479  0.004101  0.012118  -0.007723
Chlorides                    -0.013994  0.022657 -0.017605  -0.003290
FreeSulfurDioxide             0.013720  0.003176  0.006049   0.011593
TotalSulfurDioxide            1.000000  0.012816 -0.004343  -0.007133
Density                       0.012816  1.000000  0.005768  -0.009059
pH                           -0.004343  0.005768  1.000000   0.005475
Sulphates                    -0.007133 -0.009059  0.005475   1.000000
Alcohol                      -0.015957 -0.007215 -0.011548   0.004741
LabelAppeal                  -0.009747 -0.009370  0.004138  -0.003888
```

```
AcidIndex                   -0.049311  0.040413 -0.058676   0.034449
STARS                        0.029688 -0.026567 -0.009800  -0.028925

                      Alcohol  LabelAppeal  AcidIndex     STARS
INDEX               -0.007677     0.011553  -0.007097 -0.008883
TARGET               0.062062     0.356500  -0.246049  0.685381
FixedAcidity        -0.009371    -0.003366   0.178437 -0.035416
VolatileAcidity      0.004073    -0.016987   0.044642 -0.062276
CitricAcid           0.017046     0.008650   0.065697  0.008485
ResidualSugar       -0.019998     0.002320  -0.009414  0.017203
Chlorides           -0.019695     0.010509   0.025238 -0.024547
FreeSulfurDioxide   -0.018588     0.010294  -0.041717  0.018171
TotalSulfurDioxide  -0.015957    -0.009747  -0.049311  0.029688
Density             -0.007215    -0.009370   0.040413 -0.026567
pH                  -0.011548     0.004138  -0.058676 -0.009800
Sulphates            0.004741    -0.003888   0.034449 -0.028925
Alcohol              1.000000     0.001027  -0.038138  0.059214
LabelAppeal          0.001027     1.000000   0.024755  0.264700
AcidIndex           -0.038138     0.024755   1.000000 -0.170928
STARS                0.059214     0.264700  -0.170928  1.000000
```

Strong positive correlation between TARGET and (LabelAppeal & STARS)

Strong negative correlation between TARGET and AcidIndex

[12]:
```
plt.figure(figsize=(10,10))
sns.heatmap(scaled_data.corr(),annot=True,linewidth=0.
 ↪5,center=0,cmap='coolwarm')
plt.show()
```



2. DATA PREPARATION

[86]:
```
scaled_data.head()
```

[86]:

	TARGET	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	\
0	0.375	0.405714	0.610510	0.318310	0.676706	
1	0.375	0.430476	0.455951	0.342254	0.572225	
2	0.625	0.480000	0.839258	0.332394	0.530210	
3	0.375	0.453333	0.490726	0.461972	0.545083	
4	0.500	0.497143	0.482226	0.278873	0.510132	

	Chlorides	FreeSulfurDioxide	TotalSulfurDioxide	Density	pH	…	\

```
0   0.239492           0.353990            0.580319  0.495903  0.504425  …
1   0.295797           0.483871            0.263830  0.662231  0.513274  …
2   0.478985           0.652801            0.513298  0.507175  0.467257  …
3   0.295797           0.489813            0.498936  0.512953  0.311504  …
4   0.475020           0.329372            0.495213  0.504286  0.467257  …

   AcidIndex     STARS  ResidualSugar_missing  Chlorides_missing  \
0   0.554700  0.333333                    1.0                1.0
1   0.480384  0.666667                    1.0                1.0
2   0.554700  0.666667                    1.0                1.0
3   0.392232  0.000000                    1.0                1.0
4   0.620174  0.333333                    1.0                0.0

   FreeSulfurDioxide_missing  TotalSulfurDioxide_missing  pH_missing  \
0                        0.0                         1.0         1.0
1                        1.0                         1.0         1.0
2                        1.0                         1.0         1.0
3                        1.0                         1.0         1.0
4                        1.0                         1.0         1.0

   Sulphates_missing  Alcohol_missing  STARS_missing
0                1.0              1.0            1.0
1                1.0              0.0            1.0
2                1.0              1.0            1.0
3                1.0              1.0            1.0
4                1.0              1.0            1.0

[5 rows x 23 columns]
```

[89]:
```
scaled_data = scaled_data.drop("INDEX", axis = 1)
```

[18]:
```
scaled_data.head(10)
```

[18]:
```
   TARGET  FixedAcidity  VolatileAcidity  CitricAcid  ResidualSugar  \
0   0.375      0.405714         0.610510    0.318310       0.676706
1   0.375      0.430476         0.455951    0.342254       0.572225
2   0.625      0.480000         0.839258    0.332394       0.530210
3   0.375      0.453333         0.490726    0.461972       0.545083
4   0.500      0.497143         0.482226    0.278873       0.510132
5   0.000      0.560000         0.480680    0.539437       0.483361
6   0.000      0.491429         0.476043    0.400000       0.555122
7   0.500      0.468571         0.242658    0.504225       0.480387
8   0.375      0.626667         0.472952    0.604225       0.517011
9   0.750      0.449524         0.397218    0.511268       0.481874

   Chlorides  FreeSulfurDioxide  TotalSulfurDioxide   Density        pH  \
0   0.239492                NaN            0.580319  0.495903  0.504425
```

```
1   0.295797          0.483871           0.263830  0.662231  0.513274
2   0.478985          0.652801           0.513298  0.507175  0.467257
3   0.295797          0.489813           0.498936  0.512953  0.311504
4        NaN          0.329372           0.495213  0.504286  0.467257
5   0.684774          0.439728           0.445745  0.527161  0.481416
6   0.488105          0.714771           0.520745  0.509732  0.532743
7   0.480174          0.915110           0.730851  0.683258  0.481416
8   0.461538          0.290323                NaN  0.512006  0.787611
9   0.354481          0.523769           0.533511  0.280133  0.461947

   Sulphates   Alcohol  LabelAppeal  AcidIndex  STARS
0   0.344640  0.467949         0.50   0.307692   0.50
1   0.519674       NaN         0.25   0.230769   0.75
2   0.489824  0.855769         0.25   0.307692   0.75
3   0.672999  0.349359         0.25   0.153846   0.25
4   0.664858  0.589744         0.50   0.384615   0.50
5   0.599729  0.644231         0.50   0.538462   0.00
6   0.588874  0.480769         0.50   0.307692   0.00
7        NaN  0.522436         0.75   0.230769   0.75
8   0.459973  0.631410         0.50   0.153846   0.00
9   0.526459  0.554487         0.50   0.307692   1.00
```

[61]:
```
#Create flags to suggest if a variable was missing

missing_cols = ['ResidualSugar', 'Chlorides', 'FreeSulfurDioxide',␣
 ↪'TotalSulfurDioxide', 'pH', 'Sulphates', 'Alcohol', 'STARS']
for col in missing_cols:
    scaled_data[col+"_missing"] = np.where(scaled_data[col].isnull(), 0, 1)

scaled_data.head(10)
```

[61]:
```
   TARGET  FixedAcidity  VolatileAcidity  CitricAcid  ResidualSugar  \
0   0.375      0.405714         0.610510    0.318310       0.676706
1   0.375      0.430476         0.455951    0.342254       0.572225
2   0.625      0.480000         0.839258    0.332394       0.530210
3   0.375      0.453333         0.490726    0.461972       0.545083
4   0.500      0.497143         0.482226    0.278873       0.510132
5   0.000      0.560000         0.480680    0.539437       0.483361
6   0.000      0.491429         0.476043    0.400000       0.555122
7   0.500      0.468571         0.242658    0.504225       0.480387
8   0.375      0.626667         0.472952    0.604225       0.517011
9   0.750      0.449524         0.397218    0.511268       0.481874

   Chlorides  FreeSulfurDioxide  TotalSulfurDioxide   Density        pH  … \
0   0.239492                NaN            0.580319  0.495903  0.504425  …
1   0.295797           0.483871            0.263830  0.662231  0.513274  …
2   0.478985           0.652801            0.513298  0.507175  0.467257  …
```

```
3   0.295797           0.489813            0.498936  0.512953  0.311504  …
4        NaN           0.329372            0.495213  0.504286  0.467257  …
5   0.684774           0.439728            0.445745  0.527161  0.481416  …
6   0.488105           0.714771            0.520745  0.509732  0.532743  …
7   0.480174           0.915110            0.730851  0.683258  0.481416  …
8   0.461538           0.290323                 NaN  0.512006  0.787611  …
9   0.354481           0.523769            0.533511  0.280133  0.461947  …

   AcidIndex     STARS  ResidualSugar_missing  Chlorides_missing  \
0   0.307692  0.333333                      1                  1
1   0.230769  0.666667                      1                  1
2   0.307692  0.666667                      1                  1
3   0.153846  0.000000                      1                  1
4   0.384615  0.333333                      1                  0
5   0.538462       NaN                      1                  1
6   0.307692       NaN                      1                  1
7   0.230769  0.666667                      1                  1
8   0.153846       NaN                      1                  1
9   0.307692  1.000000                      1                  1

   FreeSulfurDioxide_missing  TotalSulfurDioxide_missing  pH_missing  \
0                          0                           1           1
1                          1                           1           1
2                          1                           1           1
3                          1                           1           1
4                          1                           1           1
5                          1                           1           1
6                          1                           1           1
7                          1                           1           1
8                          1                           0           1
9                          1                           1           1

   Sulphates_missing  Alcohol_missing  STARS_missing
0                  1                1              1
1                  1                0              1
2                  1                1              1
3                  1                1              1
4                  1                1              1
5                  1                1              0
6                  1                1              0
7                  0                1              1
8                  1                1              0
9                  1                1              1

[10 rows x 23 columns]
```

[62]:
```
# Add median values (IMPUTE) to the missing values in the columns

imputer = KNNImputer(n_neighbors=2)  #impute missing values
scaled_data.iloc[:,1:]=imputer.fit_transform(scaled_data.iloc[:,1:]) #replace
 ↪df with imputed missing values
scaled_data.head()
```

[62]:

	TARGET	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	\
0	0.375	0.405714	0.610510	0.318310	0.676706	
1	0.375	0.430476	0.455951	0.342254	0.572225	
2	0.625	0.480000	0.839258	0.332394	0.530210	
3	0.375	0.453333	0.490726	0.461972	0.545083	
4	0.500	0.497143	0.482226	0.278873	0.510132	

	Chlorides	FreeSulfurDioxide	TotalSulfurDioxide	Density	pH	…	\
0	0.239492	0.353990	0.580319	0.495903	0.504425	…	
1	0.295797	0.483871	0.263830	0.662231	0.513274	…	
2	0.478985	0.652801	0.513298	0.507175	0.467257	…	
3	0.295797	0.489813	0.498936	0.512953	0.311504	…	
4	0.475020	0.329372	0.495213	0.504286	0.467257	…	

	AcidIndex	STARS	ResidualSugar_missing	Chlorides_missing	\
0	0.307692	0.333333	1.0	1.0	
1	0.230769	0.666667	1.0	1.0	
2	0.307692	0.666667	1.0	1.0	
3	0.153846	0.000000	1.0	1.0	
4	0.384615	0.333333	1.0	0.0	

	FreeSulfurDioxide_missing	TotalSulfurDioxide_missing	pH_missing	\
0	0.0	1.0	1.0	
1	1.0	1.0	1.0	
2	1.0	1.0	1.0	
3	1.0	1.0	1.0	
4	1.0	1.0	1.0	

	Sulphates_missing	Alcohol_missing	STARS_missing
0	1.0	1.0	1.0
1	1.0	0.0	1.0
2	1.0	1.0	1.0
3	1.0	1.0	1.0
4	1.0	1.0	1.0

[5 rows x 23 columns]

Transform data by putting it into buckets(discretization): 3 important wine features that customers often look for are chosen and discretized/bucketed into different bins.

- Label Appeal : "Low_Appeal","Moderately_Low_Appeal", "Moderately_High_Appeal", "High_Appeal"
- Alcohol content : "V_Low_Alcohol", "Low_Alcohol", "High_Alcohol", "V_High_Alcohol"
- STARS : "Low_Rating", "Moderate_Rating", "High_Rating"

[63]:
```
scaled_data.groupby(['LabelAppeal']).size()
```

[63]:
```
LabelAppeal
0.00     504
0.25    3136
0.50    5617
0.75    3048
1.00     490
dtype: int64
```

[22]:
```
scaled_data['LabelAppeal_bin']=pd.cut(x=scaled_data['LabelAppeal'], bins=[0,0.
↪25,.50,0.75,1], labels=["Low_Appeal","Moderately_Low_Appeal",␣
↪"Moderately_High_Appeal", "High_Appeal"])
scaled_data['LabelAppeal_bin'].value_counts()
```

[22]:
```
Moderately_Low_Appeal     5617
Low_Appeal                3136
Moderately_High_Appeal    3048
High_Appeal                490
Name: LabelAppeal_bin, dtype: int64
```

The average glass of wine contains around 11% to 13% alcohol, but bottles range from as little as 5.5% alcohol by volume to as much as around 20% ABV.

- Very Low (Below 12.5 Percent)
- Low (12.5 to 13.5 Percent)
- High (13.5 to 14.5 Percent)
- Very High (More Than 14.5 Percent)

[25]:
```
scaled_data['Alcohol'].describe()
```

[25]:
```
count    12795.000000
mean         0.486883
std          0.117976
min          0.000000
25%          0.439103
50%          0.483974
75%          0.546474
max          1.000000
Name: Alcohol, dtype: float64
```

[26]:
```
scaled_data['Alcohol_bin']=pd.cut(x=scaled_data['Alcohol'], bins=4,␣
↪labels=["V_Low_Alcohol","Low_Alcohol","High_Alcohol", "V_High_Alcohol"])
```

