WINE QUALITY ANALYSIS IN VINHO VERDE WINE

By

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Introduction

Wine quality is known to be a very subjective topic. Wine taste, smell, and consistency will vary depending on many factors. Type of fruit, sugar content, age, temperature, pH level, additives, and more can affect how a glass of wine tastes to the consumer. Additionally, the consumer's taste pallet, aversion to alcohol content, and other external factors will further change how the wine is perceived. Pinpointing what "quality" truly means in terms of wine is a difficult task, but it is heavily studied for wine companies to produce higher quality products. Analyzing data gathered from wine studies can give insight into the subjectivity.

In this report, two datasets of wine from a popular Portuguese wine company called Vinho Verde are analyzed. Two types of wine are represented: red wine and white wine. They are separated since they are drastically different in taste and composition. Each dataset contains 12 attributes. There are 11 physicochemical attributes, measured and recorded by an official certification entity dealing with wine quality and marketing. The last attribute is Quality, attained through blind tastes, and rated on a scale from 0, meaning very bad, to 10, meaning excellent.

In our models, we focus on 2 attributes: pH and alcohol. The "pH" attribute quantifies the acidity or basic levels of the sample wine on a scale from 0 (very acidic) to 14 (very basic). The "alcohol" attribute describes how much alcohol is in the wine, measured in percent per volume. Through statistical inference, predictions about wine quality and the effects of these attributes can be made with a degree of confidence. Our models indicate that lowering pH levels while increasing alcohol content can lead to an increase in wine quality. Knowing this may be desirable for wine companies and their constituents because understanding the factors that increase overall wine quality can lead to improvements in production processes and profitability.

Data Cleaning and Preparation

Wines are often identified by their physicochemical attributes and sensory test to characterize the overall composition. Physicochemical attributes such as fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol in relation to a quality sensory test by individuals determine the quality of a wine. Much of the raw data is gathered through physicochemical laboratory test to quantify each attribute. To develop accurate and precise analysis the raw data provided from these tests were cleaned by developing boxplots regarding each variable to remove any anomalies. Additionally, published papers regarding the same dataset state, "during the preprocessing stage, the database was transformed to include a distinct wine sample (with all tests) per row. To avoid discarding examples, only the most common physicochemical tests were selected". Therefore, much of the data was optimized by researchers conducting the tests resulting in the raw dataset provided. By removing outliers from our data set we can interpret more accurate conclusion and develop an accurate model. The table below shows the significance of each physicochemical attribute on the composition of wine. Having a better understanding of these variables will allow for a better understanding of the data.

Table 1: Physicochemical Attributes

	Effects
fixed acidity	Provides wine with fresh and vibrant taste
volatile acidity	Measure of wines acid, acetic acid
citric acid	increase acidity, complements a specific flavor or prevent ferric hazes
residual sugar	Sweetness of the wine
chlorides	Saltiness of the wine
free sulfur dioxide	Unreacted ciomponents
total sulfur dioxide	Binds with pigments and phenolics
density	.99g/mL
pH	Most wines are slightly acidic
sulphates	Preserver and enhancer of wine
alcohol	Around 12%, higher in red
quality	Human expert opinion

Exploratory Data Analysis

General Descriptive Statistics

The data to be analyzed consists of two different datasets: red wine and white wine. The datasets were divided into red and white wine due to the difference in taste and appearance. The red wine dataset contains 1599 samples, and the white wine dataset contains 4898 samples. In both datasets, there are 12 characteristics: 11 physicochemical attributes and 1 quality attribute. The physicochemical attributes are independent variables, and the quality attribute is the dependent variable. Table 1 shows general descriptive statistics of each dataset's attributes.

Table 22: General Descriptive Statistics

	RED WINE (1599 SAMPLES)				WHITE WINE (4898 SAMPLES)			
	Mean	**Std**	**Min**	**Max**	**Mean**	**Std**	**Min**	**Max**
FIXED ACIDITY	8.32	1.74	4.60	15.90	6.86	0.84	3.80	14.20
VOLATILE ACIDITY	0.53	0.18	0.12	1.58	0.28	0.10	0.08	1.10
CITRIC ACID	0.27	0.19	0.00	1.00	0.33	0.12	0.00	1.60
RESIDUAL SUGAR	2.54	1.41	0.90	15.50	6.39	5.07	0.60	65.80
CHLORIDES	0.09	0.05	0.01	0.61	0.04	0.02	0.01	0.35
FREE SULFUR DIOXIDE	15.87	10.46	1.00	72.00	35.08	17.01	2.00	289.00
TOTAL SULFUR DIOXIDE	46.47	32.90	6.00	289.00	138.36	42.50	9.00	440.00
DENSITY	1.00	0.002	0.99	1.00	0.99	0.003	0.99	1.03
PH	3.31	0.15	2.74	4.01	3.19	0.15	2.72	3.82
SULPHATES	0.66	0.17	0.33	2.00	0.49	0.11	0.22	1.08
ALCOHOL	10.42	1.07	8.40	14.9	10.51	1.23	8.00	14.2
QUALITY	5.64	0.81	3.00	8.00	5.88	0.89	3.00	9.00

In the red wine dataset, the maximum value for a handful of attributes falls more than 3 standard deviations away from their respective mean, representing an outlier. The same is observed in the white wine dataset. “Outliers can have adverse effects on the model analysis if unaccounted for. Boxplots for both datasets are graphed and shown in Figure 1 and Figure 2 in order to visualize the general descriptive statistics and identify outliers that may affect the models.

In Figure 1, the red wine samples for fixed acidity, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, and sulphates are skewed to the right, possessing low-valued means and many outliers greater than the maximum values. Each box plot contains at least a few outliers. In Figure 2, the white wine samples for fixed acidity, volatile acidity, citric acid, chlorides, free sulfur dioxide, and sulphates seem skewed to the right. All attributes except alcohol contain outliers.

Figure 1: Boxplots for Red Wine Attributes

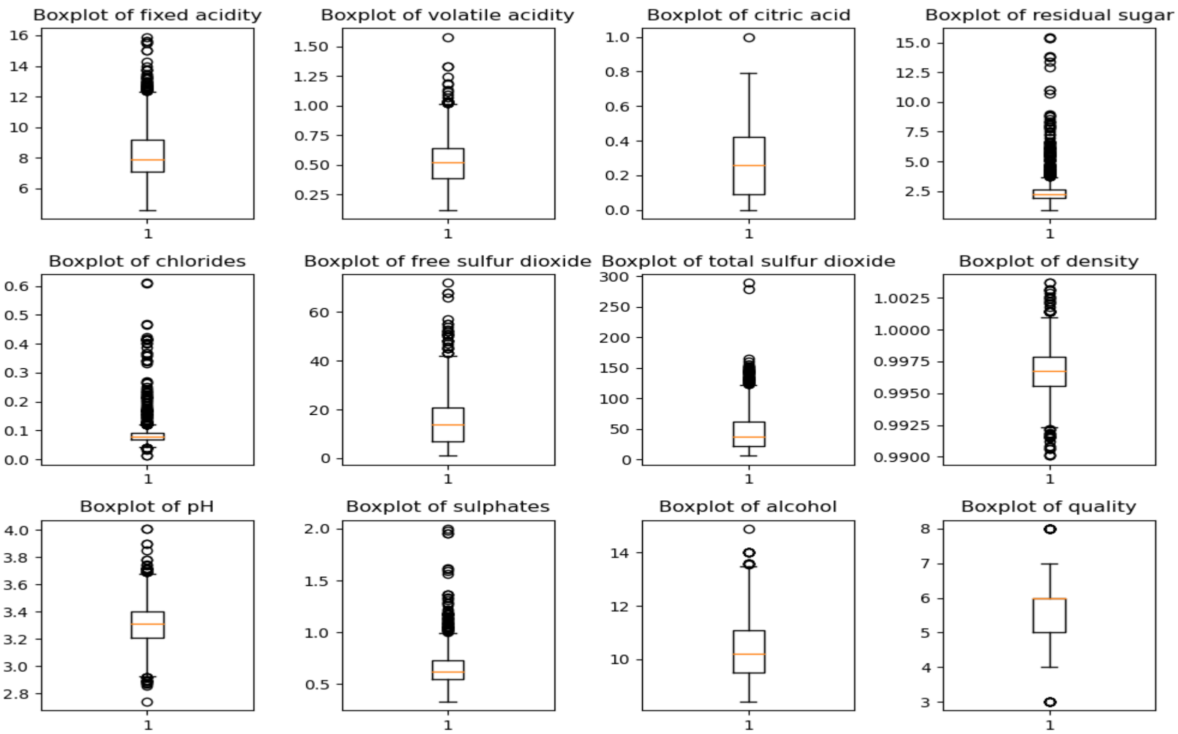
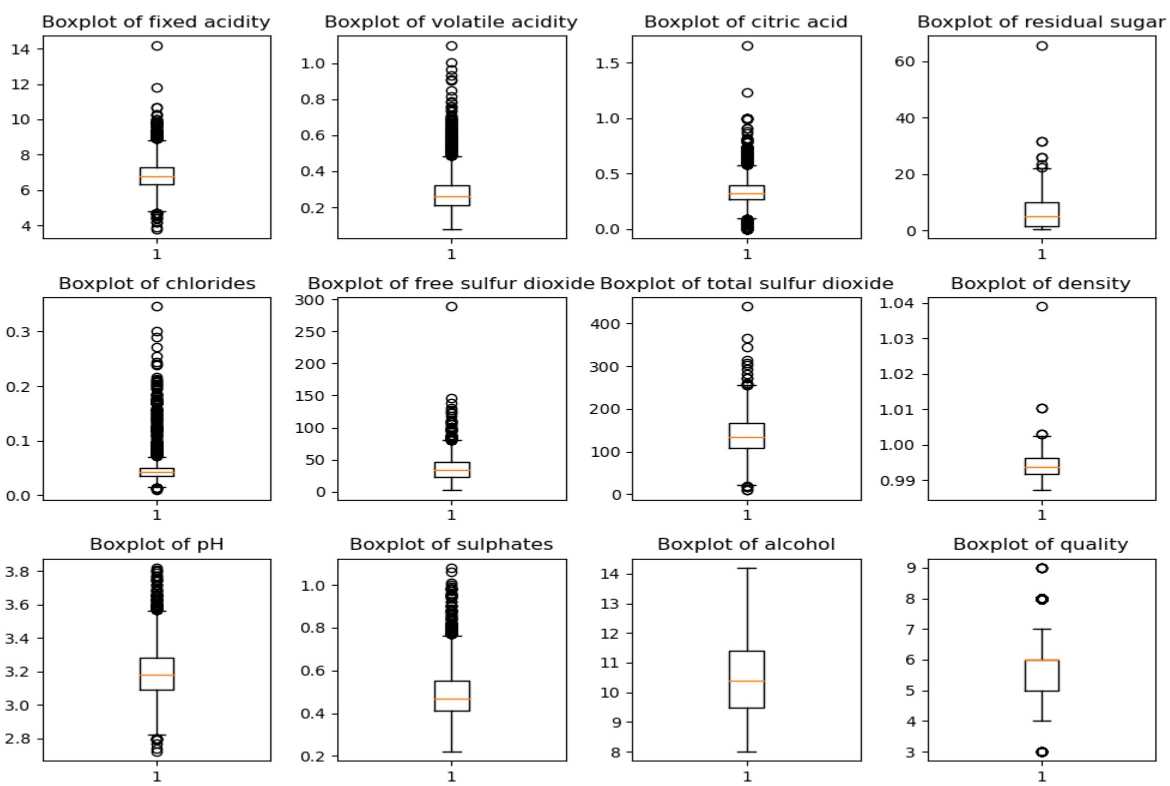


Figure 2: Boxplots for White Wine Attributes



Quantifying Outliers

The boxplots reveal many outliers in certain attributes. Table 2 quantifies the outliers and the percentage relative to the total number of samples for each dataset. For red wine, the percentages are high for chlorides and sugar. For white wine, there are double-digit percentages in volatile acidity, citric acid, and chlorides. The high number of outliers increases variability which may decrease the statistical accuracy of our models. Techniques such as nonparametric tests and certain bootstrapping techniques can assist with handling outliers.

