Akshay Bhala

Extra Credit Assignment

05/08/2020

Introduction: Predicting whether the quality of wine is bad, average or good.

Link to the data set:

https://archive.ics.uci.edu/ml/datasets/wine+quality

```
In [0]:
```

```
import numpy as np
import pandas as pd
import pickle
import matplotlib.pyplot as plt
import seaborn as sns
import plotly.express as px
from scipy import stats
import statsmodels.api as sm
from scipy import stats
from sklearn.model_selection import train_test_split
from sklearn.metrics import classification_report,confusion_matrix
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
from matplotlib import pyplot
from sklearn.model_selection import GridSearchCV
```

```
In [2]:
```

```
df = pd.read_csv('winequality-red.csv')
df.shape
```

Out[2]:

(1599, 12)

In [3]:

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

Out[3]:

```
fixed acidity
volatile acidity
citric acid
residual sugar
chlorides
                     0
free sulfur dioxide
total sulfur dioxide 0
                     0
density
sulphates
                     0
alcohol
                      0
quality
dtype: int64
```

Analysis: No Null Values

```
In [4]:
```

```
df = df.drop_duplicates()
df.shape
```

Out[4]:

(1359, 12)

Analysis: Removed 240 duplicate values

In [5]:

```
plot = plt.figure(figsize=(5,5))
plt.title("Citric Acid Vs Quality")
sns.barplot(data=df,x="quality",y="citric acid",palette="pastel")

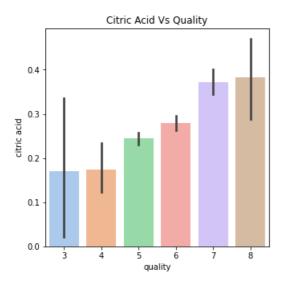
plot = plt.figure(figsize=(5,5))
plt.title("volatile Acidity Vs Quality")
sns.barplot(data=df,x="quality",y="volatile acidity",palette="rocket")

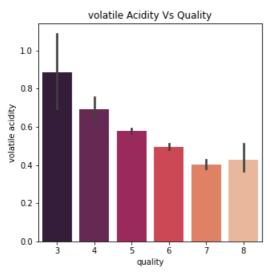
plot = plt.figure(figsize=(5,5))
plt.title("Chlorides Vs Quality")
sns.barplot(data=df,x="quality",y="chlorides",palette="pastel")

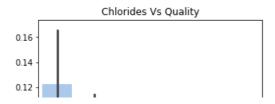
plot = plt.figure(figsize=(5,5))
plt.title("sulphates Vs Quality")
sns.barplot(data=df,x="quality",y="sulphates",palette="pastel")
```

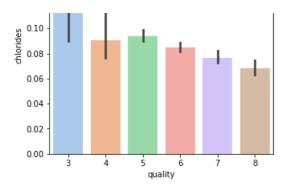
Out[5]:

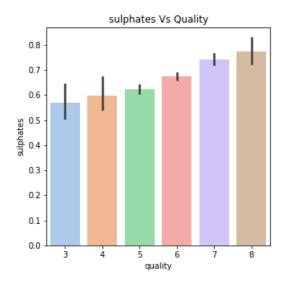
<matplotlib.axes._subplots.AxesSubplot at 0x7f1918f00588>











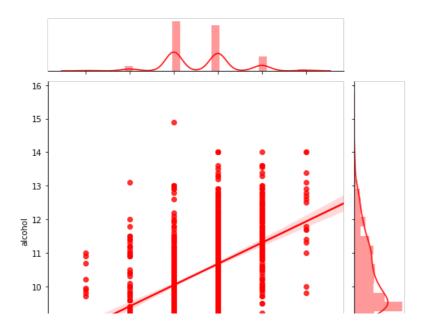
Analysis: Both citric acid and sulphates increases as the quality increases whereas chlorides and volatile acidity decreases as quality increases.