```
scaled_data['Alcohol_bin'].value_counts()
```

[26]:
```
Low_Alcohol       7171
High_Alcohol      5058
V_Low_Alcohol      328
V_High_Alcohol     238
Name: Alcohol_bin, dtype: int64
```

[27]:
```
scaled_data.groupby(['STARS']).size()
```

[27]:
```
STARS
0.00    3359
0.25    3042
0.50    3570
0.75    2212
1.00     612
dtype: int64
```

[28]:
```
scaled_data['STARS_bin']=pd.cut(x=scaled_data['STARS'], bins=3,␣
↪labels=["Low_Rating","Moderate_Rating","High_Rating"])
scaled_data['STARS_bin'].value_counts()
```

[28]:
```
Low_Rating         6401
Moderate_Rating    3570
High_Rating        2824
Name: STARS_bin, dtype: int64
```

[29]:
```
# Mathematical Transformation

# Checking the Skewness of the data

scaled_data.skew(axis = 0, skipna = True)
```

[29]:
```
TARGET                -0.326378
FixedAcidity          -0.022591
VolatileAcidity        0.020385
CitricAcid            -0.050319
ResidualSugar         -0.051587
Chlorides              0.030444
FreeSulfurDioxide      0.002126
TotalSulfurDioxide    -0.007851
Density               -0.018698
pH                     0.045805
Sulphates              0.005650
Alcohol               -0.027085
LabelAppeal            0.008431
AcidIndex              1.648883
```

```
STARS                          0.254900
ResidualSugar_missing         -4.222068
Chlorides_missing             -4.136587
FreeSulfurDioxide_missing     -4.102816
TotalSulfurDioxide_missing    -3.977563
pH_missing                    -5.425049
Sulphates_missing             -2.771394
Alcohol_missing               -4.080670
STARS_missing                  0.000000
dtype: float64
```

- If skewness value lies above +1 or below -1, data is highly skewed.
- If it lies between +0.5 to -0.5, it is moderately skewed.
- If the value is 0, then the data is symmetric

The AcidIndex feature is highly positively skewed with a value of 1.648883 ($>$ 1). Hence Square Root transformation can be applied to this feature

The missing value columns are not transformed since they are added only to indicate any missing values and hence do not posses any mathematical importance as such

[64]:
```
#Square root transformation, Applied to positive values only

scaled_data["AcidIndex"] = scaled_data["AcidIndex"]**(1/2)
scaled_data.skew(axis = 0, skipna = True)
```

[64]:
```
TARGET                        -0.326378
FixedAcidity                  -0.022591
VolatileAcidity                0.020385
CitricAcid                    -0.050319
ResidualSugar                 -0.052327
Chlorides                      0.029051
FreeSulfurDioxide              0.002722
TotalSulfurDioxide            -0.009536
Density                       -0.018698
pH                             0.045523
Sulphates                      0.005637
Alcohol                       -0.027994
LabelAppeal                    0.008431
AcidIndex                      0.767241
STARS                          0.481848
ResidualSugar_missing         -4.222068
Chlorides_missing             -4.136587
FreeSulfurDioxide_missing     -4.102816
TotalSulfurDioxide_missing    -3.977563
pH_missing                    -5.425049
Sulphates_missing             -2.771394
Alcohol_missing               -4.080670
```

```
STARS_missing                -1.079546
dtype: float64
```

[31]:
```
# Combine variable
```

From the correlation table, every feature is poorly correlated with every other feature. Hence no two variables/features are similar and therefore cannot be combined to create any new meaningful variable

[65]:
```
# PCA

scaler_pca = preprocessing.MinMaxScaler()
pcs = PCA(whiten=True) #all features
scores = pd.DataFrame(pcs.fit_transform(scaler_pca.fit_transform(scaled_data.
 ↪iloc[:,0:15])),
                      columns=['PC{}'.format(i) for i in range(0, 15)])␣
 ↪#Creating 15 PCA components
scores.head()
```

[65]:
```
        PC0       PC1       PC2       PC3       PC4       PC5       PC6  \
0 -0.018718 -0.004189 -0.047080  0.865440 -0.762556  2.210962  1.854644
1  0.398355  1.513903 -1.269654  0.314121 -0.574082 -0.073547  1.670788
2  0.787925  0.773508 -1.961440  0.081256 -0.156031 -0.602015  1.203519
3 -1.073233 -0.715158 -1.003532  1.040848  0.265641 -0.406257  0.459974
4  0.162788 -0.323682 -0.252461 -0.662229  0.398073 -0.084398  0.447525

        PC7       PC8       PC9      PC10      PC11      PC12      PC13  \
0  0.625235 -0.626340  0.429344 -1.304140 -0.596584 -0.389419  0.005775
1  1.372680 -0.018630  0.910438  1.365043 -1.564914 -0.179054 -0.383472
2  1.711803  1.273973  1.311882 -0.977383  1.468654 -2.253964  2.319961
3  0.602953 -1.113344 -0.359507 -0.233986 -0.748689 -1.071487 -1.707191
4  1.860665 -1.596815 -0.287843 -0.147443 -0.517549 -0.423088  0.757142

       PC14
0 -0.647603
1  0.199511
2 -1.089686
3  1.653986
4 -1.286271
```

Considering all the features in the dataset for PCA except for the missing_variable columns added to indicate missing variables since they don't add any valuable analytical information for PCA

[66]:
```
# Explained variance by component

pcsSummary = pd.DataFrame({'Explained Variance': pcs.explained_variance_,␣
 ↪#explained variance
```

```
                            'Explained Variance Ratio': pcs.
↪explained_variance_ratio_,  #explained variance ratio
                            'Cumulative Proportion': np.cumsum(pcs.
↪explained_variance_ratio_)}) #cumulative %
pcsSummary = pcsSummary.transpose()
pcsSummary.columns = scores.columns
pcsSummary
```

[66]:

	PC0	PC1	PC2	PC3	PC4	\
Explained Variance	0.110863	0.042521	0.034940	0.016184	0.016122	
Explained Variance Ratio	0.308623	0.118371	0.097266	0.045053	0.044882	
Cumulative Proportion	0.308623	0.426994	0.524260	0.569313	0.614194	

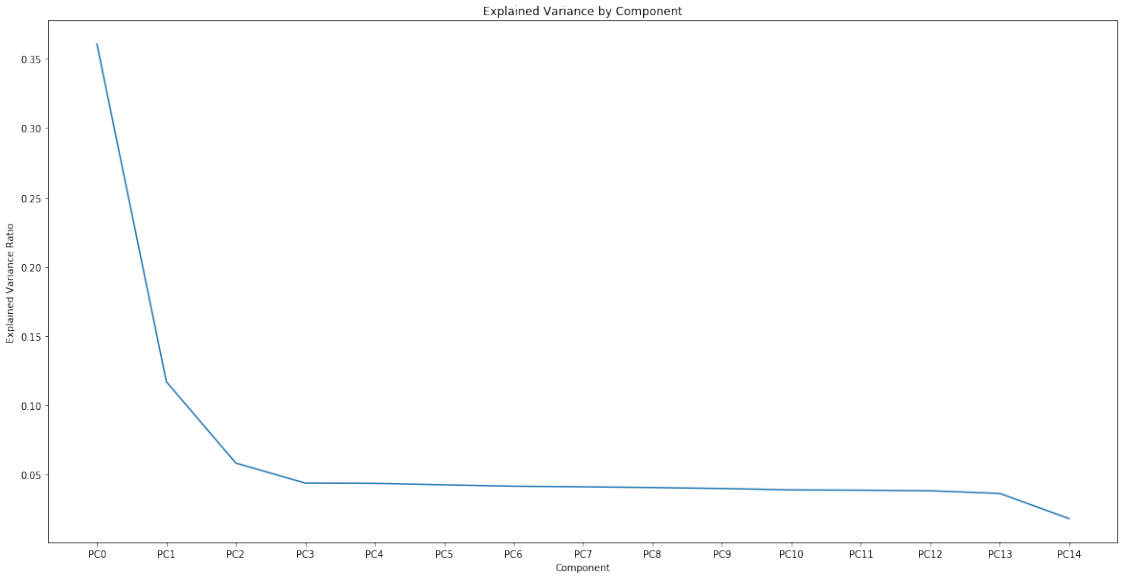
	PC5	PC6	PC7	PC8	PC9	\
Explained Variance	0.015670	0.015300	0.015149	0.014948	0.014789	
Explained Variance Ratio	0.043622	0.042592	0.042172	0.041613	0.041171	
Cumulative Proportion	0.657817	0.700408	0.742580	0.784193	0.825364	

	PC10	PC11	PC12	PC13	PC14
Explained Variance	0.014331	0.014236	0.014086	0.013362	0.006718
Explained Variance Ratio	0.039894	0.039631	0.039212	0.037198	0.018700
Cumulative Proportion	0.865258	0.904889	0.944101	0.981300	1.000000

From the Explained Variance for each component, it is seen that PC0 component explains 13.27% variance within the data, PC1 explains 4.3% and so on

[34]:
```
#scree plot

plt.figure(figsize=(20,10))
plt.plot(pcsSummary[1:2].transpose())
plt.xlabel('Component')
plt.ylabel('Explained Variance Ratio')
plt.title('Explained Variance by Component')
```

[34]:
```
Text(0.5, 1.0, 'Explained Variance by Component')
```



The elbow rule for the scree plot using MinMax scaler indicates that 4 PCA components (PC0 - PC3) could be used for analysis.

[67]:
```
#PCA- component analysis for each feature in the dataset