When comparing the outliers between both datasets, there are many outliers for residual sugar in red wine while there are only some in white wine. Additionally, there are many outliers in citric acid for white wine and very few in red wine. The difference in variability further confirms the need to separate the datasets.

Table 33: Total Outliers

	RED WINE (1599 SAMPLES)		**WHITE WINE (4898 SAMPLES)**	
	Total Outliers	**Percentage**	**Total Outliers**	**Percentage**
FIXED ACIDITY	49	3.06	119	7.44
VOLATILE ACIDITY	19	1.19	186	11.63
CITRIC ACID	1	0.06	270	16.89
RESIDUAL SUGAR	155	9.39	7	0.44
CHLORIDES	112	7	208	13.01
FREE SULFUR DIOXIDE	30	1.88	50	3.13
TOTAL SULFUR DIOXIDE	55	3.44	19	1.19
DENSITY	45	2.81	5	0.31
PH	35	2.19	75	4.69
SULPHATES	59	3.69	124	7.75
ALCOHOL	13	0.81	0	0
QUALITY	28	1.75	200	12.51

The number of outliers in chlorides range from moderate in red wine to high in white wine. Chlorides in wine are influenced by both terroir and type of grape (Coli et al, 2015). The type of grape can be controlled, but the terroir, or entire natural environment in which the wine is produced, is highly variable. Soil composition, natural weather phenomenon, humidity, temperature, and other extraneous factors can alter the terroir as often as every day. This variability may explain the variability of the data and the high number of outliers. Volatile acidity and citric acid also have a high number of outliers in white wine, but a low number in red wine. This might be explained by the way each type of wine is produced. Red wines are fermented with the grape seeds and skins while white wines are not. Mineral elements from the environment are absorbed through the roots of the vine and are mainly present in the skin, seeds, and pulp of the grape (Coli et al, 2015). The presence of these minerals in red wine may alter the chemical composition by decreasing acidity. White wine is generally more acidic than red wine, and this difference is evident in the taste.

Correlation

Another important statistic to analyze is correlation between individual attributes. High correlation between explanatory variables can lead to multicollinearity which causes large standard errors and overfitting a model. Figure 1 and Figure 2 show a correlation matrix for red wine and white wine respectively. Analyzing the red wine correlation matrix in Figure 3, fixed acidity is positively correlated with citric acid. Same with total sulfur dioxide and free sulfur dioxide. For the white wine correlation matrix in Figure 4, total sulfur dioxide and residual sugar are moderately correlated. For both datasets, residual sugar and density have a strong positive correlation, and density and alcohol have a strong negative correlation. Additionally, alcohol has a moderate positive correlation with quality. Alcohol is one of the attributes that will be analyzed in the model analysis section.

Figure 3: Correlation Matrix for Red Wine Attributes

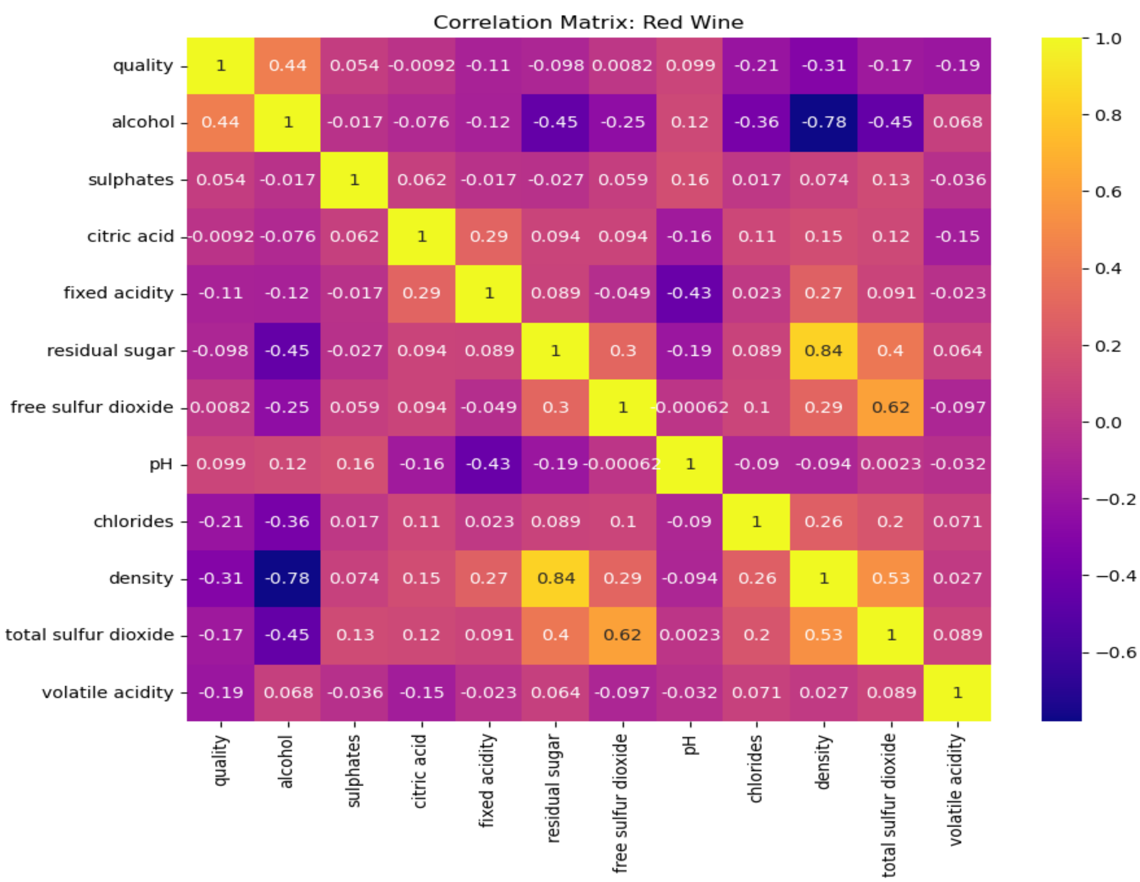
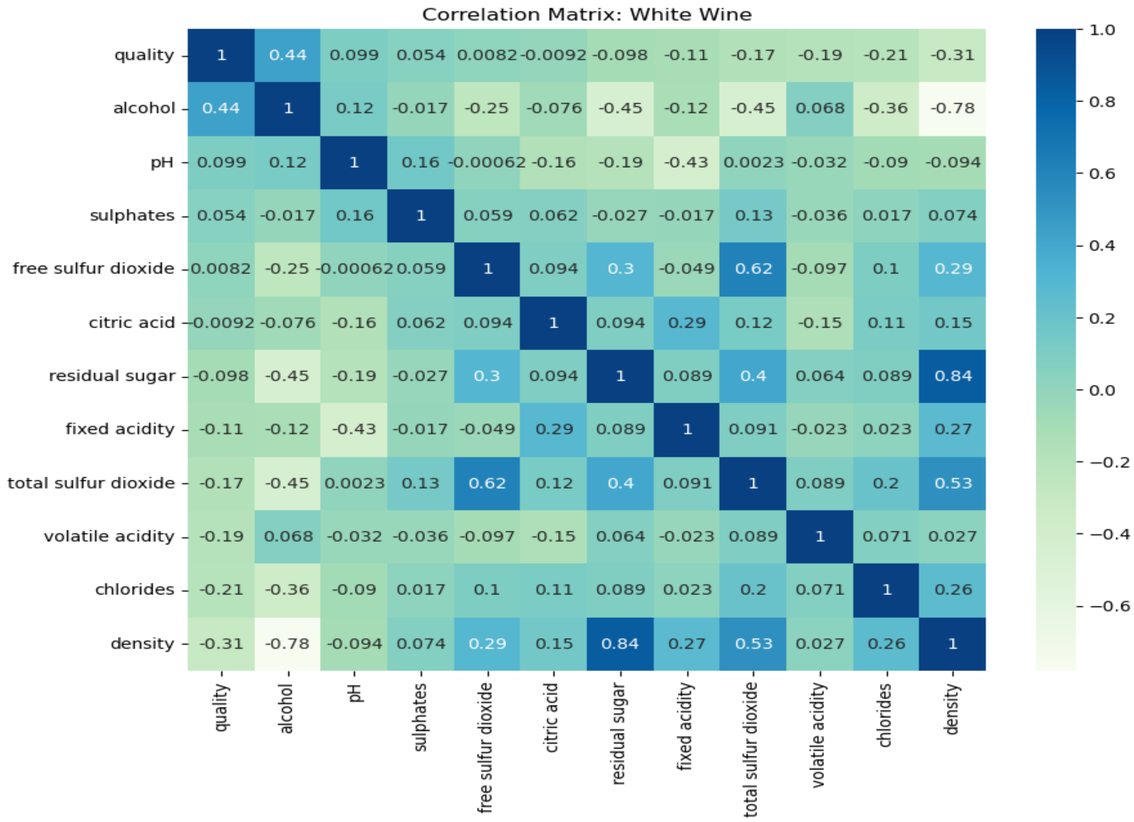


Figure 4: Correlation Matrix for White Wine Attributes



Model Selection

The model chosen for the Wine dataset is the Generalized Linear Model (GLM) from the statsmodels library. The Generalized Linear Model (GLM) is an improved version of linear regression that can handle different types of data, including those that do not follow a normal distribution, by incorporating various types of regression like multiple linear, logistic, and Poisson. In this specific case, we are using the Gaussian model. The response or dependent variable is 'quality'; all other dataset features are treated as independent variables. After removing outliers from the dataset, the GLM model is fitted with these independent variables to predict the response variable 'quality'. The process is done separately for red wine and white wine data. Two models are created and used for each type of wine, red and white.

Model Analysis

Red Wine Model Analysis

The Generalized Linear Model (GLM) for the red wine quality prediction has been trained on 1,124 observations and includes 11 predictor variables. The model summary's coefficients provide insight into each variable's impact on wine quality. For instance, 'sulphates' and 'alcohol' appear to have a significant positive effect on wine quality, as suggested by their respective positive coefficients (1.8195 and 0.2699) and small p-values (< 0.05). Similarly, 'volatile acidity', 'citric acid', 'total sulfur dioxide', and 'pH' also significantly influence but negatively.

In contrast, some variables like 'fixed acidity', 'residual sugar', 'chlorides', 'free sulfur dioxide', and 'density' exhibit large p-values (> 0.05), suggesting that these predictors might not be statistically significant in explaining the variation in wine quality. Particularly, 'density' has a very large standard error compared to its coefficient, further indicating that it may not be a reliable predictor.