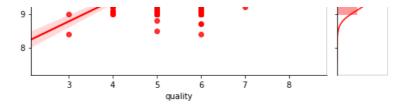
In [6]:

Out[6]:

<seaborn.axisgrid.JointGrid at 0x7f1919764e80>

<Figure size 360x360 with 0 Axes>





Analysis: Content of Alcohol increases as quality increases

In [7]:

```
df.describe()
```

Out[7]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	рН	sulph
count	1359.000000	1359.000000	1359.000000	1359.000000	1359.000000	1359.000000	1359.000000	1359.000000	1359.000000	1359.00
mean	8.310596	0.529478	0.272333	2.523400	0.088124	15.893304	46.825975	0.996709	3.309787	0.65
std	1.736990	0.183031	0.195537	1.352314	0.049377	10.447270	33.408946	0.001869	0.155036	0.17
min	4.600000	0.120000	0.000000	0.900000	0.012000	1.000000	6.000000	0.990070	2.740000	0.33
25%	7.100000	0.390000	0.090000	1.900000	0.070000	7.000000	22.000000	0.995600	3.210000	0.55
50%	7.900000	0.520000	0.260000	2.200000	0.079000	14.000000	38.000000	0.996700	3.310000	0.62
75%	9.200000	0.640000	0.430000	2.600000	0.091000	21.000000	63.000000	0.997820	3.400000	0.73
max	15.900000	1.580000	1.000000	15.500000	0.611000	72.000000	289.000000	1.003690	4.010000	2.00
4										Þ

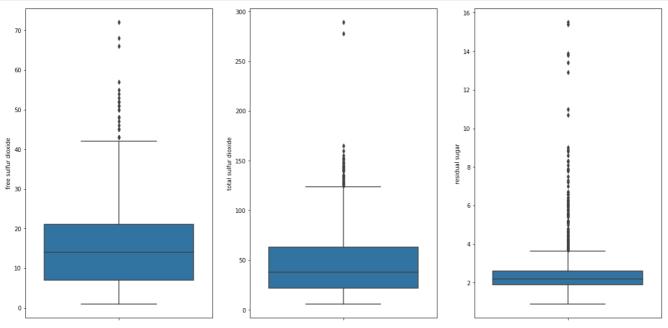
In [8]:

```
plt.figure(figsize=(20,10))
plt.subplot(1,3,1)
sns.boxplot(y= df['free sulfur dioxide'])

plt.subplot(1,3,2)
sns.boxplot(y=df['total sulfur dioxide'])

plt.subplot(1,3,3)
sns.boxplot(y=df['residual sugar'])

plt.show()
```



Analysis: After looking at data distribution i found there are some outliers which i treated using inter quartile range.

```
In [0]:
def outliers IQR(data, col):
    lower quartile = data[col].quantile(0.25)
    upper_quartile = data[col].quantile(0.75)
    IQR = upper_quartile - lower_quartile
outlier_thresh = 1.5 * IQR
    return data[data[col].between((lower quartile - outlier thresh), (upper quartile + outlier thre
sh))]
df = outliers_IQR(df, 'free sulfur dioxide')
df = outliers_IQR(df, 'total sulfur dioxide')
df = outliers_IQR(df, 'residual sugar')
df = outliers_IQR(df, 'fixed acidity')
In [10]:
df.groupby("quality")["quality"].count()
Out[10]:
quality
3
      44
4
     476
     475
6
    135
7
8
     14
Name: quality, dtype: int64
Grouping Quality into Good and Bad i.e a classification problem
In [0]:
bins =(2,5,8)
names =["bad","good"]
df["quality"] = pd.cut(df["quality"],bins=bins,labels=names)
In [12]:
df.groupby("quality")["quality"].count()
Out[12]:
quality
        528
bad
good
       624
Name: quality, dtype: int64
One hot encoding aand splitting into train and test
In [0]:
from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
df["quality"] = le.fit_transform(df["quality"])
X=df.drop("quality",axis=1)
y = df["quality"]
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.7, test_size=0.3,
random state=0)
ns probs = [0 for in range(len(y test))]
```