pcsComponents_df = pd.DataFrame(pcs.components_.transpose(), columns=pcsSummary.
 ↪columns,
                                index=scaled_data.iloc[:,0:15].columns)
pcsComponents_df
```

[67]:

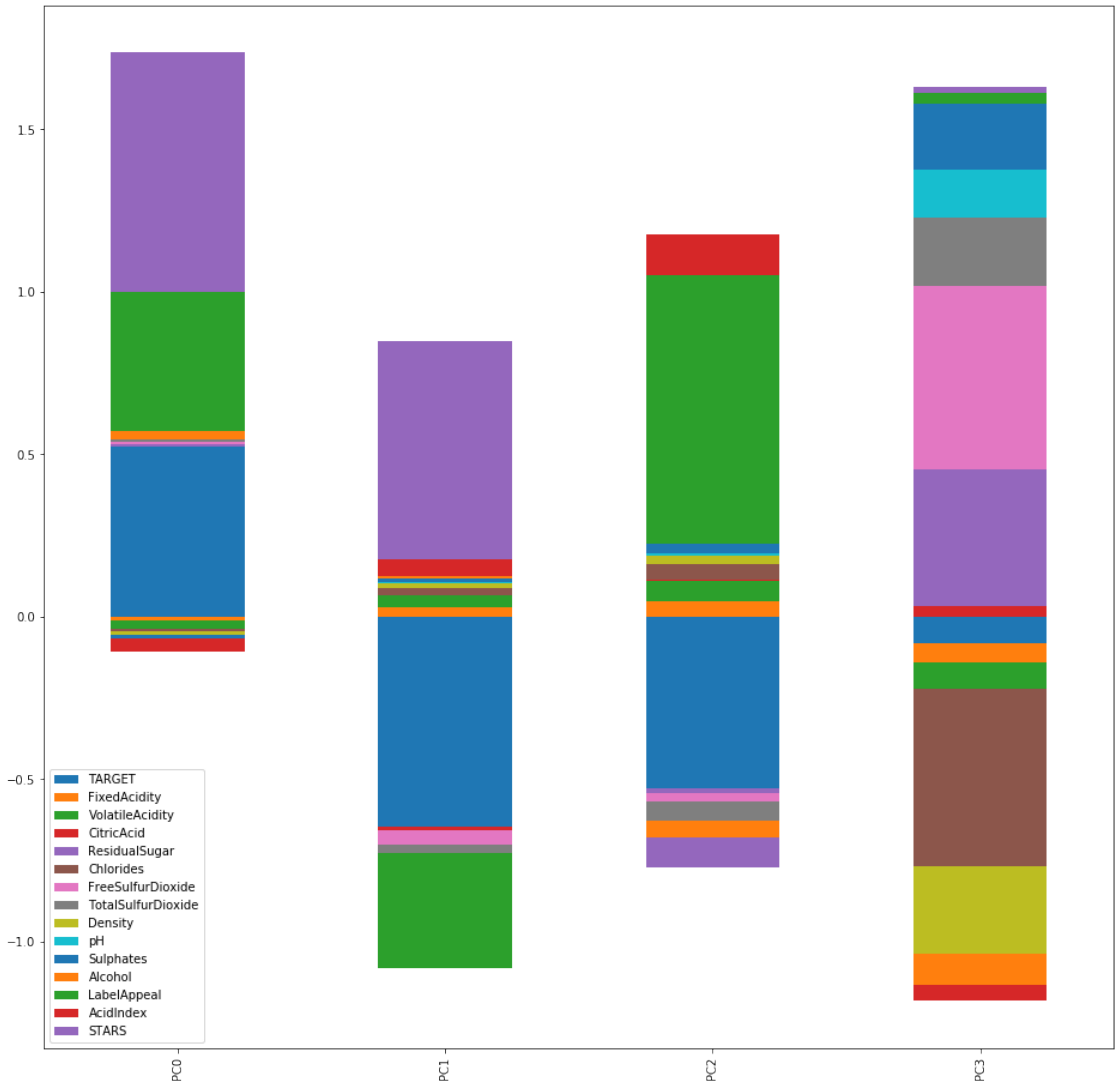
	PC0	PC1	PC2	PC3	PC4	\
TARGET	0.521507	-0.644536	-0.528205	-0.079886	0.006367	
FixedAcidity	-0.011848	0.029097	0.049139	-0.061610	0.186893	
VolatileAcidity	-0.025898	0.037666	0.059201	-0.081888	-0.024304	
CitricAcid	0.001337	-0.011237	0.005839	0.031942	0.200561	
ResidualSugar	0.006327	-0.001650	-0.015683	0.422937	-0.409218	
Chlorides	-0.005448	0.020568	0.048660	-0.542794	-0.233045	
FreeSulfurDioxide	0.007035	-0.042031	-0.025486	0.561091	-0.185932	
TotalSulfurDioxide	0.009899	-0.026998	-0.057466	0.211405	-0.244834	
Density	-0.011561	0.017155	0.025370	-0.271104	-0.715261	
pH	-0.000838	0.002353	0.007474	0.148604	-0.093272	
Sulphates	-0.012412	0.012137	0.030129	0.201878	0.227648	
Alcohol	0.025402	0.005544	-0.054081	-0.094512	0.184338	
LabelAppeal	0.428904	-0.355696	0.824087	0.033284	-0.004078	
AcidIndex	-0.040339	0.051080	0.128001	-0.049038	0.042279	
STARS	0.735174	0.670563	-0.091898	0.017326	-0.005037	

	PC5	PC6	PC7	PC8	PC9	\

```
TARGET             -0.061877  0.011546  0.035888 -0.030846  0.073692
FixedAcidity       -0.499347  0.027910 -0.162566 -0.210375  0.357784
VolatileAcidity    -0.009718  0.310969  0.284351  0.202078  0.348764
CitricAcid         -0.105745 -0.034257 -0.725123 -0.055551  0.183504
ResidualSugar       0.297626 -0.214983  0.020615 -0.442421  0.546250
Chlorides          -0.082792 -0.726983  0.103283  0.080840  0.056476
FreeSulfurDioxide  -0.447232 -0.241250 -0.027248  0.603597  0.021500
TotalSulfurDioxide  0.073655 -0.051777 -0.270795 -0.243061 -0.594589
Density            -0.393491  0.420354 -0.098726 -0.101877 -0.042643
pH                  0.119454  0.184790  0.241035  0.117437  0.024085
Sulphates          -0.496935 -0.112349  0.449239 -0.503538 -0.194202
Alcohol             0.002608  0.204697 -0.013563  0.013230  0.059015
LabelAppeal         0.041764  0.013610 -0.009210  0.002886 -0.038990
AcidIndex          -0.129485 -0.000689 -0.102464 -0.084673  0.102381
STARS              -0.010192 -0.007381 -0.005721  0.010857 -0.008636

                       PC10      PC11      PC12      PC13      PC14
TARGET             -0.040813  0.020079  0.023511 -0.046659 -0.103685
FixedAcidity       -0.459741 -0.217882  0.336500  0.306941  0.206816
VolatileAcidity    -0.459365  0.573227 -0.286522 -0.157744  0.020061
CitricAcid          0.292652  0.483017  0.038061 -0.237269  0.083538
ResidualSugar       0.048739 -0.010879 -0.111834  0.094743  0.007135
Chlorides           0.015520  0.261785  0.049904  0.145248  0.011585
FreeSulfurDioxide   0.033610 -0.015238 -0.115410  0.092197 -0.034744
TotalSulfurDioxide -0.481307  0.315090 -0.018998  0.254941 -0.029840
Density             0.224339 -0.055442 -0.038774 -0.062800  0.038813
pH                  0.208134  0.363692  0.788346  0.208157 -0.088653
Sulphates           0.235155  0.253937 -0.103517 -0.150645  0.019328
Alcohol             0.315018  0.144004 -0.373781  0.804242 -0.035289
LabelAppeal         0.014832 -0.008333 -0.021885  0.036385  0.060361
AcidIndex          -0.080471 -0.037793  0.007679 -0.013456 -0.960274
STARS              -0.005535  0.001138  0.005921 -0.024182 -0.007653
```

[68]:
```
#Analysis of the first 4 components using stacked bar plot

pcsComponents_df[['PC0','PC1','PC2', 'PC3']].transpose().plot(kind='bar',␣
↪stacked=True,figsize=(16, 16))
```

[68]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x1edb095d648>
```

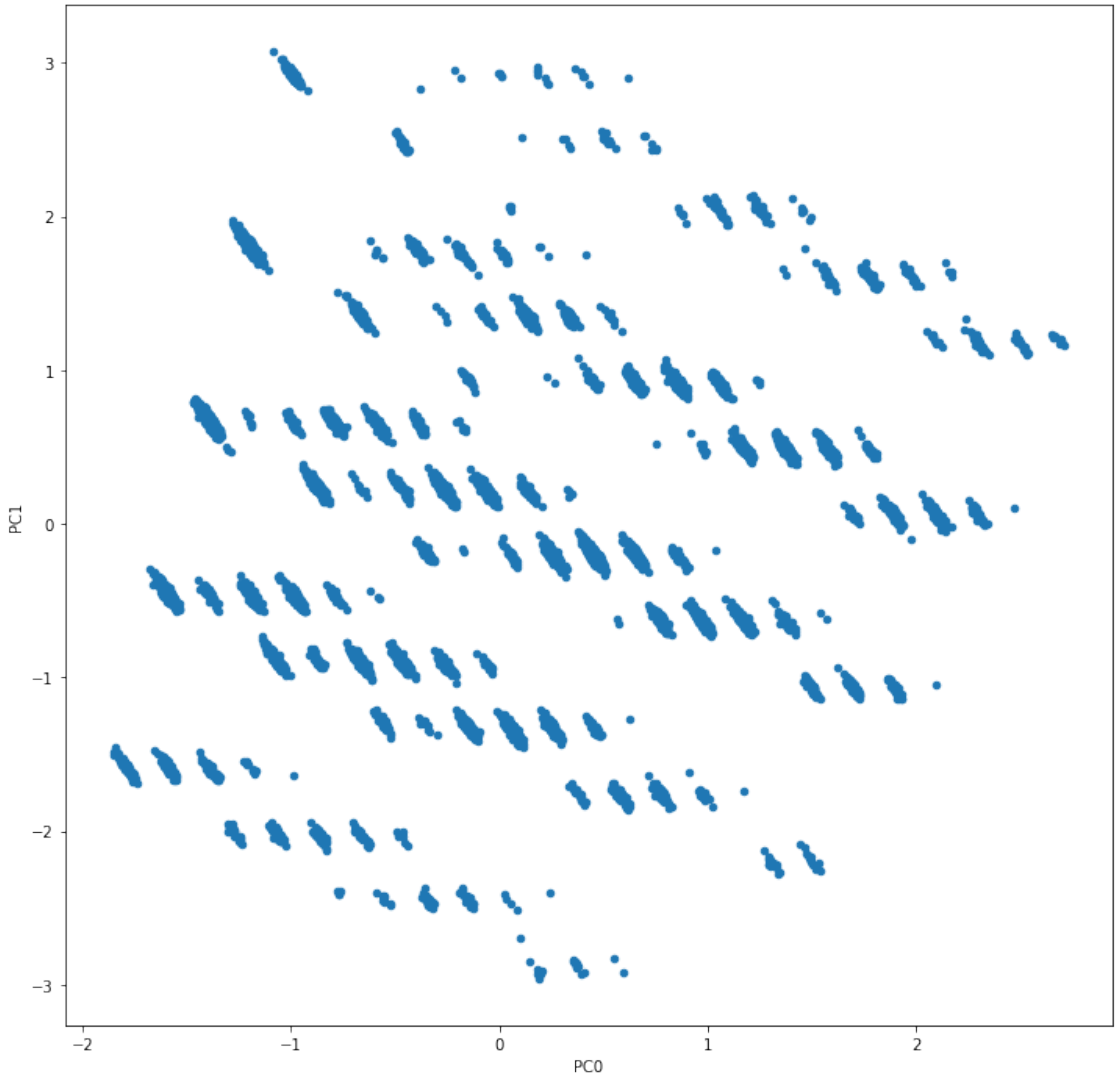


0.0.5 Analysis of PC0 - PC3 components

- PC0 : largely contains useful information on STARS, LabelAppeal & TARGET features
- PC1 : largely contains useful information on STARS, LabelAppeal & AcidIndex features
- PC2 : largely contains useful information on STARS, LabelAppeal, TARGET & AcidIndex features
- PC3 : largely contains useful information on Density, Chlorides and Sulphates features

[37]:
```
#Scatter plot of PC0 vs PC1

scores.plot.scatter(x='PC0', y='PC1',figsize=(12, 12)) # plot first 2 components
```

[37]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x1a25b92f90>
```



Scatter plot of PC0 vs PC1 shows the plot of the first two components of the PCA Analysis. It shows the how wine samples with similar chemical properties are grouped together, thereby forming different clusters

[38]:
```
#Determining the Silhouette score and inertia of the cluster by using 4␣
↪Principal Components

col_used=['PC0', 'PC1', 'PC2', 'PC3'] #number of components used

silhouette=[]
inertia=[]
clusters=[]
for i in range(2,25):  #Iterating until 30 where we see declining silhouette␣
↪and/or flattening of inertia
```