Figure 5: Red Wine Model Regression Results

```
                 Generalized Linear Model Regression Results
==============================================================================
Dep. Variable:                quality   No. Observations:                 1124
Model:                            GLM   Df Residuals:                     1112
Model Family:                Gaussian   Df Model:                           11
Link Function:               Identity   Scale:                         0.33074
Method:                          IRLS   Log-Likelihood:                -967.05
Date:                Sat, 17 Jun 2023   Deviance:                       367.79
Time:                        11:47:23   Pearson chi2:                     368.
No. Iterations:                     3   Pseudo R-squ. (CS):             0.4471
Covariance Type:            nonrobust
========================================================================================
                           coef    std err          z      P>|z|      [0.025      0.975]
----------------------------------------------------------------------------------------
const                   13.3441     27.333      0.488      0.625     -40.228      66.916
fixed acidity            0.0181      0.031      0.580      0.562      -0.043       0.079
volatile acidity        -0.8159      0.150     -5.457      0.000      -1.109      -0.523
citric acid             -0.3364      0.168     -1.997      0.046      -0.666      -0.006
residual sugar           0.0096      0.051      0.189      0.850      -0.090       0.110
chlorides               -1.1807      1.414     -0.835      0.404      -3.953       1.591
free sulfur dioxide      0.0029      0.003      1.041      0.298      -0.003       0.008
total sulfur dioxide    -0.0023      0.001     -2.254      0.024      -0.004      -0.000
density                 -9.4483     27.902     -0.339      0.735     -64.135      45.239
pH                      -0.5278      0.233     -2.261      0.024      -0.985      -0.070
sulphates                1.8195      0.176     10.310      0.000       1.474       2.165
alcohol                  0.2699      0.034      7.931      0.000       0.203       0.337
========================================================================================
```

The Pseudo R-squared value is approximately 0.4471, which indicates that the model explains around 44.71% of the variability in wine quality, leaving a substantial portion unexplained. This suggests there may be other factors not included in the model that could contribute to red wine's quality, or non-linear relationships that this GLM does not capture.

White Wine Model Analysis

This Generalized Linear Model (GLM) for white wine quality prediction has been trained on a larger set of 3,815 observations. It reveals that the statistically significant factors influencing white wine quality include 'fixed acidity', 'volatile acidity', 'residual sugar', 'chlorides', 'free sulfur dioxide', 'density', 'pH', 'sulphates', and 'alcohol'.

Among these, 'density' and 'volatile acidity' exhibit a substantial negative relationship with quality. Interestingly, unlike red wine, 'residual sugar' and 'pH' positively influences white wine quality. 'Citric acid' and 'total sulfur dioxide', however, do not have a statistically significant impact, indicating that they may not be crucial in predicting white wine quality.

Figure 6: White Wine Model Regression Results

Generalized Linear Model Regression Results

Dep. Variable:	quality	No. Observations:	3815
Model:	GLM	Df Residuals:	3803
Model Family:	Gaussian	Df Model:	11
Link Function:	Identity	Scale:	0.43001
Method:	IRLS	Log-Likelihood:	-3797.4
Date:	Mon, 19 Jun 2023	Deviance:	1635.3
Time:	17:28:35	Pearson chi2:	1.64e+03
No. Iterations:	3	Pseudo R-squ. (CS):	0.2766
Covariance Type:	nonrobust		

	coef	std err	z	P>|z|	[0.025	0.975]
const	174.4951	24.946	6.995	0.000	125.602	223.388
fixed acidity	0.1173	0.025	4.697	0.000	0.068	0.166
volatile acidity	-1.7875	0.150	-11.939	0.000	-2.081	-1.494
citric acid	0.0518	0.134	0.387	0.699	-0.211	0.314
residual sugar	0.0834	0.009	8.919	0.000	0.065	0.102
chlorides	-3.8680	1.335	-2.898	0.004	-6.484	-1.252
free sulfur dioxide	0.0035	0.001	3.652	0.000	0.002	0.005
total sulfur dioxide	0.0003	0.000	0.630	0.529	-0.001	0.001
density	-174.5434	25.282	-6.904	0.000	-224.095	-124.992
pH	0.7944	0.119	6.696	0.000	0.562	1.027
sulphates	0.7817	0.116	6.750	0.000	0.555	1.009
alcohol	0.1028	0.031	3.293	0.001	0.042	0.164

Despite the model accounting for these factors, it explains only about 27.66% of the variability in white wine quality (as denoted by the Pseudo R-squared value), suggesting other important factors or non-linear relationships might not be captured in the model. While the deviance of 1635.3 indicates a reasonable model fit, the model may benefit from further enhancements such as considering additional predictors or refining variable interactions.

Summary

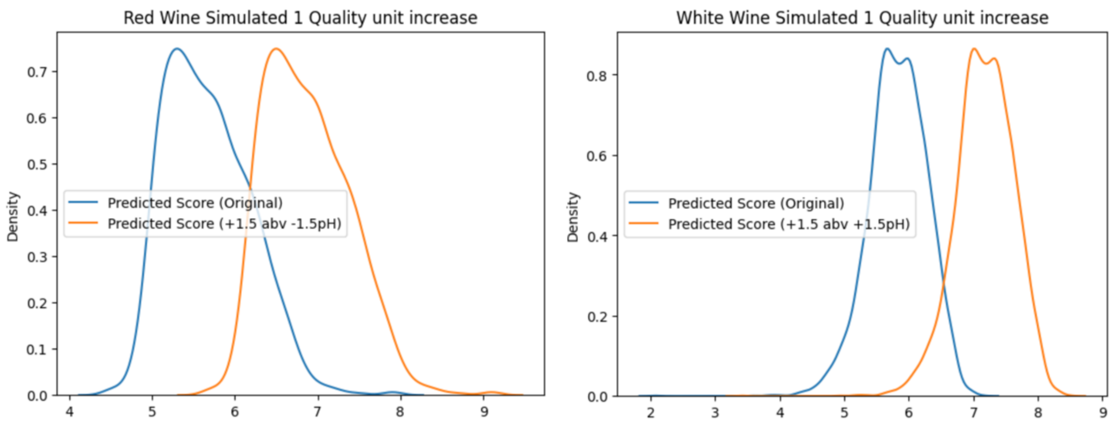
In summary, while the model's reveal some interesting patterns and appears to predict some quality variance, the relatively low R-squared value and high p-values for certain predictors suggest room for further refinement.

Conclusion

While the predictive models developed in this study do not achieve perfect accuracy, they successfully identify the attributes that correlate with higher wine quality. These insights can prove invaluable to experienced winemakers, enabling them to refine their products and enhance their wine ratings through simple modifications.

Our model identified two modifiable attributes post-fermentation: ' pH' and 'alcohol'. The model suggests that wines with a higher alcohol content generally receive higher quality scores. In contrast, red wines exhibiting lower pH values tend to achieve higher quality ratings. White wines exhibiting higher pH achieve higher quality scores. Based on the current red and white wine datasets, our model predicts that a change in pH by 1.5 units, coupled with an increase in alcohol by 1.5 units, could potentially increase the quality score by one unit across all wines.

Figure 7: Wine Simulated 1 Quality Increase



Recommendation

Our model predicts winemakers can increase quality scores by 1 unit by changing pH by 1.5 units and increasing alcohol by 1.5 units. To accomplish this, we recommend using an acidifying agent to decrease pH or using carbonate salts to increase pH. To increase alcohol content, we recommend back-adding higher alcohol wine or increasing fermentable sugars. Commonly used acidifiers in beer and wine include phosphoric acid and lactic acid. We recommend using phosphoric acid to decrease pH levels in the wine since it does not contain adverse flavors that the lactic acid may contain. To increase alcohol, we recommend blending a higher-alcohol wine or adding additional fermentable sugars such as dextrose. pH can be brought down to a low of 2.74 units for red wine and raised to 3.82 units for white wine. Alcohol can be raised to 14.9 units in red wine and 14.2 units in white wine.

Figure 8: Wine pH and alcohol summary

Red Wine pH and alcohol summary

	pH	alcohol
count	1599.000000	1599.000000
mean	3.311113	10.422983
std	0.154386	1.065668
min	2.740000	8.400000
25%	3.210000	9.500000
50%	3.310000	10.200000
75%	3.400000	11.100000
max	4.010000	14.900000

White Wine pH and alcohol summary

	pH	alcohol
count	4898.000000	4898.000000
mean	3.188267	10.514267
std	0.151001	1.230621
min	2.720000	8.000000
25%	3.090000	9.500000
50%	3.180000	10.400000
75%	3.280000	11.400000
max	3.820000	14.200000

Figure 9: Red Wine alcohol/pH quality correlation

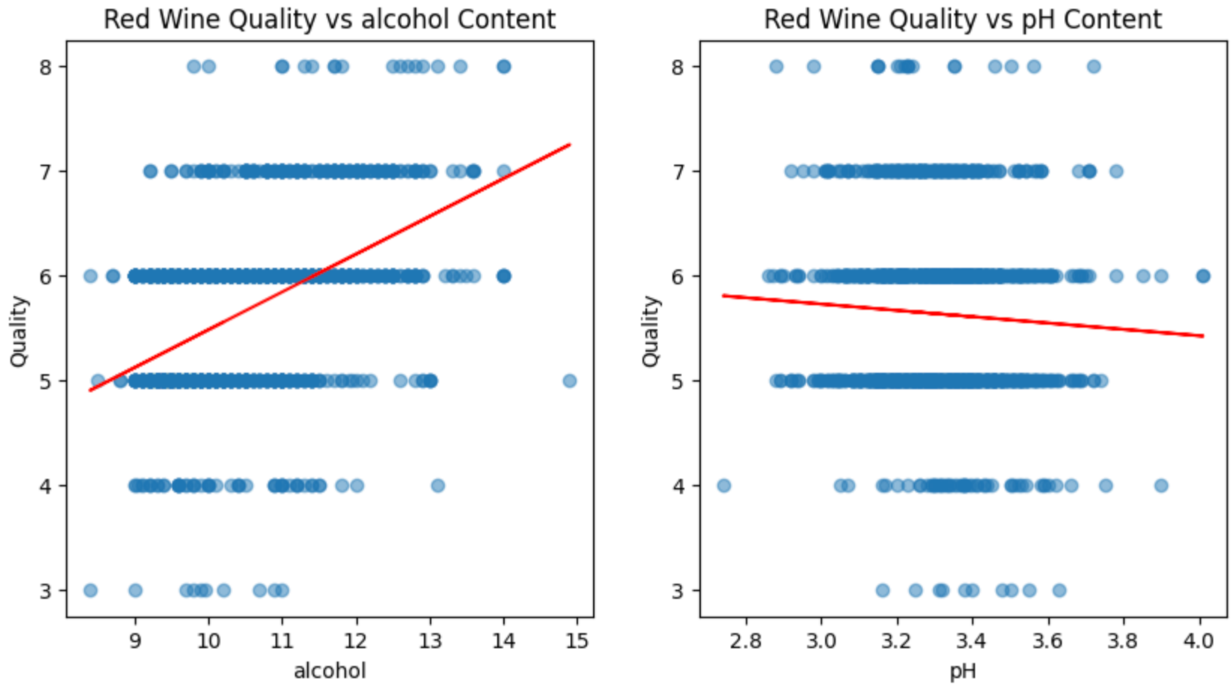
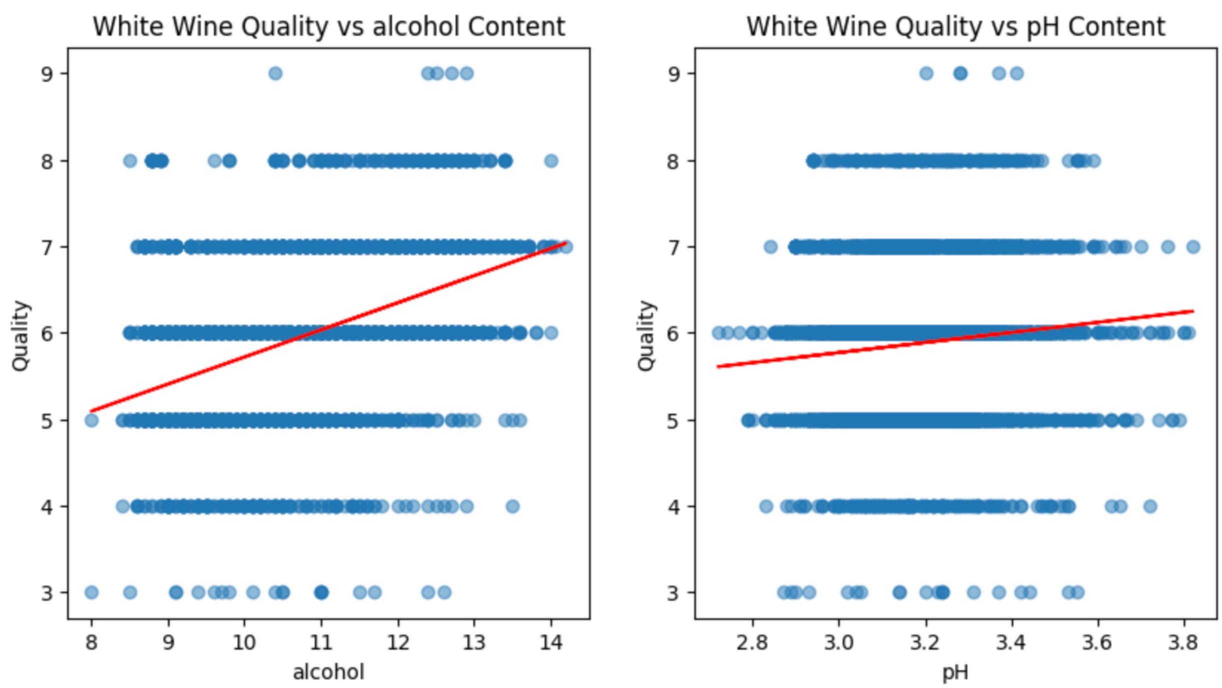