Machine Learning Models

1. Random Forest

```
from sklearn.ensemble import RandomForestClassifier
rf = RandomForestClassifier()
rf.fit(X_train, y_train)
predictions = rf.predict(X test)
print("\n Confusion Matrix \n", confusion matrix(y test, predictions))
print("\n Classification Report \n", classification_report(y_test, predictions))
 Confusion Matrix
 [[106 54]
 [ 38 148]]
 Classification Report
              precision recall f1-score
                                             support
                                  0.70
           Ω
                  0.74
                            0.66
                                                 160
           1
                  0.73
                            0.80
                                      0.76
                                                 186
                                      0.73
                                                 346
   accuracy
                  0.73 0.73
                                     0.73
                                                 346
  macro avg
                  0.73
                           0.73
                                      0.73
                                                 346
weighted avg
In [29]:
from sklearn.ensemble import RandomForestClassifier
param grid = { 'bootstrap': [True],
   'max depth': [10, 50, 100],
    'max features': [2, 3],
    'min_samples_leaf': [3, 5],
    'min_samples_split': [8, 10, 12],
    'n_estimators': [100, 200, 300]}
grid = GridSearchCV(RandomForestClassifier(),param grid,n jobs=5)
grid = grid.fit(X_train,y_train)
grid predictions = grid.predict(X test)
print("\n Best Parameters \n", grid.best_params_)
Best Parameters
 {'bootstrap': True, 'max depth': 50, 'max features': 2, 'min samples leaf': 3,
'min_samples_split': 12, 'n_estimators': 200}
In [30]:
print("\n Confusion Matrix \n",confusion_matrix(y_test,grid_predictions))
print("\n Classification Report \n", classification report(y test, grid predictions))
Confusion Matrix
 [[109 51]
 [ 37 149]]
 Classification Report
              precision recall f1-score support
                 0.75
                           0.68
           Ω
                                     0.71
                                                 160
                  0.74
                            0.80
                                      0.77
                                                 186
                                      0.75
                                                346
   accuracy
                  0.75
                           0.74
                                     0.74
                                                 346
  macro avg
                                      0.74
                                                 346
weighted avg
                  0.75
                           0.75
In [34]:
tune1 = pd.DataFrame(data=None, index=
['RF','RF Best'],columns=['Accuracy','Precision','Recall','F1 Score','Hyper Parameters'])
tune1['Accuracy']= [0.73,0.75]
tune1['Precision'] = [0.73,0.75]
tune1['Recall']= [0.73,0.74]
tune1['F1 Score'] = [0.73,0.74]
tune1['Hyper_Parameters']= [['max_depth = None','n_estimator = 100','bootstrap = True',
'max features = auto', 'min samples leaf = 1', 'min samples split = 2'], ['max depth =
50', 'n estimator = 200', 'bootstrap = True', 'max features = 2', 'min samples leaf = 3',
```

```
'min_samples_split = 12']]
tune1
```

Out[34]:

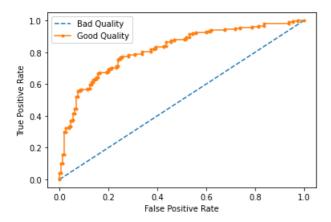
Hyper_Parameters	F1_Score	Recall	Precision	Accuracy	
[max_depth = None, n_estimator = 100, bootstra	0.73	0.73	0.73	0.73	RF
[max_depth = 50, n_estimator = 200, bootstrap	0.74	0.74	0.75	0.75	RF_Best

Analysis: A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting.n_estimators represents the number of trees in the forest. Usually the higher the number of trees the better to learn the data. However, adding a lot of trees can slow down the training process considerably. max_depth represents the depth of each tree in the forest. The deeper the tree, the more splits it has and it captures more information about the data. As Depth increases there is a chance of overfitting. min_samples_split represents the minimum number of samples required to split an internal node. When we increase this parameter, each tree in the forest becomes more constrained as it has to consider more samples at each node. There is a chance of underfitting when we require all of the sample at each node.min_samples_leaf is The minimum number of samples required to be at a leaf node. This parameter is similar to min_samples_splits, however, this describe the minimum number of samples of samples at the leafs, the base of the tree.Increasing this value can cause underfitting.max_features represents the number of features to consider when looking for the best split. As this value increases there is a chance of overfitting. After tuning random forest model the accuracy remained constant at 73% but recall and f1 score increased by 1% which is now 74%.