```
    kmeans = KMeans(n_clusters=i, random_state=0).fit(scores[col_used])
    silhouette.append(silhouette_score(scores[col_used],kmeans.labels_))␣
 ↪#creating a list of silhouette scores
    inertia.append(kmeans.inertia_) #creating the list of inertia
    clusters.append(i)

print('The max silhouette value is: ',max(silhouette))
```

```
The max silhouette value is:  0.24214354066802526
```

[39]:
```
#Evaluating KMeans Clustering for the dataset

kmeans_eval=pd.DataFrame({'silhouette_score': silhouette,'inertia':␣
 ↪inertia,},index=clusters) #put silhouette and inertia in df
kmeans_eval.head(8)
```

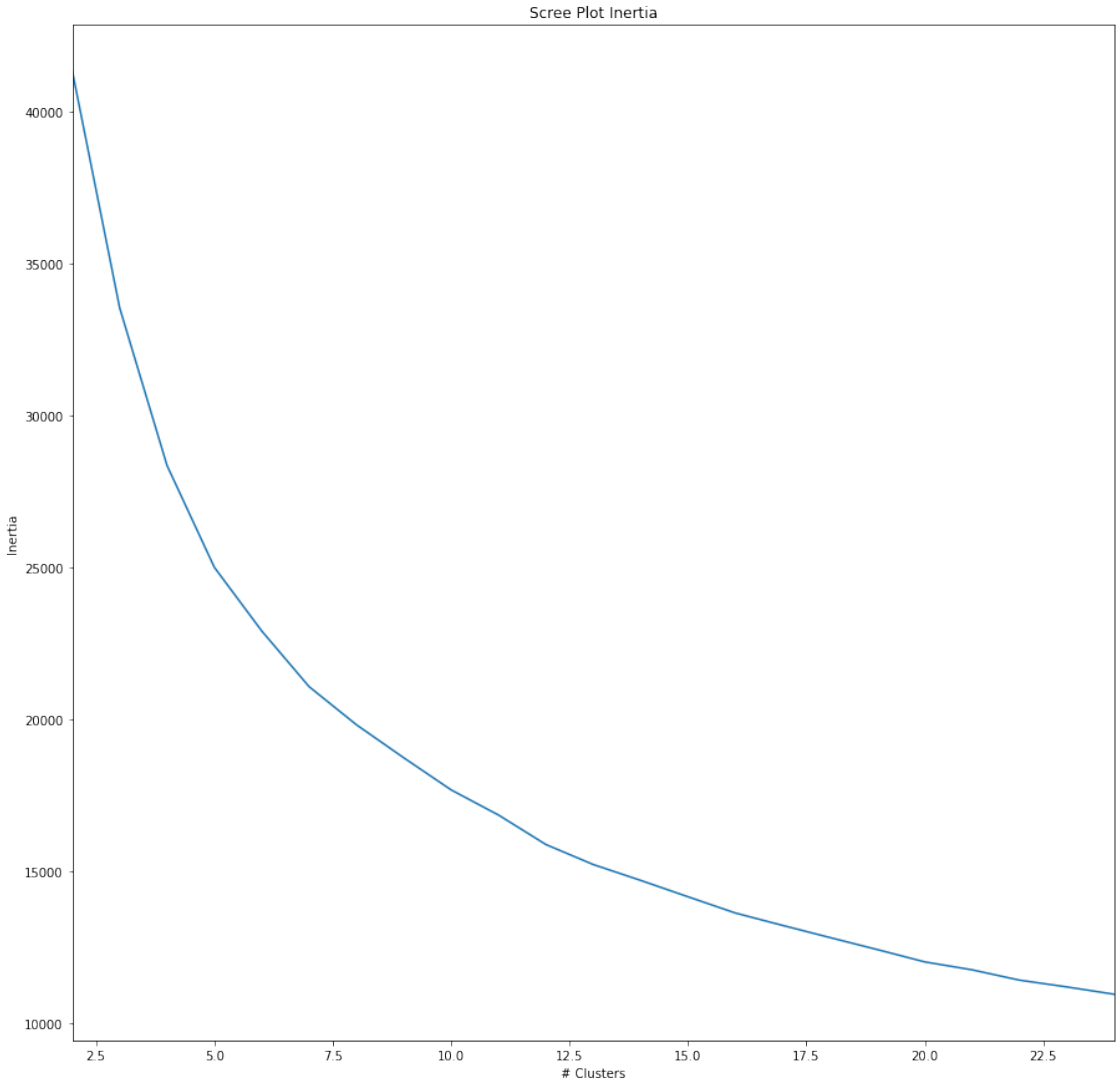
[39]:

	silhouette_score	inertia
2	0.242144	41339.738732
3	0.233252	33551.737085
4	0.240989	28365.859952
5	0.234598	25013.768859
6	0.230951	22921.680077
7	0.232437	21089.350881
8	0.215680	19835.755857
9	0.212783	18748.378666

The maximum Silhouette score is for a k value of 4

[40]:
```
#Plotting the Scree Plot Inertia to identify the likely number of clusters

kmeans_eval['inertia'].plot(figsize=(15, 15))#use elbow method of finding # of␣
 ↪components to cluster
plt.xlabel('# Clusters')
plt.ylabel('Inertia')
plt.title('Scree Plot Inertia')
```

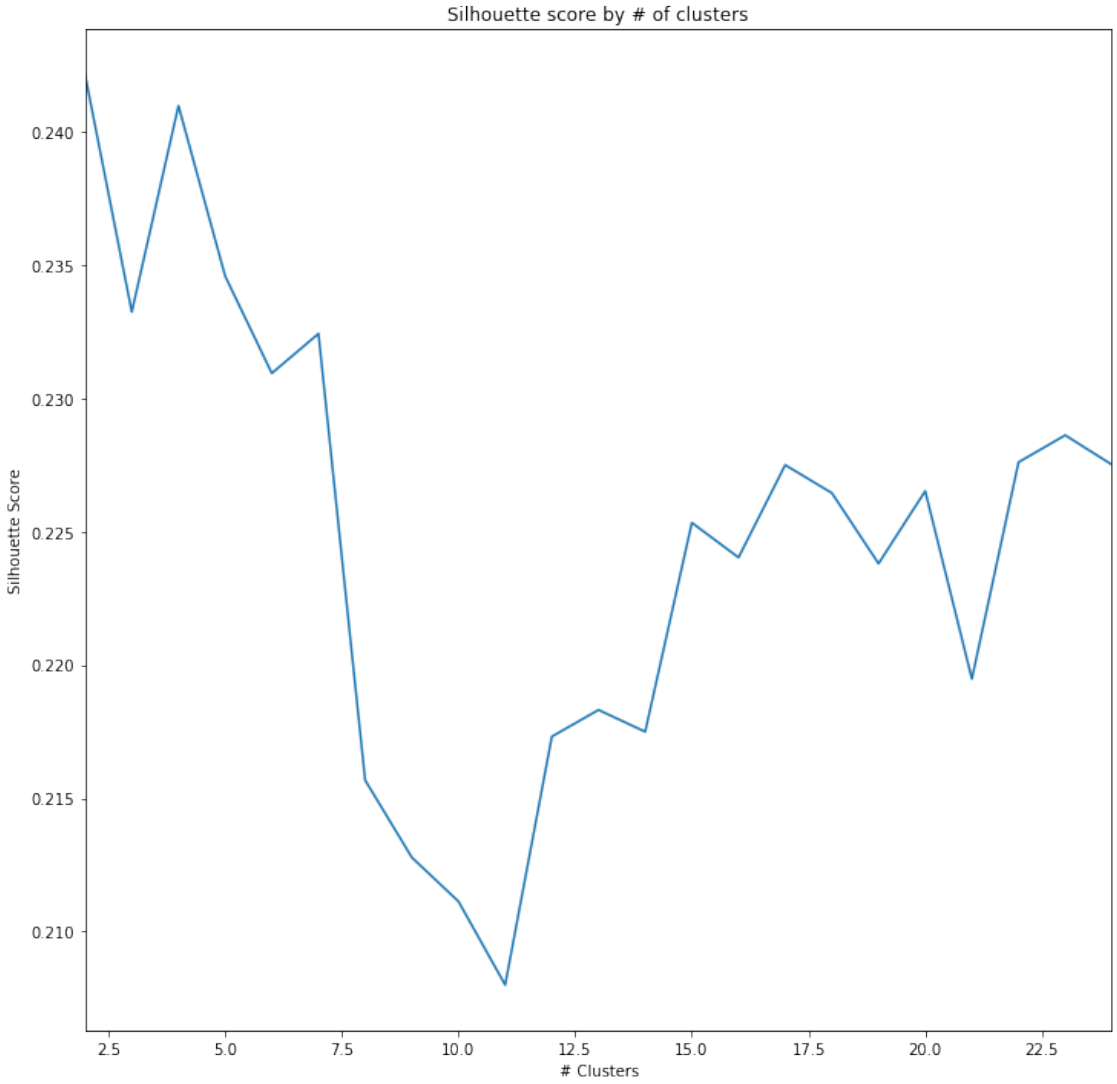
[40]:
```
Text(0.5, 1.0, 'Scree Plot Inertia')
```



Based on the elbow rule, the scree plot indicates that around 8 clusters can be used for KMeans clustering

[41]:
```
#Silhouette score plot further gives an idea on the number of clusters

kmeans_eval['silhouette_score'].plot(figsize=(12, 12)) #plot silhouete_score to␣
 ↪visually look for highest value & corresponding cluster
plt.xlabel('# Clusters')
plt.ylabel('Silhouette Score')
plt.title('Silhouette score by # of clusters')
```

[41]:
```
Text(0.5, 1.0, 'Silhouette score by # of clusters')
```



The plot peaks at a value of 4. Hence choosing to divide the data into 4 clusters

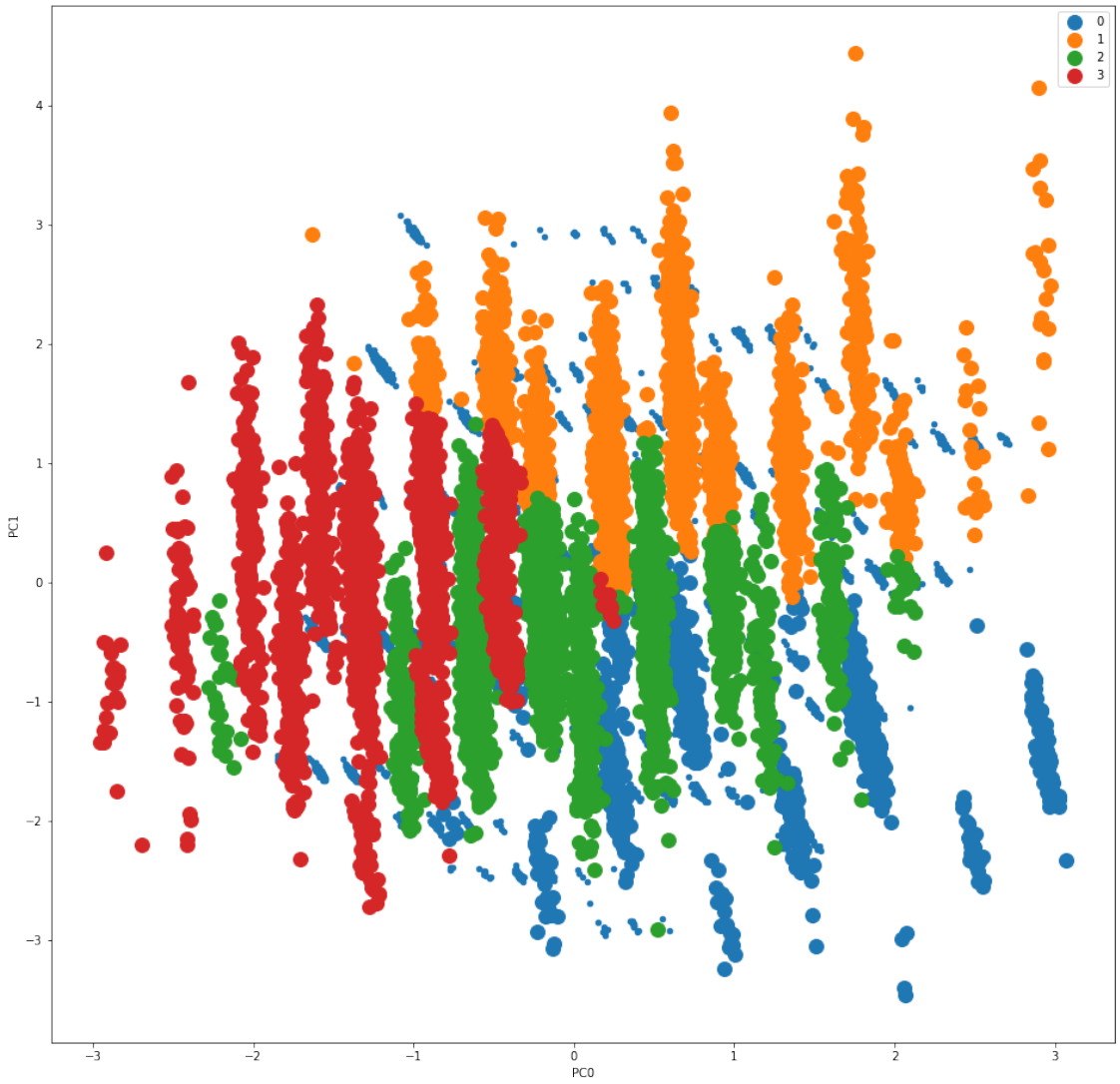
[42]:
```
print(kmeans_eval['silhouette_score'])
```

```
2     0.242144
3     0.233252
4     0.240989
5     0.234598
6     0.230951
7     0.232437
8     0.215680
9     0.212783
10    0.211130
11    0.207999
```

```
12    0.217317
13    0.218318
14    0.217499
15    0.225341
16    0.224038
17    0.227509
18    0.226457
19    0.223810
20    0.226531
21    0.219483
22    0.227614
23    0.228626
24    0.227521
Name: silhouette_score, dtype: float64
```

[43]:
```
#Taking clusters 4 provides a well define plot

cols=['PC0','PC1', 'PC2', 'PC3'] # PCA Components used for clustering

kmeans= KMeans(n_clusters=4).fit(scores[cols])
scores['cluster']=kmeans.labels_

groups = scores.groupby('cluster')

scaled_data['cluster']=scores['cluster']
ax = scores.plot.scatter(x='PC0', y='PC1', figsize=(16, 16))
points = scores[['PC0','PC1']]


for name, group in groups:
    ax.plot(group.PC1, group.PC2, marker='o', linestyle='', ms=12, label=name)␣
 ↪#grouping subplots
ax.legend()
```

[43]: <matplotlib.legend.Legend at 0x1a24f89810>



The dataset is divided into 4 different clusters Cluster 0 : Cluster having high STARS, LabelAppeal & TARGET features Cluster 1 : Cluster having medium STARS, LabelAppeal & TARGET features Cluster 2 : Cluster having very low STARS, LabelAppeal & TARGET features Cluster 3 : Cluster having low STARS, LabelAppeal & TARGET features

3. BUILD MODELS

[69]:
```
scaled_data.columns
```

[69]:
```
Index(['TARGET', 'FixedAcidity', 'VolatileAcidity', 'CitricAcid',
       'ResidualSugar', 'Chlorides', 'FreeSulfurDioxide', 'TotalSulfurDioxide',
       'Density', 'pH', 'Sulphates', 'Alcohol', 'LabelAppeal', 'AcidIndex',
       'STARS', 'ResidualSugar_missing', 'Chlorides_missing',
       'FreeSulfurDioxide_missing', 'TotalSulfurDioxide_missing', 'pH_missing',
       'Sulphates_missing', 'Alcohol_missing', 'STARS_missing'],
```

```
      dtype='object')
```

[70]:
```
# Data Partitioning

predictors = ['FixedAcidity', 'VolatileAcidity', 'CitricAcid',
       'ResidualSugar', 'Chlorides', 'FreeSulfurDioxide', 'TotalSulfurDioxide',
       'Density', 'pH', 'Sulphates', 'Alcohol', 'LabelAppeal', 'AcidIndex',
       'STARS']

outcome = 'TARGET'

X = pd.get_dummies(scaled_data[predictors], drop_first=True)
y = df[outcome]
train_X, temp_X, train_y, temp_y = train_test_split(X, y, test_size=0.5,␣
↪random_state=1)
valid_X, test_X, valid_y, test_y = train_test_split(temp_X, temp_y, test_size=0.
↪3, random_state=1)

print('Training : ', train_X.shape)
print('Validation : ', valid_X.shape)
print('Test : ', test_X.shape)

#train model using training data
train_X
```

```
Training :  (6397, 14)
Validation :  (4478, 14)
Test :  (1920, 14)
```

[70]:

	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	Chlorides	\
7763	0.485714	0.344668	0.914085	0.249117	0.339810	
422	0.045714	0.415765	0.464789	0.285927	0.729183	
9428	0.607619	0.533230	0.254930	0.481874	0.732355	
1095	0.405714	0.521638	0.267606	0.496747	0.482554	
2309	0.476190	0.435858	0.674648	0.686373	0.478588	
…	…	…	…	…	…	
10955	0.626667	0.471406	0.488732	0.514594	0.477795	
905	0.413333	0.523957	0.504225	0.661089	0.291039	
5192	0.447619	0.267388	0.566197	0.699015	0.622522	
12172	0.653333	0.443586	0.516901	0.523517	0.417129	
235	0.531429	0.499227	0.515493	0.485592	0.411182	

	FreeSulfurDioxide	TotalSulfurDioxide	Density	pH	Sulphates	\
7763	0.478778	0.499734	0.582619	0.509735	0.540027	
422	0.491511	0.770213	0.506323	0.495575	0.617368	
9428	0.943124	0.680319	0.519583	0.536283	0.500678	
1095	0.738540	0.542553	0.125030	0.591150	0.521031	

```
2309            0.298812            0.671809  0.498745  0.389381   0.411126
…                  …                   …        …         …          …
10955           0.339559            0.551064  0.348425  0.527434   0.795115
905             0.466893            0.503723  0.515794  0.231858   0.290366
5192            0.448217            0.210638  0.522377  0.745133   0.332429
12172           0.731749            0.528723  0.274118  0.460177   0.439620
235             0.500849            0.526596  0.582193  0.467257   0.477612

        Alcohol  LabelAppeal  AcidIndex     STARS
7763   0.842949         0.75   0.554700  0.333333
422    0.371795         0.75   0.620174  0.000000
9428   0.467949         0.75   0.554700  0.333333
1095   0.198718         0.50   0.392232  0.000000
2309   0.455128         1.00   0.480384  0.666667
…         …           …         …         …
10955  0.637821         0.50   0.277350  0.000000
905    0.500000         0.25   0.554700  0.666667
5192   0.467949         0.75   0.554700  1.000000
12172  0.358974         0.75   0.480384  0.333333
235    0.554487         0.25   0.733799  0.000000

[6397 rows x 14 columns]
```

Regression Model

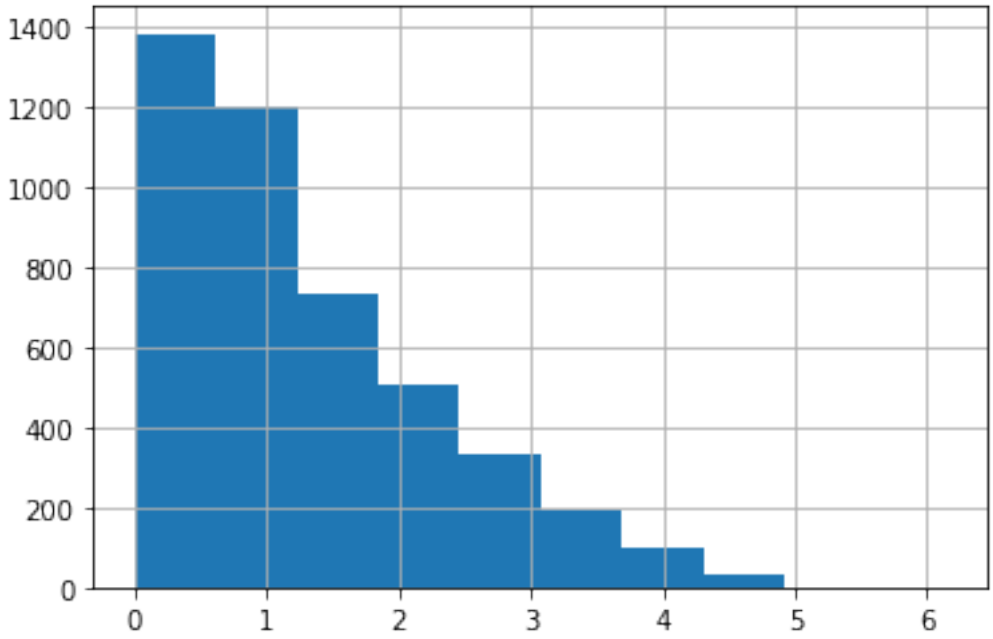
[71]:
```
def findsubsets(s, n):
    return list(map(set, itertools.combinations(s, n)))
```

[72]:
```
def exhaustive(model,train_X,train_y,valid_X,valid_y):
    low_err=600000**2

    for x in range(len(train_X.columns),0,-1):
        n=x
        ss=findsubsets(train_X.columns,n)
        print("_"*50)
        print(str(len(ss))+" model(s) using "+ str(n)+ " features")
        for z in range(0,len(ss)):

            model = model
            reg  = model.fit(train_X[ss[z]], train_y)

            pred_train = reg.predict(train_X[ss[z]])
            mse_train= mean_squared_error(train_y, pred_train)
            rmse_train=mse_train**.5
            mad_train=mean_absolute_error(train_y,pred_train)

            pred_valid = reg.predict(valid_X[ss[z]])
```

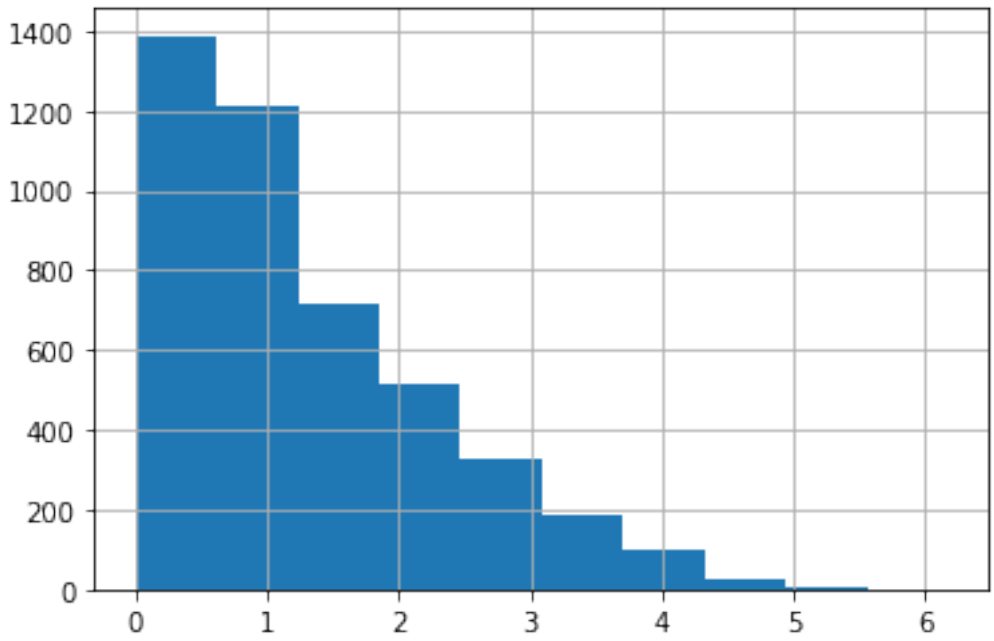
```
            mse_valid= mean_squared_error(valid_y, pred_valid)
            rmse_valid=mse_valid**.5
            mad_valid=mean_absolute_error(valid_y,pred_valid)