Figure 10: White Wine alcohol/pH quality correlation



Appendix: Github

https://github.com/p-parks/AAI-500-Team-4-Final-Project/tree/main

Appendix: Code Output

In [ ]:

```
# imports
import pandas as pd
from scipy import stats
import statsmodels.api as sm
import random
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from scipy.stats import norm
from sklearn.metrics import mean_absolute_error
from tabulate import tabulate
```

Datasets

In [ ]:

```
wine_white = pd.read_csv('../Dataset/wine+quality/winequality-white.csv',
sep=';')
wine_white.describe()
```

Out[ ]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
count	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000
mean	6.854788	0.278241	0.334192	6.391415	0.045772	35.308085	138.360657	0.994027	3.188267	0.489847	10.514267	5.877909
std	0.843868	0.100795	0.121020	5.072058	0.021848	17.007137	42.498065	0.002991	0.151001	0.114126	1.230621	0.885639
min	3.800000	0.080000	0.000000	0.600000	0.009000	2.000000	9.000000	0.987110	2.720000	0.220000	8.000000	3.000000
25%	6.300000	0.210000	0.270000	1.700000	0.036000	23.000000	108.000000	0.991723	3.090000	0.410000	9.500000	5.000000
50%	6.800000	0.260000	0.320000	5.200000	0.043000	34.000000	134.000000	0.993740	3.180000	0.470000	10.400000	6.000000
75%	7.300000	0.320000	0.390000	9.900000	0.050000	46.000000	167.000000	0.996100	3.280000	0.550000	11.400000	6.000000

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
max	14.200000	1.100000	1.660000	65.800000	0.346000	289.000000	440.000000	1.038980	3.820000	1.080000	14.200000	9.000000

In [ ]:

```
wine_red = pd.read_csv('../Dataset/wine+quality/winequality-red.csv',
sep=';')
wine_red.describe()
```

Out[ ]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
count	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000
mean	8.319637	0.527821	0.270976	2.538806	0.087467	15.874922	46.467792	0.996747	3.311113	0.658149	10.422983	5.636023
std	1.741096	0.179060	0.194801	1.409928	0.047065	10.460157	32.895324	0.001887	0.154386	0.169507	1.065668	0.807569
min	4.600000	0.120000	0.000000	0.900000	0.012000	1.000000	6.000000	0.990070	2.740000	0.330000	8.400000	3.000000
25%	7.100000	0.390000	0.090000	1.900000	0.070000	7.000000	22.000000	0.995600	3.210000	0.550000	9.500000	5.000000
50%	7.900000	0.520000	0.260000	2.200000	0.079000	14.000000	38.000000	0.996750	3.310000	0.620000	10.200000	6.000000
75%	9.200000	0.640000	0.420000	2.600000	0.090000	21.000000	62.000000	0.997835	3.400000	0.730000	11.100000	6.000000
max	15.900000	1.580000	1.000000	15.500000	0.611000	72.000000	289.000000	1.003690	4.010000	2.000000	14.900000	8.000000

In [ ]:

```
columns = [
    'fixed acidity',
    'volatile acidity',
    'citric acid',
    'residual sugar',
    'chlorides',
    'free sulfur dioxide',
    'total sulfur dioxide',
    'density',
    'pH',
    'sulphates',
    'alcohol',
```

```
    'quality'
]
```

Boxplot all data to view outliers

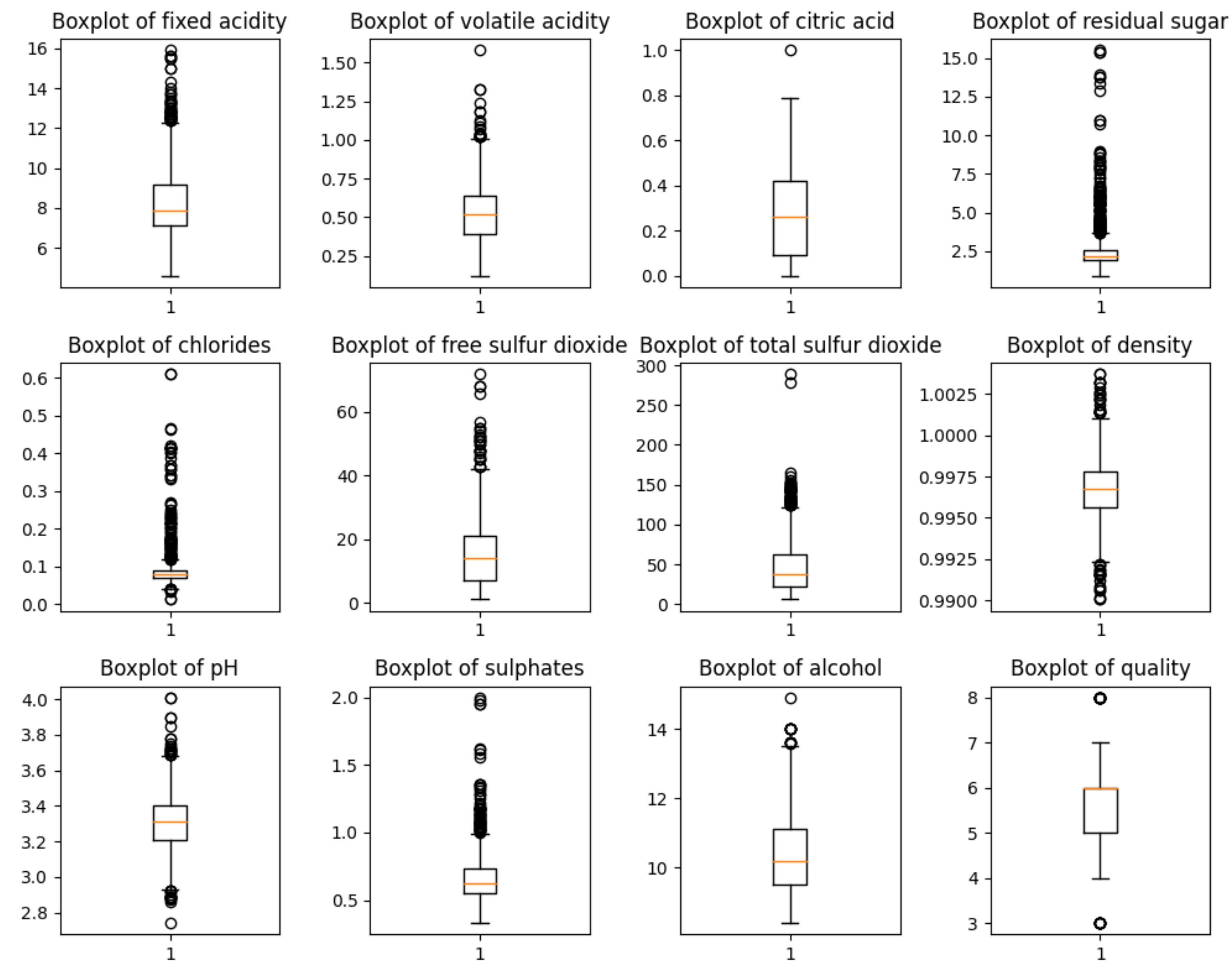
In [ ]:

```
def do_boxplot(data):
    # fig, axes = plt.subplots(nrows=3, ncols=4, figsize=(15,10))
    # 6/19/23 ACaterio: Lowering figsize to fit into screenshot for EDA in
the report
    fig, axes = plt.subplots(nrows=3, ncols=4, figsize=(10,8))
    axes = axes.ravel()
    for i, column in enumerate(columns):
        axes[i].boxplot(data[column])
        axes[i].set_title(f'Boxplot of {column}')
    plt.tight_layout()
    plt.show()
```

In [ ]:

```
print('BoxPlots Red Wine')
do_boxplot(wine_red)
```

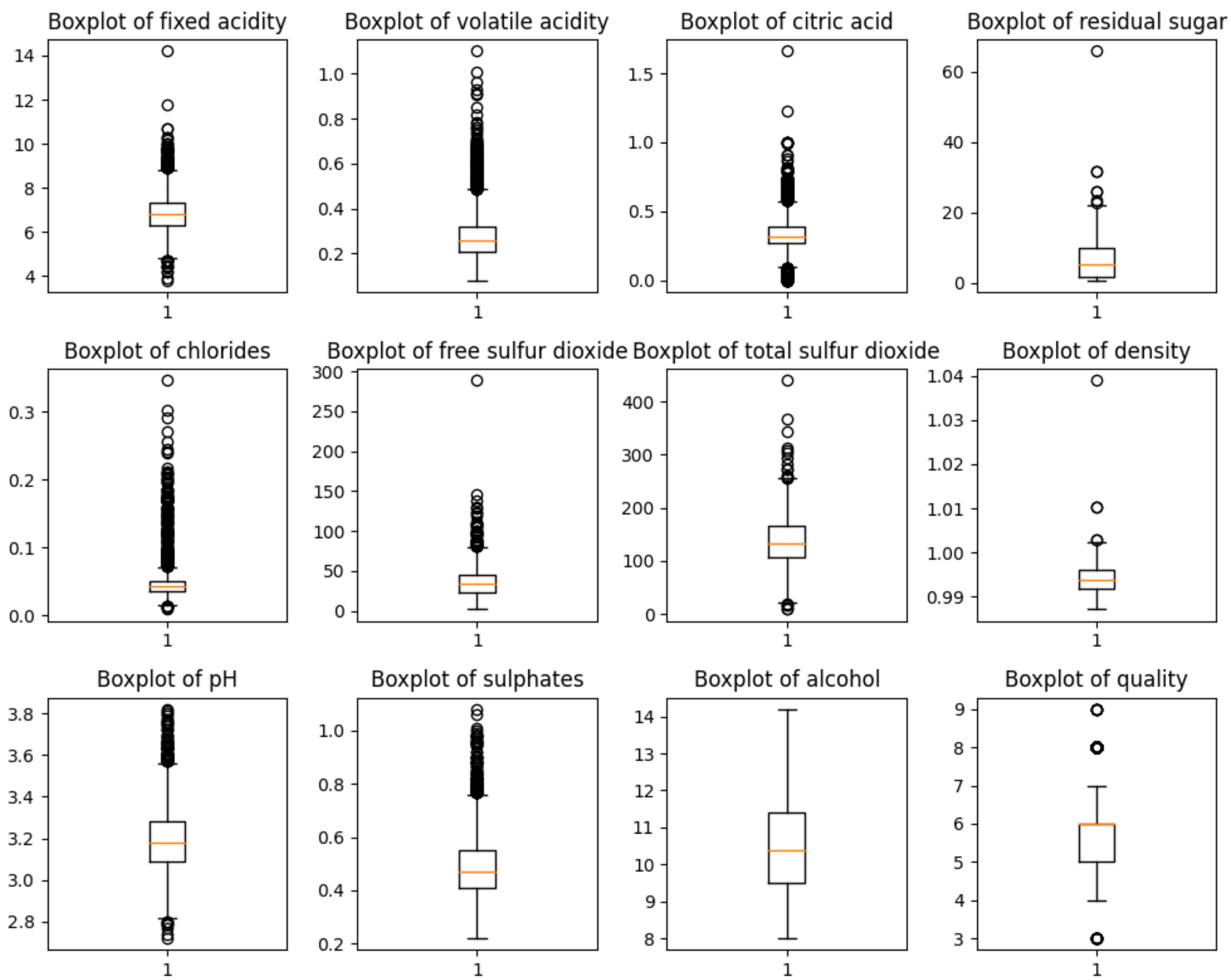
```
BoxPlots Red Wine
```



In [ ]:

```
print('BoxPlots White Wine')
do_boxplot(wine_white)
```

```
BoxPlots White Wine
```



In [ ]:

```
wine_red_n = len(wine_red)
wine_white_n = len(wine_white)

def countOutliers(df, df_str, n):
    Q1 = df.quantile(0.25)
    Q3 = df.quantile(0.75)
    IQR = Q3 - Q1
    outliers = ((df < (Q1 - 1.5 * IQR)) | (df > (Q3 + 1.5 * IQR))).sum()
    outliers = outliers.tolist()
    arr = []
    for i in range(len(outliers)):
        arr.append([])
        outlier_perc = round(outliers[i]/len(wine_red)*100,2)
        arr[i].append(columns[i])
        arr[i].append(outliers[i])
        arr[i].append(outlier_perc)
```

```
    print(tabulate(arr, headers=['Attribute', 'Total Outliers', 'Percentage'], tablefmt="fancy_grid"))
```

In [ ]:

```
countOutliers(wine_red, "Red Wine", wine_red_n)
```

Attribute	Total Outliers	Percentage
fixed acidity	49	3.06
volatile acidity	19	1.19
citric acid	1	0.06
residual sugar	155	9.69
chlorides	112	7
free sulfur dioxide	30	1.88
total sulfur dioxide	55	3.44
density	45	2.81
pH	35	2.19
sulphates	59	3.69
alcohol	13	0.81
quality	28	1.75

In [ ]:

```
countOutliers(wine_white, "White Wine", wine_white_n)
```

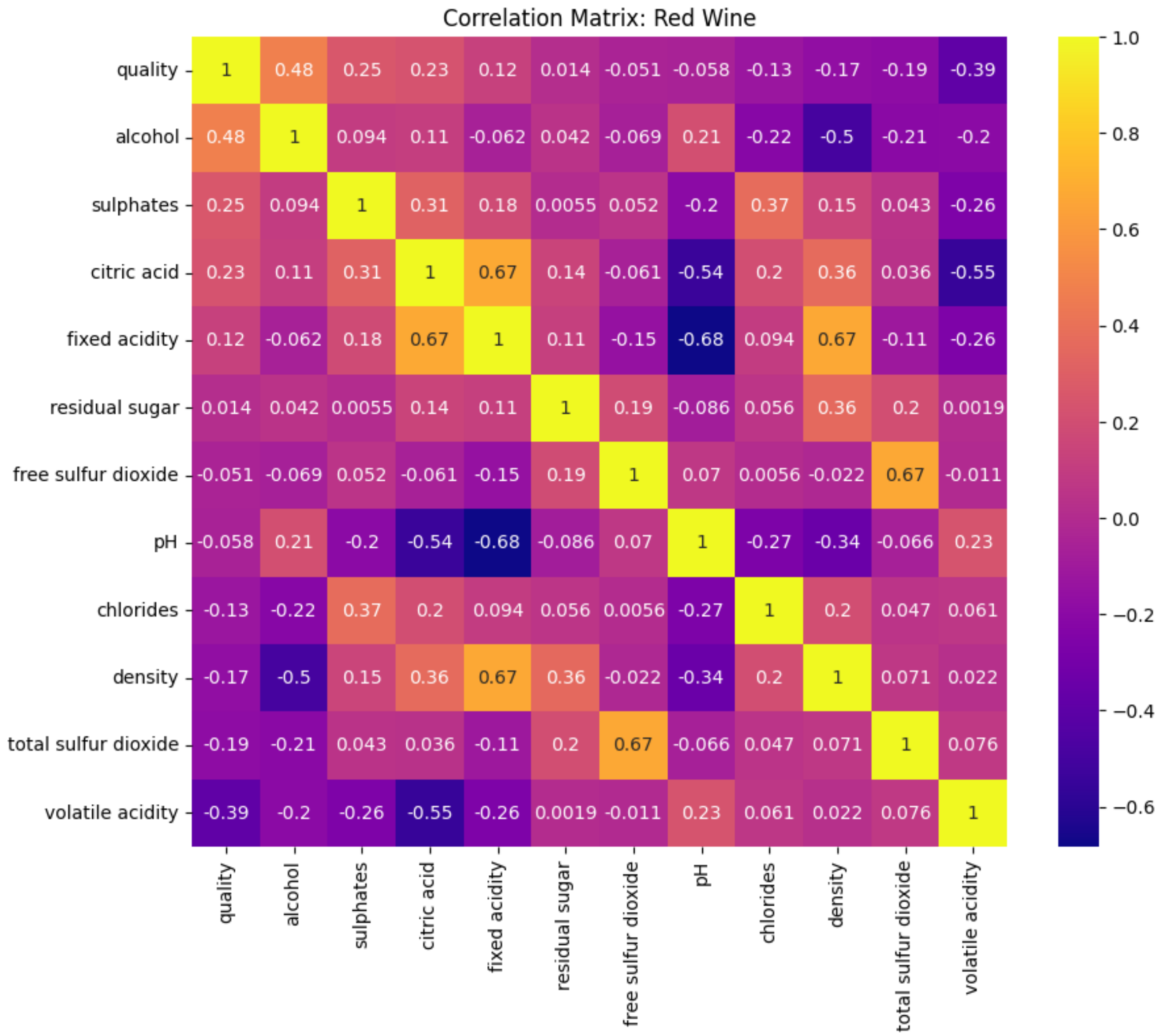
Attribute	Total Outliers	Percentage
fixed acidity	119	7.44
volatile acidity	186	11.63
citric acid	270	16.89
residual sugar	7	0.44
chlorides	208	13.01

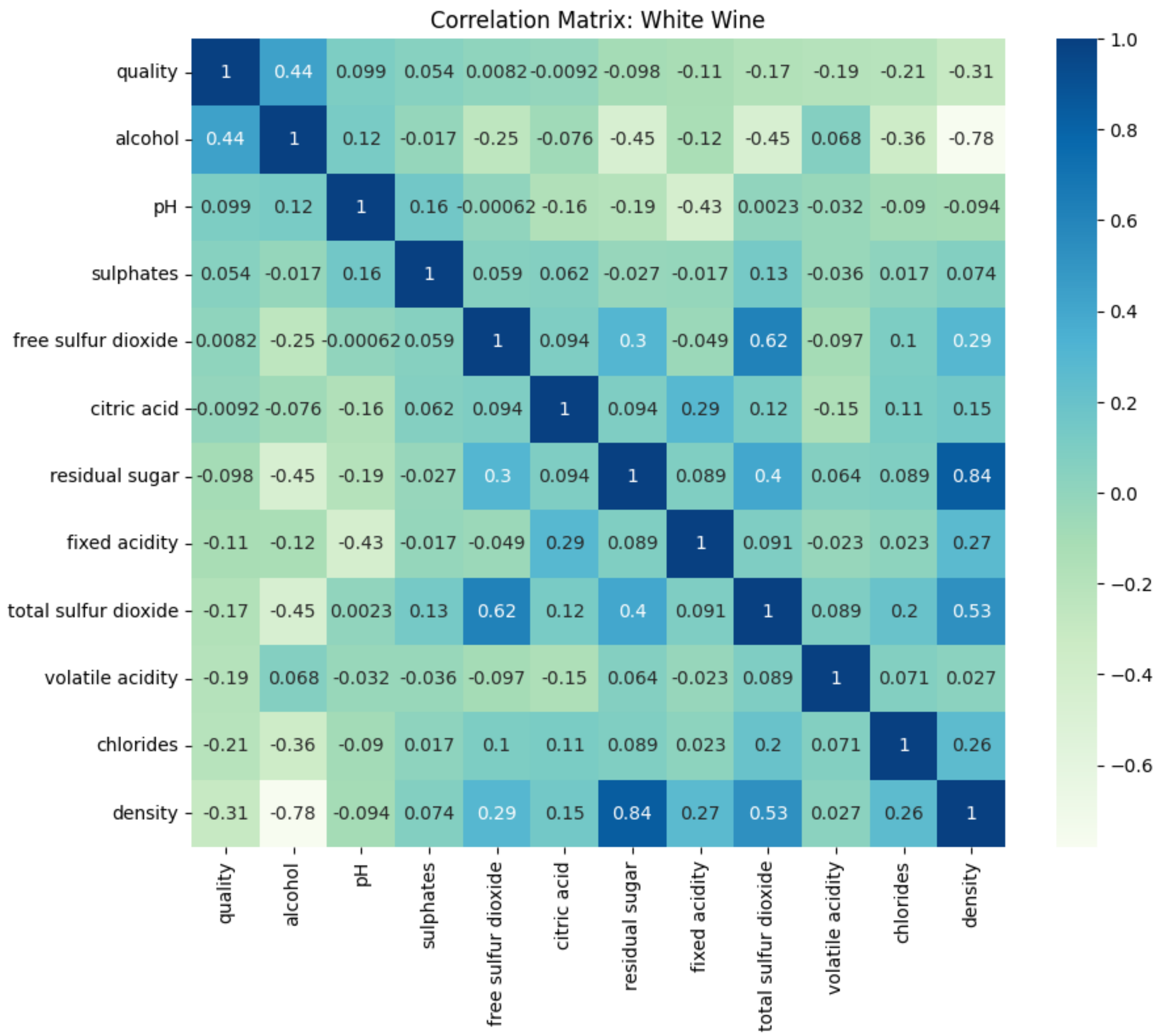
free sulfur dioxide	50	3.13
total sulfur dioxide	19	1.19
density	5	0.31
pH	75	4.69
sulphates	124	7.75
alcohol	0	0
quality	200	12.51

Correlation and Variation

In [ ]:

```
def createCorrMatr(df, df_str, color):
    cols_df = df.corr().nlargest(len(columns), 'quality')['quality'].index
    correl = df[cols_df].corr()
    plt.figure(figsize=(10,8))
    plt.title(f"Correlation Matrix: {df_str}")
    sns.heatmap(correl, annot=True, cmap = color)

createCorrMatr(wine_red, 'Red Wine', 'plasma')
createCorrMatr(wine_white, 'White Wine', 'GnBu')
```


Correlation Matrix: Red Wine
quality
alcohol
sulphates
citric acid
fixed acidity
residual sugar
free sulfur dioxide
pH
chlorides
density
total sulfur dioxide
volatile acidity



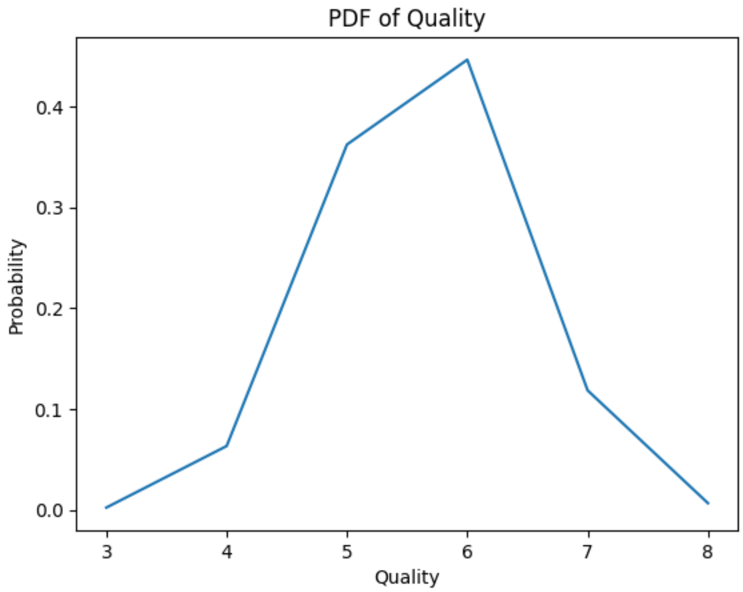
Probability of Scores

In [ ]:

```
def get_probability(df):
    df.sort_values(by=['quality'], inplace=True)
    df_mean = np.mean(df["quality"])
    df_std = np.std(df["quality"])
    pdf = stats.norm.pdf(df["quality"], df_mean, df_std)

    plt.xlabel('Quality')
    plt.ylabel('Probability')
    plt.title('PDF of Quality')
    plt.plot(df["quality"], pdf)
```

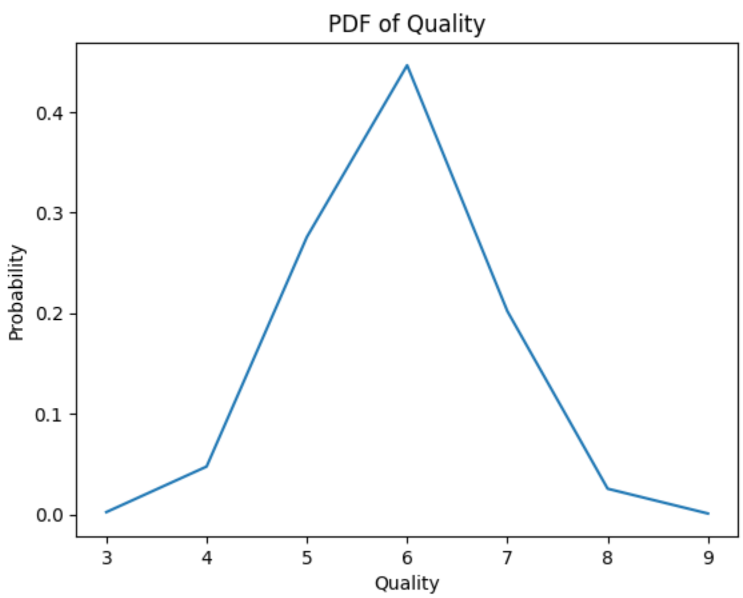
In [ ]:

```
get_probability(wine_red)
```



In [ ]:

```
get_probability(wine_white)
```



Remove all outliers

In [ ]:

```
def remove_all_outliers(data_source):
    data = data_source.copy()
    for column in columns:
        Q1 = data[column].quantile(0.25)
        Q3 = data[column].quantile(0.75)
        IQR = Q3 - Q1
        data = data[(data[column] >= Q1 - 1.5*IQR) & (data[column] <= Q3 +
1.5*IQR)]
    return data
```

In [ ]:

```
wine_red_cleaned = remove_all_outliers(wine_red)
wine_white_cleaned = remove_all_outliers(wine_white)
```

Generalized Linear Model Regression

In [ ]:

```
def create_glm_fitted_model(df):
    X = df.drop('quality', axis=1)
    y = df['quality']

    X = sm.add_constant(X)

    # Create the model
    model = sm.GLM(y, X)
    return model.fit()
```

In [ ]:

```
wine_red_results = create_glm_fitted_model(wine_red)
print(wine_red_results.summary())
                 Generalized Linear Model Regression Results
==============================================================================
=
Dep. Variable:                quality   No. Observations:
1599
Model:                            GLM   Df Residuals:
1587
Model Family:                Gaussian   Df Model:
11
Link Function:               Identity   Scale:
0.41992
Method:                          IRLS   Log-Likelihood:                -
1569.1
Date:                Sat, 24 Jun 2023   Deviance:
666.41
Time:                        18:16:51   Pearson chi2:
666.
No. Iterations:                     3   Pseudo R-squ. (CS):
0.4286
Covariance Type:            nonrobust
==============================================================================
===========
                          coef    std err          z      P>|z|      [0.025
0.975]
------------------------------------------------------------------------------
-----------
const                  21.9652     21.195      1.036      0.300     -19.575
63.506
```

```
fixed acidity            0.0250      0.026      0.963      0.336      -0.026
0.076
volatile acidity        -1.0836      0.121     -8.948      0.000      -1.321
-0.846
citric acid             -0.1826      0.147     -1.240      0.215      -0.471
0.106
residual sugar           0.0163      0.015      1.089      0.276      -0.013
0.046
chlorides               -1.8742      0.419     -4.470      0.000      -2.696
-1.052
free sulfur dioxide      0.0044      0.002      2.009      0.045       0.000
0.009
total sulfur dioxide    -0.0033      0.001     -4.480      0.000      -0.005
-0.002
density                -17.8812     21.633     -0.827      0.408     -60.281
24.519
pH                      -0.4137      0.192     -2.159      0.031      -0.789
-0.038
sulphates                0.9163      0.114      8.014      0.000       0.692
1.140
alcohol                  0.2762      0.026     10.429      0.000       0.224
0.328
==============================================================================
===========
The variables 'volatile acidity', 'chlorides', 'free sulfur dioxide', 'total
sulfur dioxide', 'pH', 'sulphates', and 'alcohol' are statistically
significant predictors of wine quality because their p-values are less than
0.05.
```

In [ ]:

```
wine_white_results = create_glm_fitted_model(wine_white)
print(wine_white_results.summary())
                 Generalized Linear Model Regression Results
==============================================================================
=
Dep. Variable:                quality   No. Observations:
4898
Model:                            GLM   Df Residuals:
4886
Model Family:                Gaussian   Df Model:
11
Link Function:               Identity   Scale:
0.56454
Method:                          IRLS   Log-Likelihood:                -
5543.7
Date:                Sat, 24 Jun 2023   Deviance:
2758.3
```

```
Time:                        18:16:51   Pearson chi2:
2.76e+03
No. Iterations:                     3   Pseudo R-squ. (CS):
0.3240
Covariance Type:            nonrobust
==============================================================================
===========
                           coef    std err          z      P>|z|      [0.025
0.975]
------------------------------------------------------------------------------
-----------
const                  150.1928     18.804      7.987      0.000     113.337
187.048
fixed acidity            0.0655      0.021      3.139      0.002       0.025
0.106
volatile acidity        -1.8632      0.114    -16.373      0.000      -2.086
-1.640
citric acid              0.0221      0.096      0.231      0.818      -0.166
0.210
residual sugar           0.0815      0.008     10.825      0.000       0.067
0.096
chlorides               -0.2473      0.547     -0.452      0.651      -1.318
0.824
free sulfur dioxide      0.0037      0.001      4.422      0.000       0.002
0.005
total sulfur dioxide    -0.0003      0.000     -0.756      0.450      -0.001
0.000
density               -150.2842     19.075     -7.879      0.000    -187.670
-112.899
pH                       0.6863      0.105      6.513      0.000       0.480
0.893
sulphates                0.6315      0.100      6.291      0.000       0.435
0.828
alcohol                  0.1935      0.024      7.988      0.000       0.146
0.241
==============================================================================
===========
The variables 'volatile acidity', 'residual sugar', 'free sulfur dioxide',
'density', 'pH', 'sulphates', and 'alcohol' are statistically significant
predictors of wine quality because their p-values are less than 0.05.
```

In [ ]:

```
wine_red_cleaned_results = create_glm_fitted_model(wine_red_cleaned)
print(wine_red_cleaned_results.summary())
                 Generalized Linear Model Regression Results
==============================================================================
=
```

```
Dep. Variable:                quality   No. Observations:
1124
Model:                            GLM   Df Residuals:
1112
Model Family:                Gaussian   Df Model:
11
Link Function:               Identity   Scale:
0.33074
Method:                          IRLS   Log-Likelihood:                -
967.05
Date:                Sat, 24 Jun 2023   Deviance:
367.79
Time:                        18:16:51   Pearson chi2:
368.
No. Iterations:                     3   Pseudo R-squ. (CS):
0.4471
Covariance Type:            nonrobust
=============================================================================
===========
                           coef    std err          z      P>|z|      [0.025
0.975]
-----------------------------------------------------------------------------
-----------
const                   13.3441     27.333      0.488      0.625     -40.228
66.916
fixed acidity            0.0181      0.031      0.580      0.562      -0.043
0.079
volatile acidity        -0.8159      0.150     -5.457      0.000      -1.109
-0.523
citric acid             -0.3364      0.168     -1.997      0.046      -0.666
-0.006
residual sugar           0.0096      0.051      0.189      0.850      -0.090
0.110
chlorides               -1.1807      1.414     -0.835      0.404      -3.953
1.591
free sulfur dioxide      0.0029      0.003      1.041      0.298      -0.003
0.008
total sulfur dioxide    -0.0023      0.001     -2.254      0.024      -0.004
-0.000
density                 -9.4483     27.902     -0.339      0.735     -64.135
45.239
pH                      -0.5278      0.233     -2.261      0.024      -0.985
-0.070
sulphates                1.8195      0.176     10.310      0.000       1.474
2.165
```

```
alcohol                  0.2699      0.034      7.931      0.000       0.203
0.337
==============================================================================
===========
```

In [ ]:

```
wine_white_cleaned_results = create_glm_fitted_model(wine_white_cleaned)
print(wine_white_cleaned_results.summary())
                 Generalized Linear Model Regression Results
==============================================================================
=
Dep. Variable:                quality   No. Observations:
3815
Model:                            GLM   Df Residuals:
3803
Model Family:                Gaussian   Df Model:
11
Link Function:               Identity   Scale:
0.43001
Method:                          IRLS   Log-Likelihood:                -
3797.4
Date:                Sat, 24 Jun 2023   Deviance:
1635.3
Time:                        18:16:51   Pearson chi2:
1.64e+03
No. Iterations:                     3   Pseudo R-squ. (CS):
0.2766
Covariance Type:            nonrobust
==============================================================================
===========
                           coef    std err          z      P>|z|      [0.025
0.975]
------------------------------------------------------------------------------
-----------
const                  174.4951     24.946      6.995      0.000     125.602
223.388
fixed acidity            0.1173      0.025      4.697      0.000       0.068
0.166
volatile acidity        -1.7875      0.150    -11.939      0.000      -2.081
-1.494
citric acid              0.0518      0.134      0.387      0.699      -0.211
0.314
residual sugar           0.0834      0.009      8.919      0.000       0.065
0.102
chlorides               -3.8680      1.335     -2.898      0.004      -6.484
-1.252
```

```
free sulfur dioxide       0.0035      0.001      3.652      0.000       0.002
0.005
total sulfur dioxide      0.0003      0.000      0.630      0.529      -0.001
0.001
density                -174.5434     25.282     -6.904      0.000    -224.095
-124.992
pH                        0.7944      0.119      6.696      0.000       0.562
1.027
sulphates                 0.7817      0.116      6.750      0.000       0.555
1.009
alcohol                   0.1028      0.031      3.293      0.001       0.042
0.164
==============================================================================
===========
```

Predictions

In [ ]:

```
def quality_histogram(X, y, results):
    predicted_scores = []
    actual_scores = []
    for row_iter in range(len(X)):
        row = X.iloc[row_iter]
        predicted_quality = results.predict(row)
        predicted_scores.append(predicted_quality[0])
        actual_scores.append(y.iloc[row_iter])

    sns.kdeplot(predicted_scores, label='Predicted Score')
    sns.kdeplot(actual_scores, label="Actual Score")

    plt.legend()
    plt.show()

def predict_wine_using_df(df_source, results):
    df = df_source.copy()

    get_mse_predictions(df, results)

    X = df.drop('quality', axis=1)
    X = sm.add_constant(X)
    y = df['quality']
    index = random.randint(0, len(df))
    row = X.iloc[index]
    predicted_quality = results.predict(row)
    print('Predicted wine quality:', predicted_quality[0])
    print('Predicted wine quality rounded:', round(predicted_quality[0]))
    print('Actual wine quality:', y.iloc[index])
```

```
    quality_histogram(X, y, results)
```

In [ ]:

```
def get_mse_predictions(df, results):
    X = df.drop('quality', axis=1)
    X = sm.add_constant(X)
    y = df['quality']
    predictions = results.predict(X)
    mae = mean_absolute_error(y, predictions)
    print(f'Mean Absolute Error: {mae}')
```

In [ ]:

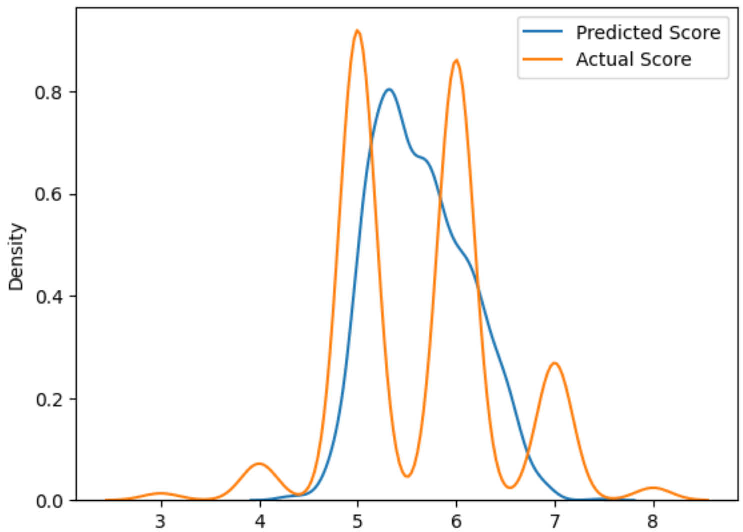
```
def predict_simulated_best_wine(data_source, results):
    print('Take the best scoring wine in the dataset and make it even
better.')
    # new_wine = {
    #     'const': [1],
    #     'fixed acidity': [8.5],
    #     'volatile acidity': [0.8],
    #     'citric acid': [0.56],
    #     'residual sugar': [1.8],
    #     'chlorides': [0.077],
    #     'free sulfur dioxide': [10.0],
    #     'total sulfur dioxide': [37.0],
    #     'density': [0.9968],
    #     'pH': [3.2],
    #     'sulphates': [0.68],
    #     'alcohol': [9.8]
    # }
    data = data_source.copy()
    # get the best scoring wine in the real dataset
    X = sm.add_constant(data)
    max_quality_index = X['quality'].idxmax()
    max_quality_row = X.loc[max_quality_index]
    actual_score = max_quality_row['quality']
    print(f'Actual quality: {actual_score}')
    max_quality_row = max_quality_row.drop('quality')

    # Statistically significant values for both red and white wines
    # tldr how to get a 11/10 wine
    max_quality_row['alcohol'] = 15 #high alcohol
    max_quality_row['sulphates'] = 2 #high sulphates
    max_quality_row['volatile acidity'] = 0.1 #low volatile acidity
    max_quality_row['total sulfur dioxide'] = 30 # low total sulfur dioxide
    max_quality_row['pH'] = 2 # low pH

    print(max_quality_row)
```

```
    predicted_quality = results.predict(max_quality_row)
    print(f'\nPredicted wine quality: {round(predicted_quality[0])}\n')
```

In [ ]:

```
print('\nRed Wine prediction: \n')
predict_wine_using_df(wine_red, wine_red_results)
```

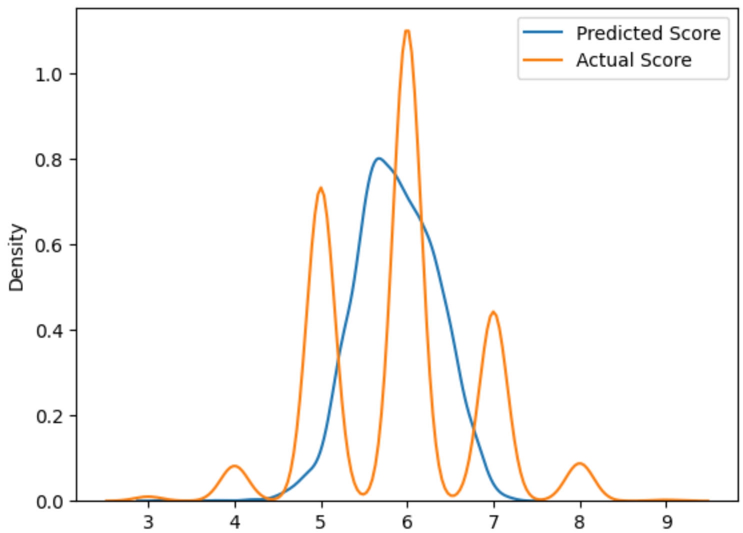
```
Red Wine prediction:

Mean Absolute Error: 0.500489963564491
Predicted wine quality: 6.4713673724387
Predicted wine quality rounded: 6
Actual wine quality: 6
```



In [ ]:

```
print('\nWhite Wine prediction: \n')
predict_wine_using_df(wine_white, wine_white_results)
```

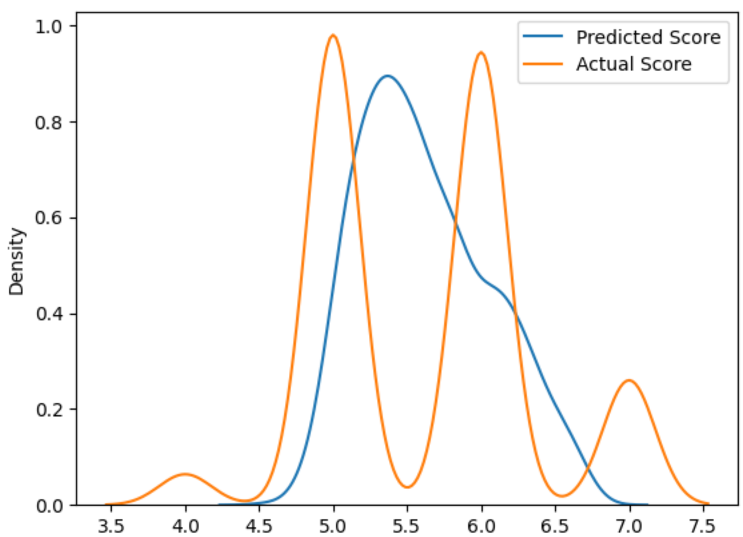
```
White Wine prediction:

Mean Absolute Error: 0.5836349500279457
Predicted wine quality: 5.6392830408493975
Predicted wine quality rounded: 6
Actual wine quality: 6
```



In [ ]:

```
print('\nRed Wine Cleaned prediction: \n')
predict_wine_using_df(wine_red_cleaned, wine_red_cleaned_results)
```

```
Red Wine Cleaned prediction:

Mean Absolute Error: 0.4593529800397901
Predicted wine quality: 5.2065795461938
Predicted wine quality rounded: 5
Actual wine quality: 5
```

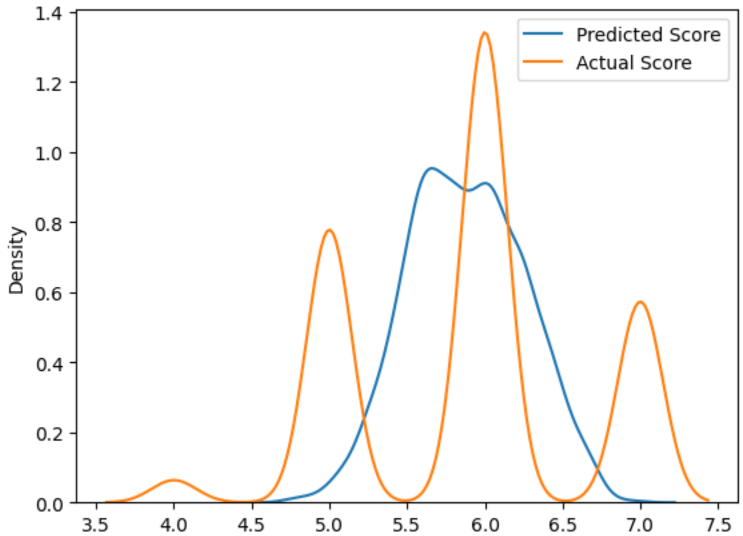


In [ ]:

```
print('\nWhite Wine Cleaned prediction: \n')
predict_wine_using_df(wine_white_cleaned, wine_white_cleaned_results)
```

```
White Wine Cleaned prediction:
```

```
Mean Absolute Error: 0.5287723085610089
Predicted wine quality: 6.218434120248082
Predicted wine quality rounded: 6
Actual wine quality: 6
```



In [ ]:

```
print('\nRed Wine prediction: \n')
predict_simulated_best_wine(wine_red, wine_red_cleaned_results)
```

```
Red Wine prediction:

Take the best scoring wine in the dataset and make it even better.
Actual quality: 8.0
const                    1.0000
fixed acidity            5.5000
volatile acidity         0.1000
citric acid              0.0300
residual sugar           1.8000
chlorides                0.0440
free sulfur dioxide     28.0000
total sulfur dioxide    30.0000
density                  0.9908
pH                       2.0000
sulphates                2.0000
alcohol                 15.0000
Name: 1269, dtype: float64

Predicted wine quality: 11
```

In [ ]:

```
print('\nWhite Wine prediction: \n')
predict_simulated_best_wine(wine_white, wine_white_cleaned_results)
```

```
White Wine prediction:

Take the best scoring wine in the dataset and make it even better.
Actual quality: 9.0
const                    1.000
fixed acidity            9.100
volatile acidity         0.100
citric acid              0.450
residual sugar          10.600
chlorides                0.035
free sulfur dioxide     28.000
total sulfur dioxide    30.000
density                  0.997
pH                       2.000
sulphates                2.000
alcohol                 15.000
Name: 774, dtype: float64

Predicted wine quality: 7
```

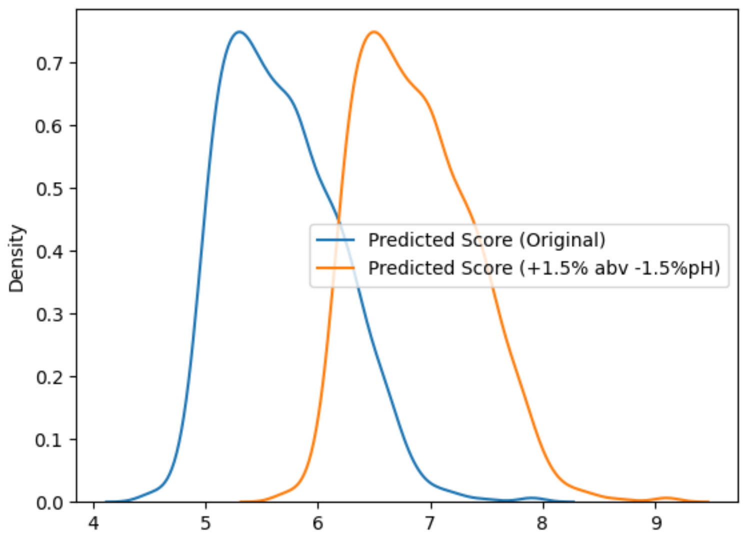
In [ ]:

```
def predict_simulated_best_wine_only_modify_pH_and_alcohol(data_source, results):
    predicted_scores_original = []
    predicted_scores_with_modifications = []
    score_diff = []

    data = data_source.copy()
    X = sm.add_constant(data)

    for row_iter in range(len(data)):
        row = X.loc[row_iter]
        row = row.drop('quality')
        predicted_quality = results.predict(row)
        row['alcohol'] = row['alcohol'] + 1.5
        row['pH'] = row['pH'] - 1.5
        predicted_quality_modified = results.predict(row)
        predicted_scores_original.append(predicted_quality[0])
predicted_scores_with_modifications.append(predicted_quality_modified[0])
        score_diff = predicted_quality_modified[0] - predicted_quality[0]

    sns.kdeplot(predicted_scores_original, label='Predicted Score (Original)')
```

```
    sns.kdeplot(predicted_scores_with_modifications, label="Predicted Score
(+1.5% abv -1.5%pH)")

    plt.legend()
    plt.show()
    print(f'Average Score difference (Score point out of 10):
{np.mean(score_diff)}')
```

In [ ]:

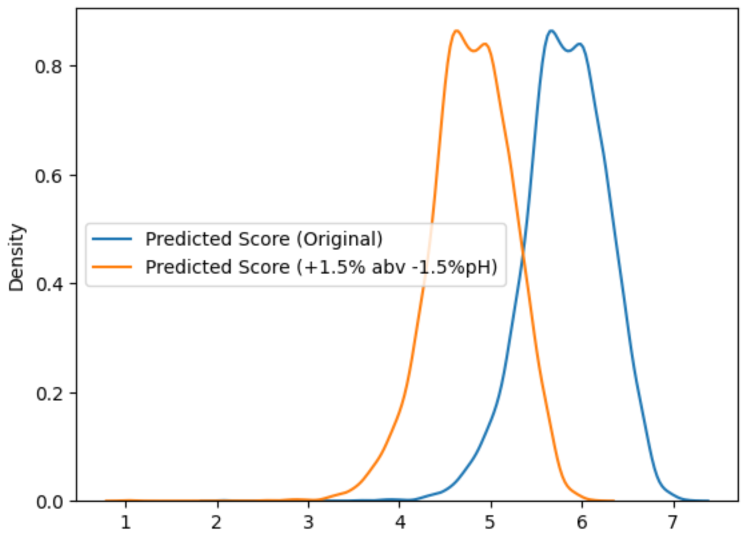
```
# pH and Alcohol and both easily adjustable post fermentation.
# What would happen to our wine scores if we increased alcohol and decreased
pH?

predict_simulated_best_wine_only_modify_pH_and_alcohol(wine_red,
wine_red_cleaned_results)
```




```
Average Score difference (Score point out of 10): 1.1965024634214307
```

In [ ]:

```
predict_simulated_best_wine_only_modify_pH_and_alcohol(wine_white,
wine_white_cleaned_results)
```




```
Average Score difference (Score point out of 10): -1.0374215502692428

Increasing alcohol percentage by 1.5 and lowering pH by 1.5 gains an average
of 1 whole score point.
```

In [ ]:

```
subset = wine_red[["pH", "alcohol"]]
description = subset.describe()
print('Red Wine pH and alcohol summary')
print(description)
Red Wine pH and alcohol summary
                pH      alcohol
count  1599.000000  1599.000000
mean      3.311113    10.422983
std       0.154386     1.065668
min       2.740000     8.400000
25%       3.210000     9.500000
50%       3.310000    10.200000
75%       3.400000    11.100000
max       4.010000    14.900000
```

In [ ]:

```
subset = wine_white[["pH", "alcohol"]]
description = subset.describe()
print('White Wine pH and alcohol summary')
print(description)
White Wine pH and alcohol summary
                pH      alcohol
count  4898.000000  4898.000000
mean      3.188267    10.514267
std       0.151001     1.230621
min       2.720000     8.000000
25%       3.090000     9.500000
```

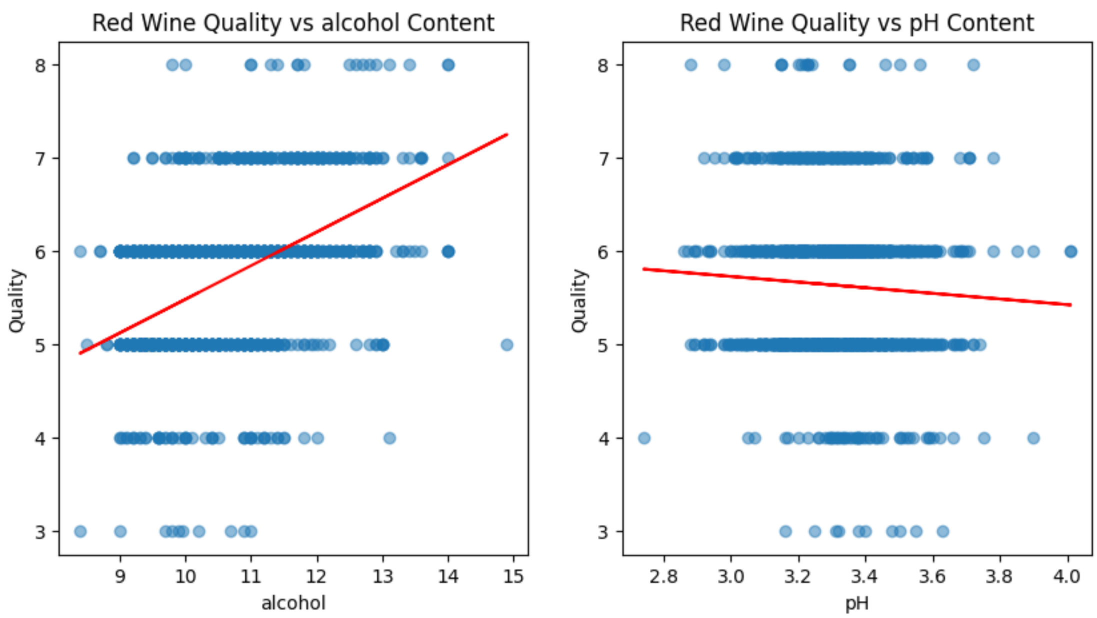
```
50%       3.180000   10.400000
75%       3.280000   11.400000
max       3.820000   14.200000
```

In [ ]:

```
def do_regression_and_plot(df, param, axs, label):
    X = df[[param]]
    y = df['quality']

    # Add a constant to the independent value
    X = sm.add_constant(X)

    # Perform regression
    model = sm.GLM(y, X)
    results = model.fit()
    axs.scatter(X[param], y, alpha=0.5)

    # Fitted line
    y_pred = results.predict(X)
    axs.plot(X[param], y_pred, color='red')

    axs.set_xlabel(param)
    axs.set_ylabel('Quality')
    axs.set_title(label + ' Wine Quality vs ' + param + ' Content')

def create_scatterplot(df, label):
    # Create two subplots side by side
    fig, axs = plt.subplots(1, 2, figsize=(10, 5)) # 1 row, 2 columns

    # Scatter plot for first set of data
    do_regression_and_plot(df, 'alcohol', axs[0], label)

    # Scatter plot for second set of data
    do_regression_and_plot(df, 'pH', axs[1], label)

    # Display the plots
    plt.show()
```

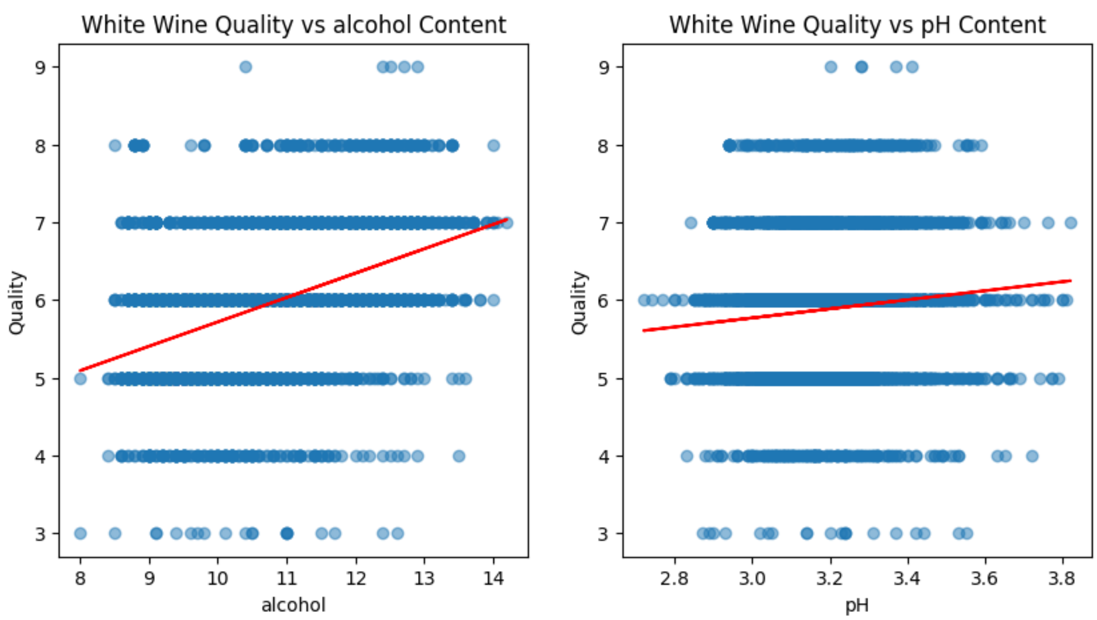
In [ ]:

```
create_scatterplot(wine_red, 'Red')
```



In [ ]:

```
create_scatterplot(wine_white, 'White')
```



Bibliography

1. https://archive.ics.uci.edu/dataset/186/wine+quality
2. http://www3.dsi.uminho.pt/pcortez/wine5.pdf
3. http://www3.dsi.uminho.pt/pcortez/wine5.pdf
4. https://www.scielo.br/j/cta/a/HQsrPrPMNZYgRzSKtrjHyHh/?format=pdf

5. https://r4ds.had.co.nz/exploratory-data-analysis.html
6. https://towardsdatascience.com/exploratory-data-analysis-8fc1cb20fd15
7. https://www.vinhoverde.pt/en/homepage
8. https://www.vinhoverde.pt/en/homepage