In [18]:

```
lr probs = grid.predict proba(X test)
lr probs = lr_probs[:, 1]
ns auc = roc_auc_score(y_test, ns_probs)
lr auc = roc auc score(y test, lr probs)
# summarize scores
print('No Disease: ROC AUC=%.3f' % (ns auc))
print('Disease: ROC AUC=%.3f' % (lr auc))
# calculate roc curves
ns_fpr, ns_tpr, _ = roc_curve(y_test, ns_probs)
lr_fpr, lr_tpr, _ = roc_curve(y_test, lr_probs)
# plot the roc curve for the model
pyplot.plot(ns fpr, ns tpr, linestyle='--', label='Bad Quality')
pyplot.plot(lr_fpr, lr_tpr, marker='.', label='Good Quality')
# axis labels
pyplot.xlabel('False Positive Rate')
pyplot.ylabel('True Positive Rate')
# show the legend
pyplot.legend()
# show the plot
pyplot.show()
```

No Disease: ROC AUC=0.500 Disease: ROC AUC=0.818



Analysis: The Roc curve with an auc score of 0.818 proves that our model is a good fit

```
In [19]:
```

In [35]:

```
from sklearn.svm import SVC
svm L = SVC()
svm_L.fit(X_train, y_train)
Out[19]:
SVC(C=1.0, break_ties=False, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='scale', kernel='rbf',
    max iter=-1, probability=False, random state=None, shrinking=True,
    tol=0.001, verbose=False)
In [20]:
predictions = svm L.predict(X test)
print("\n Confusion Matrix \n", confusion_matrix(y_test, predictions))
print("\n Classification report \n", classification report(y test, predictions))
 Confusion Matrix
 [[ 46 114]
 [ 18 168]]
 Classification report
              precision
                          recall f1-score
                                               support
           0
                   0.72
                             0.29
                                       0.41
                                                  160
           1
                   0.60
                            0.90
                                       0.72
                                                  186
   accuracy
                                       0.62
                                                  346
                           0.60
                  0.66
                                       0.56
                                                  346
   macro avg
                                       0.58
weighted avg
                   0.65
                             0.62
                                                  346
In [21]:
param grid = {'C': [0.1,1,10], 'kernel': ['linear','rbf'],'probability' : [True]}
grid = GridSearchCV(SVC(),param_grid,n_jobs=3)
grid = grid.fit(X_train,y_train)
grid predictions = grid.predict(X test)
print("\n Best Parameters \n", grid.best_params_)
 Best Parameters
 {'C': 10, 'kernel': 'linear', 'probability': True}
In [22]:
predictions = grid.predict(X test)
print("\n Confusion Matrix \n", confusion_matrix(y_test, grid_predictions))
print("\n Classification report \n",classification_report(y_test,grid_predictions))
 Confusion Matrix
 [[118 42]
 [ 44 142]]
 Classification report
              precision
                           recall f1-score
                                               support
           0
                  0.73
                             0.74
                                       0.73
                                                  160
           1
                   0.77
                             0.76
                                       0.77
                                                  186
                                       0.75
                                                  346
   accuracy
                  0.75
                            0.75
   macro avg
                                       0.75
                                                  346
                   0.75
                             0.75
                                       0.75
                                                  346
weighted avg
```

Line 1 and Distriction (data Water States Classed Large District 1 and 1

Out[35]:

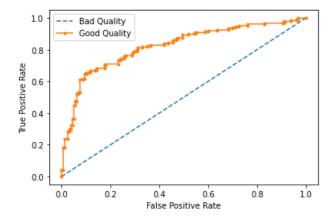
	Accuracy	Precision	Recall	F1_Score	Hyper_Parameters
svc	0.62	0.66	0.60	0.56	[C = 1, kernel = rbf]
SVC_Best	0.75	0.75	0.75	0.75	[C = 10, kernel = linear]

Analysis: C is the penalty parameter of the error term. It controls the trade off between smooth decision boundary and classifying the training points correctly. Increasing C values may lead to overfitting the training data. As we go beyond C = 10 there is a chance of overfitting. As i hypertuned both kernel and penalty parameter the model showed significant improvent i.e accuracy increased from 62% to 75% as well as f1 has increased from 56% to 75% and as the dataset is balanced i am using accuracy as the performance metric.