            if rmse_valid < low_err:
                low_err=rmse_valid
                low_err_features=list(ss[z])
                print("_"*100)
                print(low_err_features)
                print("_"*50)
                print("train mse: "+str(mse_train))
                print("train rmse: "+str(rmse_train))
                print("train mad: "+str(mad_train))
                print("valid mse: "+str(mse_valid))
                print("valid rmse: "+str(rmse_valid))
                print("valid mad: "+str(mad_valid))
                abs(valid_y-pred_valid).hist()
                plt.show()
```

[73]:
```
exhaustive(model=LinearRegression(normalize=False,n_jobs=-1),
           train_X=train_X, train_y=train_y,valid_X=valid_X,valid_y=valid_y )
```

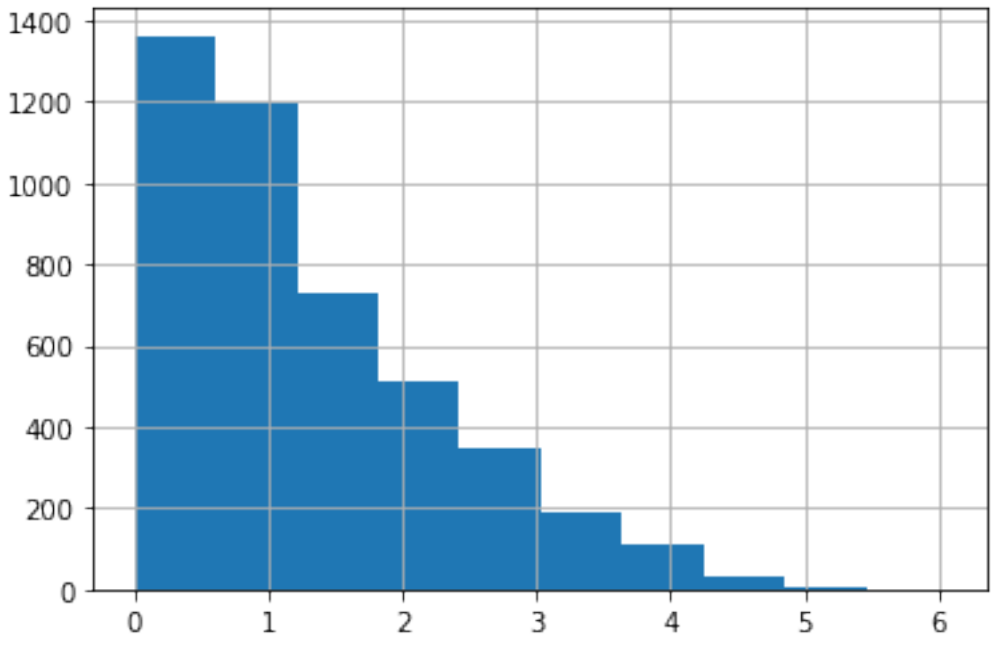
```
--------------------------------------------------
1 model(s) using 14 features

--------------------------------------------------------------------------------
--------------------
['FreeSulfurDioxide', 'LabelAppeal', 'FixedAcidity', 'ResidualSugar', 'Density',
'VolatileAcidity', 'CitricAcid', 'AcidIndex', 'pH', 'Chlorides', 'Alcohol',
'TotalSulfurDioxide', 'STARS', 'Sulphates']
--------------------------------------------------
train mse: 2.790001493519296
train rmse: 1.6703297559222539
train mad: 1.3133503316562167
valid mse: 2.716628491184453
valid rmse: 1.6482197945615302
valid mad: 1.2971813722209837
```



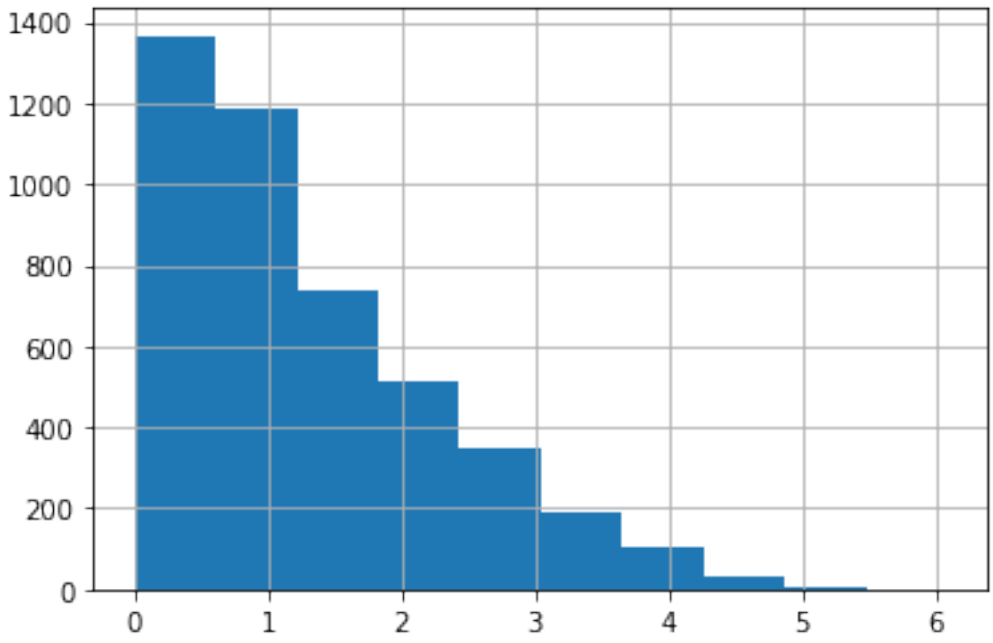

```
--------------------------------------------------
14 model(s) using 13 features
--------------------------------------------------------------------------------
--------------------
['FreeSulfurDioxide', 'LabelAppeal', 'FixedAcidity', 'ResidualSugar', 'Density',
'VolatileAcidity', 'CitricAcid', 'AcidIndex', 'Chlorides', 'Alcohol',
'TotalSulfurDioxide', 'STARS', 'Sulphates']
--------------------------------------------------
train mse: 2.794249556436931
train rmse: 1.671600896277856
train mad: 1.3145415387682173
valid mse: 2.7152970771883393
valid rmse: 1.647815850508891
valid mad: 1.2970602072911015
```



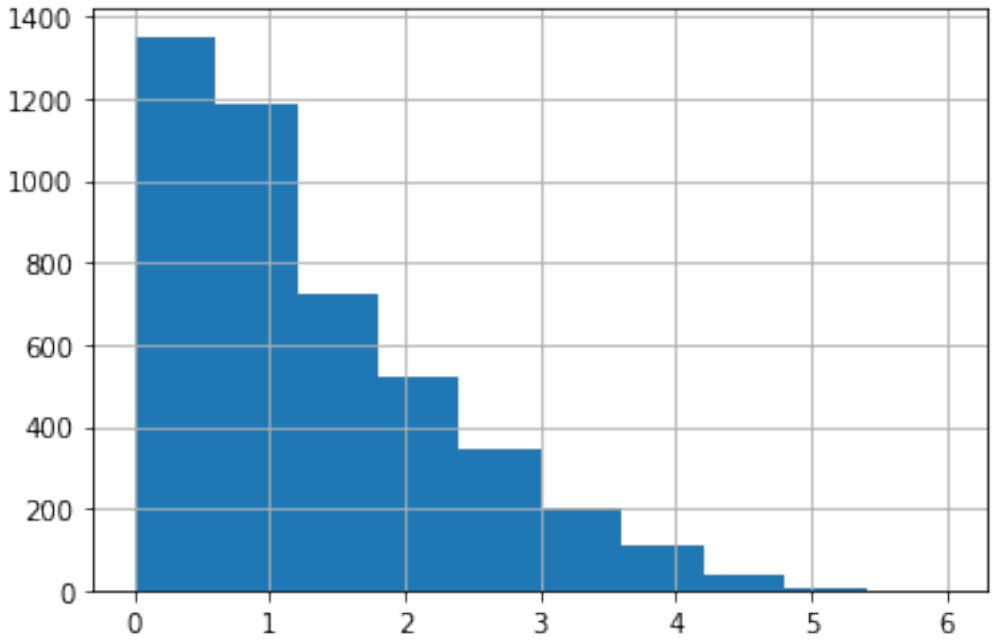

```
--------------------------------------------------------------------------------
--------------------
['FreeSulfurDioxide', 'LabelAppeal', 'FixedAcidity', 'Density',
'VolatileAcidity', 'CitricAcid', 'AcidIndex', 'pH', 'Chlorides', 'Alcohol',
'TotalSulfurDioxide', 'STARS', 'Sulphates']
--------------------------------------------------
train mse: 2.790847318073315
train rmse: 1.670582927625359
train mad: 1.3136779354331738
valid mse: 2.7140244514030605
valid rmse: 1.6474296499101442
valid mad: 1.2957674331408267
```




```
--------------------------------------------------
91 model(s) using 12 features
--------------------------------------------------------------------------------
--------------------
['FreeSulfurDioxide', 'LabelAppeal', 'FixedAcidity', 'Density',
'VolatileAcidity', 'CitricAcid', 'AcidIndex', 'Chlorides', 'Alcohol',
'TotalSulfurDioxide', 'STARS', 'Sulphates']
--------------------------------------------------
train mse: 2.7950385435514726
train rmse: 1.6718368770760719
train mad: 1.3147459896942166
valid mse: 2.712801631012163
valid rmse: 1.6470584783219335
valid mad: 1.295888954355542
```




```
--------------------------------------------------
364 model(s) using 11 features
--------------------------------------------------------------------------------
--------------------
['FreeSulfurDioxide', 'LabelAppeal', 'Density', 'VolatileAcidity', 'CitricAcid',
'AcidIndex', 'Chlorides', 'Alcohol', 'TotalSulfurDioxide', 'STARS', 'Sulphates']
--------------------------------------------------
train mse: 2.795764392186343
train rmse: 1.672053944161594
train mad: 1.314887190864838
valid mse: 2.7118929590193472
valid rmse: 1.6467826083060713
valid mad: 1.2955668232447082
```




```
--------------------------------------------------
1001 model(s) using 10 features
--------------------------------------------------
2002 model(s) using 9 features
--------------------------------------------------
3003 model(s) using 8 features
--------------------------------------------------
3432 model(s) using 7 features
--------------------------------------------------
3003 model(s) using 6 features
--------------------------------------------------
2002 model(s) using 5 features
--------------------------------------------------
1001 model(s) using 4 features
--------------------------------------------------
364 model(s) using 3 features
--------------------------------------------------
91 model(s) using 2 features
--------------------------------------------------
14 model(s) using 1 features
```

0.0.6 Observations :

364 model(s) using the below 11 features is the MULTIPLE LINEAR REGRESSION model with the least RMSE error for the Validation dataset : ['Density', 'Chlorides', 'Alcohol', 'LabelAppeal', 'AcidIndex', 'TotalSulfurDioxide', 'FreeSulfurDioxide', 'VolatileAcidity',

'CitricAcid', 'Sulphates', 'STARS']

- valid mse: 2.7118929590193472
- valid rmse: 1.6467826083060713
- valid mad: 1.2955668232447082

0.0.7 Regularization / Shrinkage:

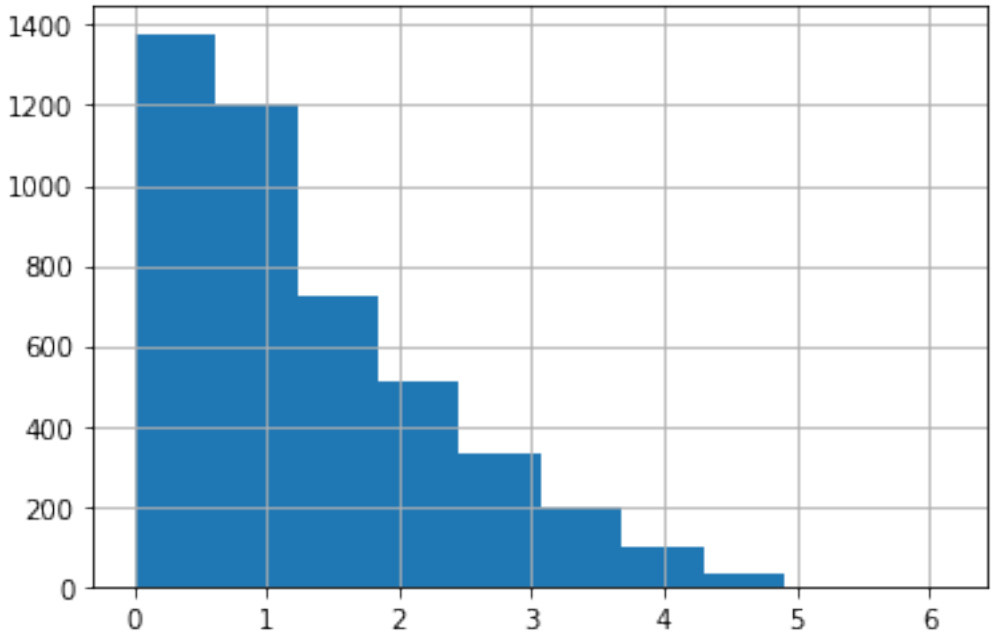
- Regularization/Shrinkage -> "shrinks" the coefficients towards zero.

[74]:
```
def reg_shrink(model,train_X,train_y,valid_X,valid_y):
        model = model
        reg  = model.fit(train_X, train_y)


        pred_train = reg.predict(train_X)
        mse_train= mean_squared_error(train_y, pred_train)
        rmse_train=mse_train**.5
        mad_train=mean_absolute_error(train_y,pred_train)

        pred_valid = reg.predict(valid_X)
        mse_valid= mean_squared_error(valid_y, pred_valid)
        rmse_valid=mse_valid**.5
        mad_valid=mean_absolute_error(valid_y,pred_valid)

        print("train mse: "+str(mse_train))
        print("train rmse: "+str(rmse_train))
        print("train mad: "+str(mad_train))
        print("valid mse: "+str(mse_valid))
        print("valid rmse: "+str(rmse_valid))
        print("valid mad: "+str(mad_valid))
        abs(valid_y-pred_valid).hist()

        coefficients=pd.DataFrame(reg.coef_)
        coefficients.index=train_X.columns
        print(coefficients)
```

[75]:
```
reg_shrink(model=LassoCV(normalize=True,cv=5),
           train_X=train_X, train_y=train_y,valid_X=valid_X,valid_y=valid_y )
```

```
train mse: 2.790033143576006
train rmse: 1.6703392300895066
train mad: 1.313546076374775
valid mse: 2.7163762268298384
valid rmse: 1.6481432664758966
valid mad: 1.2972378408043703
                           0
FixedAcidity       -0.212325
VolatileAcidity    -1.015237
```

```
CitricAcid            0.284082
ResidualSugar         0.224805
Chlorides            -0.516046
FreeSulfurDioxide     0.390058
TotalSulfurDioxide    0.691048
Density              -0.272034
pH                   -0.537041
Sulphates            -0.332735
Alcohol               0.668827
LabelAppeal           2.144188
AcidIndex            -4.500159
STARS                 1.844331
```



0.0.8 Observations :

The LASSO CV model with the least RMSE error for the Validation dataset has the below error metrics :

- valid mse: 2.7163762268298384
- valid rmse: 1.6481432664758966
- valid mad: 1.2972378408043703

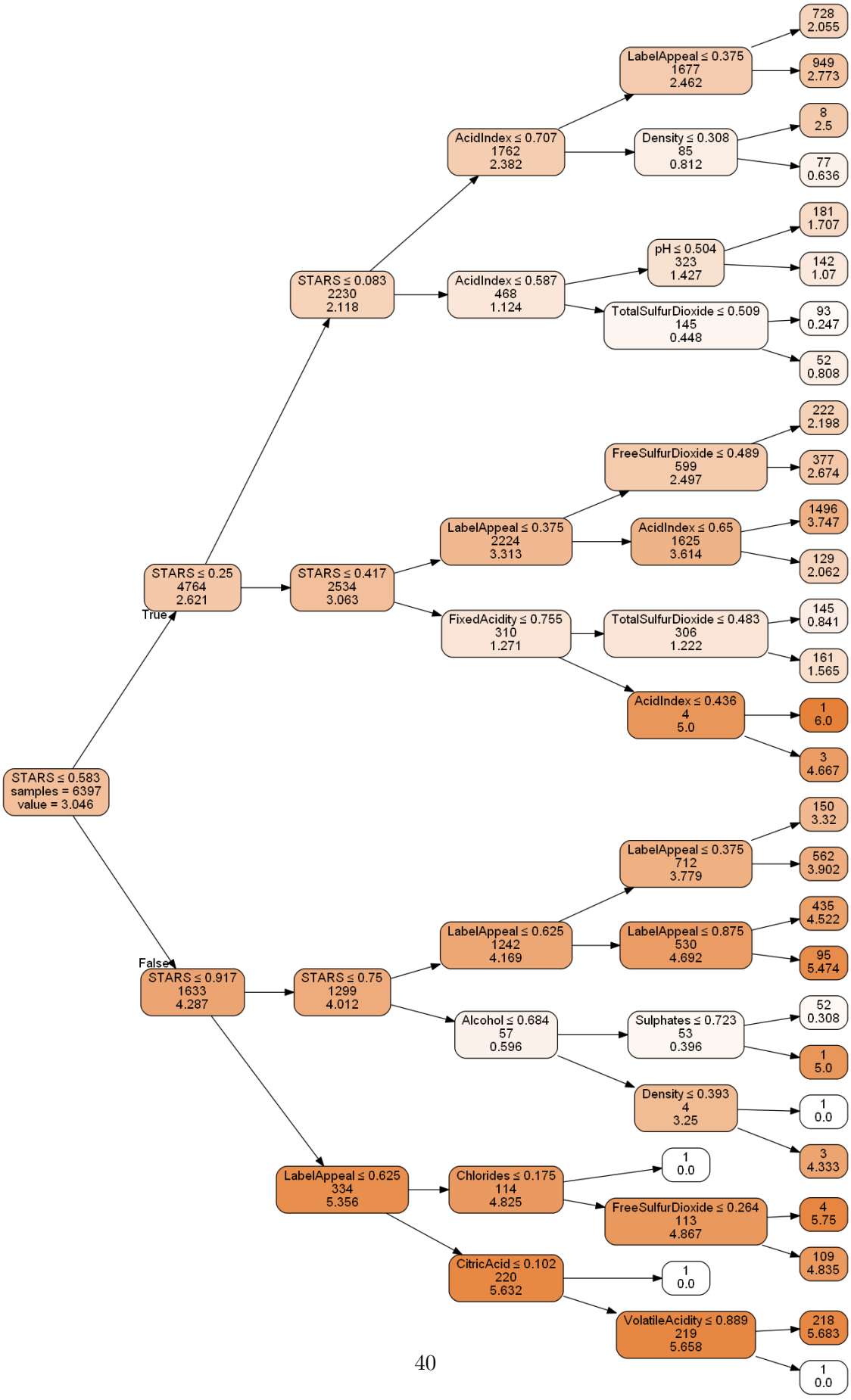
Decision Tree Regressor

[76]:
```
# Shallow tree

shallowTree = DecisionTreeRegressor(max_depth=5)
```

```
shallowTree.fit(train_X, train_y)
print('Tree has {} nodes'.format(shallowTree.tree_.node_count))
plotDecisionTree(shallowTree, feature_names=train_X.columns, rotate=True,␣
↪impurity=False)
```

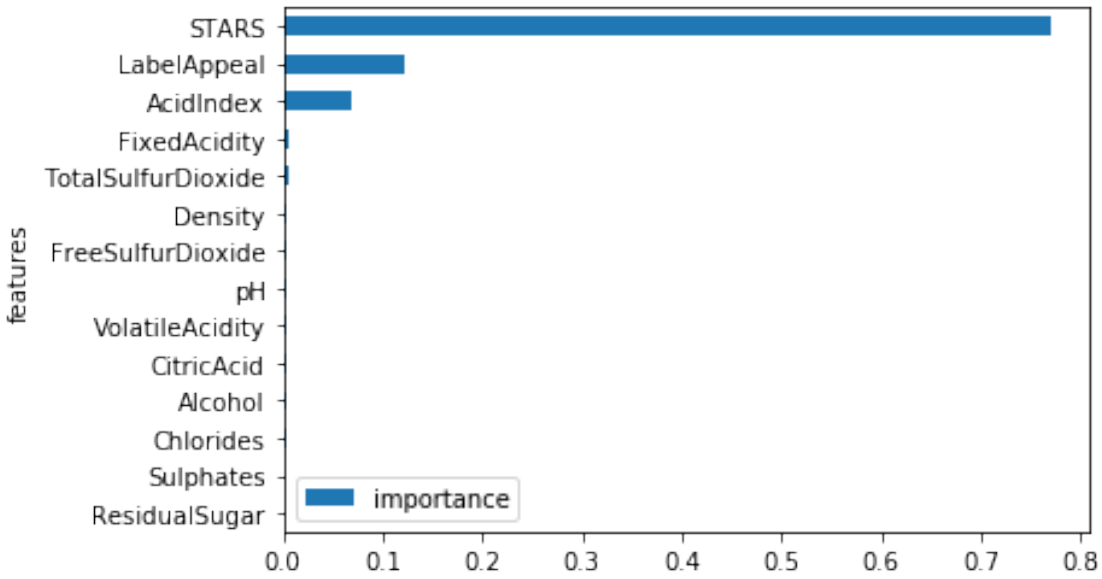
```
Tree has 59 nodes
```

[76]:


STARS ≤ 0.583
samples = 6397
value = 3.046
True
False
STARS ≤ 0.25
4764
2.621
STARS ≤ 0.917
1633
4.287
STARS ≤ 0.083
2230
2.118
STARS ≤ 0.417
2534
3.063
STARS ≤ 0.75
1299
4.012
LabelAppeal ≤ 0.625
334
5.356
AcidIndex ≤ 0.707
1762
2.382
AcidIndex ≤ 0.587
468
1.124
LabelAppeal ≤ 0.375
2224
3.313
FixedAcidity ≤ 0.755
310
1.271
LabelAppeal ≤ 0.625
1242
4.169
Alcohol ≤ 0.684
57
0.596
Chlorides ≤ 0.175
114
4.825
CitricAcid ≤ 0.102
220
5.632
LabelAppeal ≤ 0.375
1677
2.462
Density ≤ 0.308
85
0.812
pH ≤ 0.504
323
1.427
TotalSulfurDioxide ≤ 0.509
145
0.448
FreeSulfurDioxide ≤ 0.489
599
2.497
AcidIndex ≤ 0.65
1625
3.614
TotalSulfurDioxide ≤ 0.483
306
1.222
AcidIndex ≤ 0.436
4
5.0
LabelAppeal ≤ 0.375
712
3.779
LabelAppeal ≤ 0.875
530
4.692
Sulphates ≤ 0.723
53
0.396
Density ≤ 0.393
4
3.25
FreeSulfurDioxide ≤ 0.264
113
4.867
VolatileAcidity ≤ 0.889
219
5.658
728
2.055
949
2.773
8
2.5
77
0.636
181
1.707
142
1.07
93
0.247
52
0.808
222
2.198
377
2.674
1496
3.747
129
2.062
145
0.841
161
1.565
1
6.0
3
4.667
150
3.32
562
3.902
435
4.522
95
5.474
52
0.308
1
5.0
1
0.0
3
4.333
1
0.0
4
5.75
109
4.835
1
0.0
218
5.683
1
0.0

[77]:
```
# Variable importance

importance_shallow = pd.DataFrame({'features': train_X.columns,
                           'importance': shallowTree.feature_importances_})
importance_shallow.index=importance_shallow.features
importance_shallow.sort_values(by='importance', ascending=True).plot.barh()
```

[77]: <matplotlib.axes._subplots.AxesSubplot at 0x1edea374648>



STARS, LabelAppeal, ACidIndex and VolatileAcidity seem to be the prime contributers to TARGET in the shallow tree

[78]:
```
print("Prediction error of Validation set for the Shallow Tree")
print("RMSE: ", str(mean_squared_error(valid_y, shallowTree.predict(valid_X))**.
 ↪5))
```

```
Prediction error of Validation set for the Shallow Tree
RMSE:  1.5707220727754558
```

Random Forest Regressor

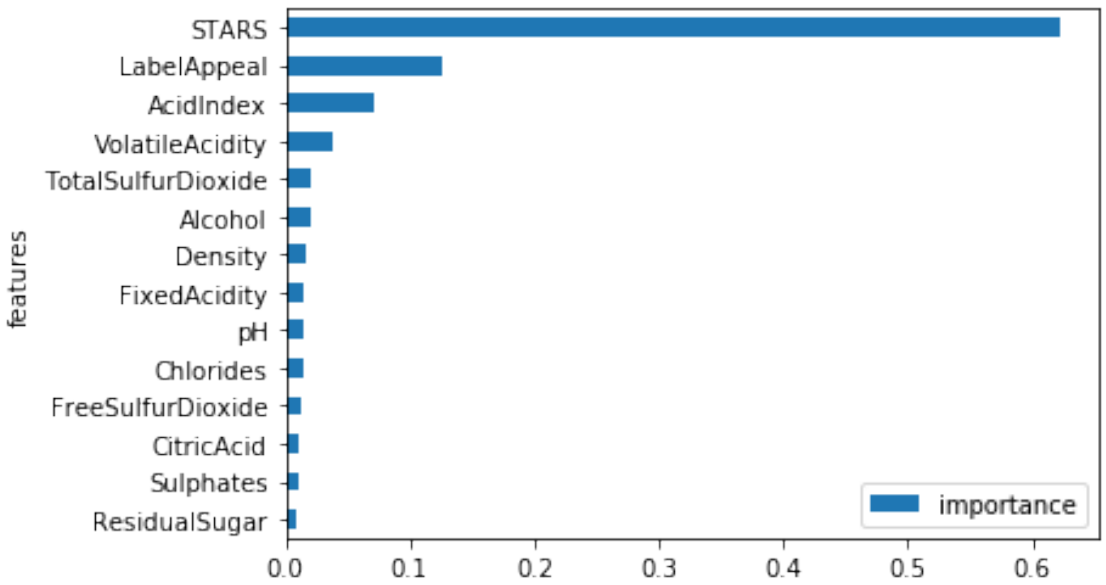
[79]:
```
# user grid search to find optimized tree - RandomForestRegressor

param_grid = {
    'max_depth': [9],
    'min_samples_split':[5],
```

```
    'max_leaf_nodes': [52],
}
gridSearch = GridSearchCV(RandomForestRegressor(random_state=1),
                          param_grid, cv=5, n_jobs=-1)
gridSearch.fit(train_X, train_y)
print('Improved parameters: ', gridSearch.best_params_)

rf = gridSearch.best_estimator_

print("RMSE: "+str(mean_squared_error(valid_y, rf.predict(valid_X))**.5))
```

```
Improved parameters:  {'max_depth': 9, 'max_leaf_nodes': 52,
'min_samples_split': 5}
RMSE: 1.5071431234386243
```

[80]:
```
# Variable importance
importance = pd.DataFrame({'features': train_X.columns,
                           'importance': rf.feature_importances_})
importance.index=importance.features
importance.sort_values(by='importance', ascending=True).plot.barh()
```

[80]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x1edea685888>
```



Gradient Boosting Regressor

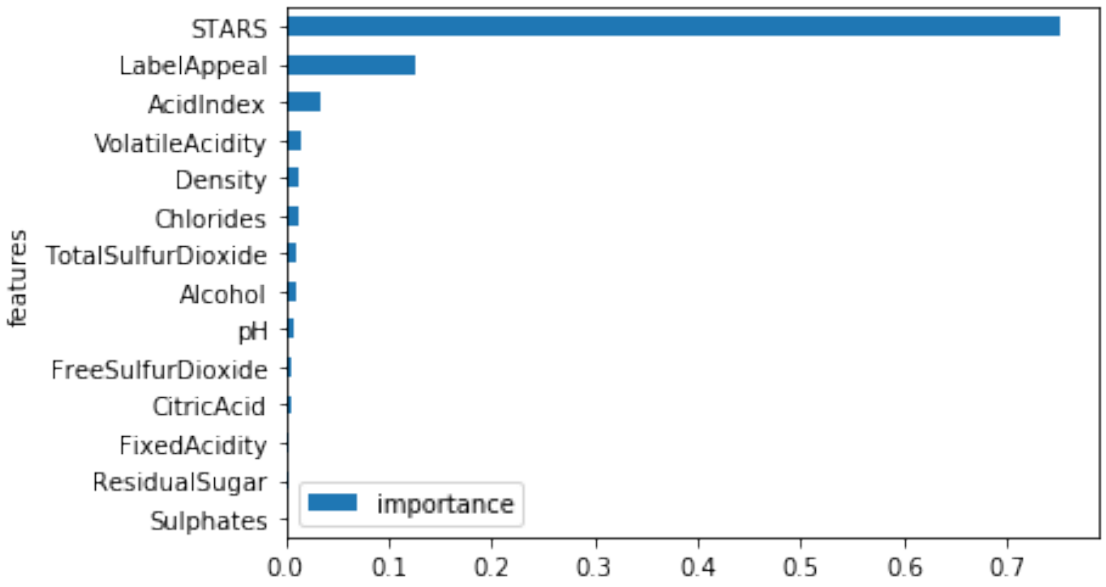
[85]:
```
# user grid search to find optimized tree - GradientBoostingRegressor

param_grid = {
```

```
    'learning_rate':list(np.arange(0.01,0.22,.01)),  #choose initial high␣
 ↪learning rate
    'min_samples_split': list(np.arange(3,7)),
    'max_leaf_nodes': list(np.arange(4,7)),
}

gridSearch = GridSearchCV(GradientBoostingRegressor(random_state=1),
                          param_grid, cv=5, n_jobs=-1)
gridSearch.fit(train_X, train_y)
print('Improved parameters: ', gridSearch.best_params_)

gbm = gridSearch.best_estimator_

print("RMSE: "+str(mean_squared_error(valid_y, gbm.predict(valid_X))**.5))
```

```
Improved parameters:  {'learning_rate': 0.19, 'max_leaf_nodes': 6,
'min_samples_split': 5}
RMSE: 1.4719045877616919
```

[68]:
```
# Variable importance
importance = pd.DataFrame({'features': train_X.columns,
                           'importance': gbm.feature_importances_})
importance.index=importance.features
importance.sort_values(by='importance', ascending=True).plot.barh()
```

[68]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x2a0a1ddc048>
```



AdaBoost Regressor

[82]:
```
clf = AdaBoostRegressor(DecisionTreeRegressor(max_depth=8,min_samples_split=5,
 ↪min_samples_leaf=5,max_features=14,random_state=1),
                        n_estimators=100, random_state=1)

param_grid = {}
gridSearch = GridSearchCV(clf, param_grid, cv=5, n_jobs=-1)
gridSearch.fit(train_X, train_y)

clf = gridSearch.best_estimator_

print(clf)
print("RMSE of Validation: "+str((mean_squared_error(valid_y, clf.
 ↪predict(valid_X))**.5)))
print("RMSE of Training: "+str((mean_squared_error(train_y, clf.
 ↪predict(train_X))**.5)))
```

```
AdaBoostRegressor(base_estimator=DecisionTreeRegressor(ccp_alpha=0.0,
                                                       criterion='mse',
                                                       max_depth=8,
                                                       max_features=14,
                                                       max_leaf_nodes=None,
min_impurity_decrease=0.0,
                                                       min_impurity_split=None,
                                                       min_samples_leaf=5,
                                                       min_samples_split=5,
min_weight_fraction_leaf=0.0,
                                                       presort='deprecated',
                                                       random_state=1,
                                                       splitter='best'),
                  learning_rate=1.0, loss='linear', n_estimators=100,
                  random_state=1)
RMSE of Validation: 1.6430020448391252
RMSE of Training: 1.3742985204508331
```

Bagging Regressor

[83]:
```
clf = BaggingRegressor(DecisionTreeRegressor(max_depth=6,min_samples_split=2,
 ↪min_samples_leaf=5,max_features=10,random_state=1),
                       n_estimators=100, random_state=1)

param_grid = {}
gridSearch = GridSearchCV(clf, param_grid, cv=5, n_jobs=-1)
gridSearch.fit(train_X, train_y)
```

```
clf = gridSearch.best_estimator_

print(clf)
print("RMSE of Validation: "+str((mean_squared_error(valid_y, clf.
 ↪predict(valid_X))**.5)))
print("RMSE of Training: "+str((mean_squared_error(train_y, clf.
 ↪predict(train_X))**.5)))
```

```
BaggingRegressor(base_estimator=DecisionTreeRegressor(ccp_alpha=0.0,
                                                      criterion='mse',
                                                      max_depth=6,
                                                      max_features=10,
                                                      max_leaf_nodes=None,
                                                      min_impurity_decrease=0.0,
                                                      min_impurity_split=None,
                                                      min_samples_leaf=5,
                                                      min_samples_split=2,
min_weight_fraction_leaf=0.0,
                                                      presort='deprecated',
                                                      random_state=1,
                                                      splitter='best'),
                 bootstrap=True, bootstrap_features=False, max_features=1.0,
                 max_samples=1.0, n_estimators=100, n_jobs=None,
                 oob_score=False, random_state=1, verbose=0, warm_start=False)
RMSE of Validation: 1.5054425258629212
RMSE of Training: 1.4298412821838515
```

0.0.9 Observations :

The Bagging Regressor model has lower RMSE error for the Validation dataset than the AdaBoost model :

- Bagging Regressor RMSE: 1.5054425258629212
- AdaBoost Regressor: 1.6430020448391252

MLP Regressor

[84]:
```
mlp_model = MLPRegressor(hidden_layer_sizes=(100,), activation='relu',␣
 ↪solver='lbfgs')

param_grid = {}
gridSearch = GridSearchCV(mlp_model, param_grid, cv=5, n_jobs=-1)
gridSearch.fit(train_X, train_y)

mlp_model = gridSearch.best_estimator_

print(mlp_model)
```

```
print("RMSE of Validation: "+str((mean_squared_error(valid_y, mlp_model.
 ↪predict(valid_X))**.5)))
print("RMSE of Training: "+str((mean_squared_error(train_y, mlp_model.
 ↪predict(train_X))**.5)))
```

```
MLPRegressor(activation='relu', alpha=0.0001, batch_size='auto', beta_1=0.9,
             beta_2=0.999, early_stopping=False, epsilon=1e-08,
             hidden_layer_sizes=(100,), learning_rate='constant',
             learning_rate_init=0.001, max_fun=15000, max_iter=200,
             momentum=0.9, n_iter_no_change=10, nesterovs_momentum=True,
             power_t=0.5, random_state=None, shuffle=True, solver='lbfgs',
             tol=0.0001, validation_fraction=0.1, verbose=False,
             warm_start=False)
RMSE of Validation: 1.602453487496162
RMSE of Training: 1.5953849964181932
```

4. MODEL SELECTION

The Models and the associated RMSE for the WINE database are summarized below:

Model	RMSE
Linear Regression	1.6467826083060713
LassoCV model	1.6481432664758966
Decision Tree Regressor	1.5707220727754558
Random Forest Regressor	1.5071431234386243
Gradient Boosting Regressor	1.4719045877616919
AdaBoost Regressor	1.6430020448391252
Bagging Regressor	1.5054425258629212
MLP Regressor	1.602453487496162

CONCLUSION

- Analysis of the data reveals that the chemical predictor variables do not add sufficient predictive power above the STARS ratings and LabelAppeal measurement.
- It is evident from this dataset that wine sales are largely dependent on the ratings of wine experts and how much customers are appealed by the Label.
- Dataset has been analyzed using PCA and grouped into 4 distinct clusters.Any future prediction of a test data can classify the TARGET sales into one of these clusters.

0.0.10 Model Selection & Justification

- The Gradient Boosting Regressor & Bagging Regressor seem to have the lowest RMSE for the validation set.
- They have a low implementation cost as compared to other models and can thus be used as a predictive algorithm to determine Wine sales

The Wine dataset was explored, analyzed, divided into clusters and predictive

models were built for future analysis. The models did not scale the TARGET outcome variable thus making prediction a whole lot easier. The Gradient Boosting and Bagging Regressor models could be used for wine sales prediction