In [23]:

```
lr probs = grid.predict proba(X test)
lr probs = lr probs[:, 1]
ns auc = roc auc score(y test, ns probs)
lr_auc = roc_auc_score(y_test, lr_probs)
# summarize scores
print('No Disease: ROC AUC=%.3f' % (ns auc))
print('Disease: ROC AUC=%.3f' % (lr auc))
# calculate roc curves
ns_fpr, ns_tpr, _ = roc_curve(y_test, ns_probs)
lr_fpr, lr_tpr, _ = roc_curve(y_test, lr_probs)
# plot the roc curve for the model
pyplot.plot(ns fpr, ns tpr, linestyle='--', label='Bad Quality')
pyplot.plot(lr_fpr, lr_tpr, marker='.', label='Good Quality')
# axis labels
pyplot.xlabel('False Positive Rate')
pyplot.ylabel('True Positive Rate')
# show the legend
pyplot.legend()
# show the plot
pyplot.show()
```

No Disease: ROC AUC=0.500 Disease: ROC AUC=0.823



Analysis: The roc curve shows that our model is a good fit and has an auc score of 0.823

In [37]:

```
tune1 = pd.DataFrame(data=None, index=
['RF_Best','SVC_Best'],columns=['Accuracy','Precision','Recall','F1_Score','Hyper_Parameters'])
```

```
tune1['Accuracy']= [0.75,0.75]
tune1['Precision']= [0.75,0.75]
tune1['Recall']= [0.74,0.75]
tune1['F1_Score']= [0.74,0.75]
tune1['Hyper_Parameters']= [['max_depth = 50','n_estimator = 200','bootstrap = True',
'max_features = 2','min_samples_leaf = 3', 'min_samples_split = 12'],['C = 10', 'kernel = linear']
]
tune1
```

Out[37]:

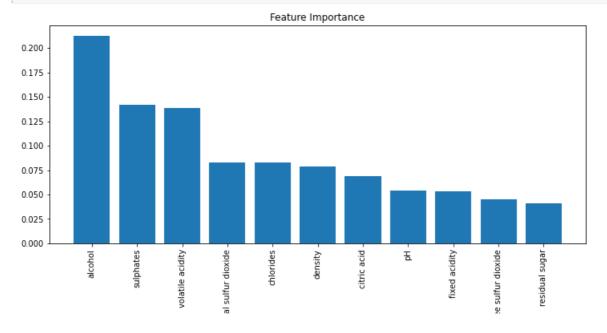
Hyper_Parameters	F1_Score	Recall	Precision	Accuracy	
[max_depth = 50, n_estimator = 200, bootstrap	0.74	0.74	0.75	0.75	RF_Best
[C = 10, kernel = linear]	0.75	0.75	0.75	0.75	SVC_Best

Analysis: Both the machine learning models showed same accuracy which is 75%. Hence i used random forest for getting feature importance.

Feature Importance

```
In [24]:
```

```
rf =
RandomForestClassifier(bootstrap=True, max depth=50, max features=2, min samples leaf=5, min samples sp
lit=10, n estimators=200)
model = rf.fit(X train, y train)
importances = model.feature importances
indices = np.argsort(importances)[::-1]
feature names = list(X.columns)
# Rearrange feature names so they match the sorted feature importances
names = [feature names[i] for i in indices]
# Create plot
plt.figure(figsize=(12,5))
# Create plot title
plt.title("Feature Importance")
# Add bars
plt.bar(range(X.shape[1]), importances[indices])
# Add feature names as x-axis labels
plt.xticks(range(X.shape[1]), names, rotation=90)
# Show plot
plt.show()
```



tot fre

Analysis: Alcohol, Sulphates, and volatile acidity are the 3 most important features used to predict the quality of wine.

In [0]: