

PROJECT 4 WINE ANALYSIS

11.25.2024

Problem Statement

VinoVista, a renowned winery, is committed to producing consistently exceptional wines. However, they have observed variability in the quality of their vinho verde batches. To address this challenge, VinoVista seeks a predictive model that can accurately assess the quality of wine batches based on their chemical properties before bottling.

Project Goal:

The primary objective of this project is to develop a robust machine learning model capable of predicting wine quality on a scale of 0-10. This model will utilize a dataset containing various chemical properties of wine, such as acidity, pH, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, sulfates, and alcohol content.

Resources:

Wine Quality Dataset from UC Irvine Machine Learning Repository with 4899 samples

Predicting Wine Quality

Collaborators:

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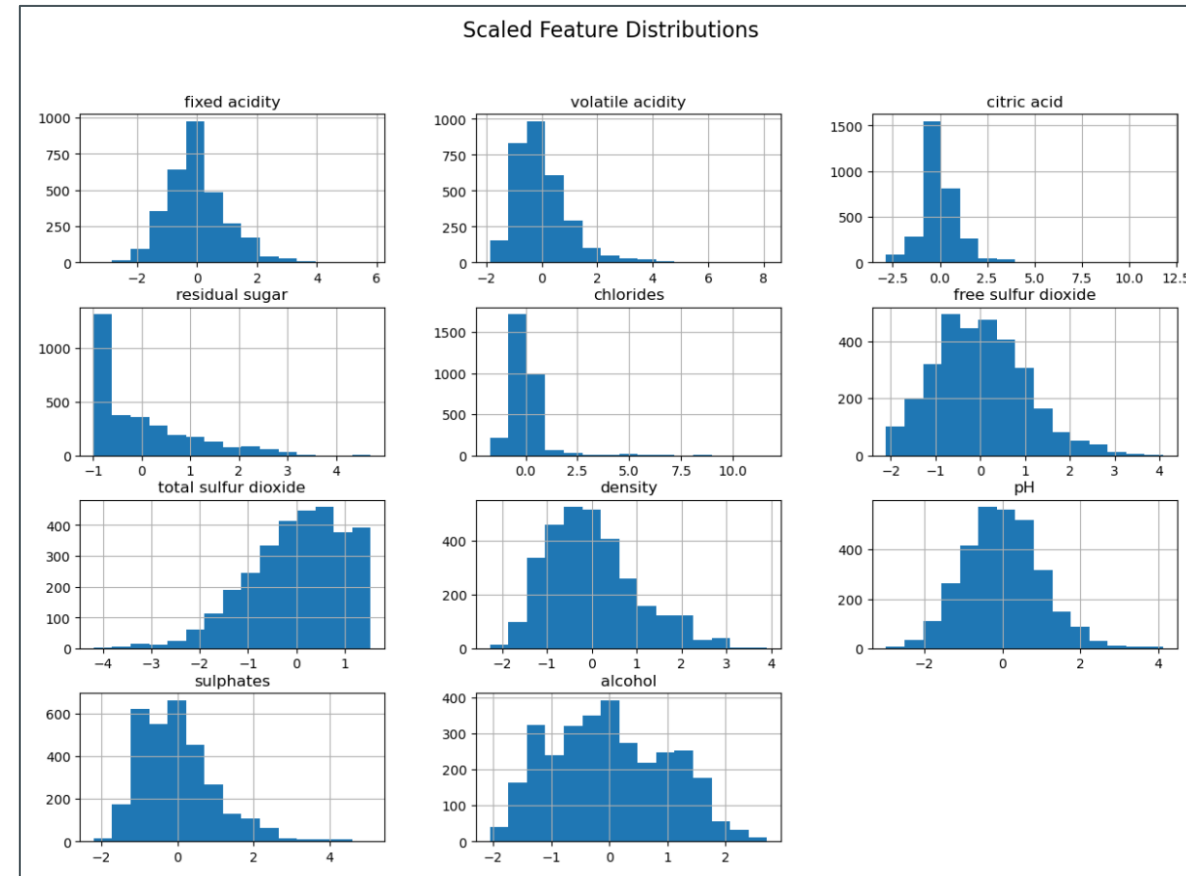
QUICK TAKE

- This data set was chosen because it contains information about the chemical properties of vinho verde, such as acidity, sugar levels, and alcohol content and the data is modeled after the physicochemical wine tests.
- The number of samples in our dataset after filtering is 3,090. We used Quality as our target and there are 11 total features.
- We cleaned our database by checking for null values, dropping any outliers in 'total sulfur dioxide' above 150 as that is likely a data entry error. Our quality values range from 1-10, so we created binary classification to use in our machine learning models. We chose 7 and above as good; 6 and below as not good.
- We checked for multi collinearity among our features for possible features that could be dropped to increase our precision and recall values and filtered our data to only keep wines that pH values between 3 and 4, as this is the nominal level for white wines.

QUICK TAKE

- The 3 acid categories are what combine to make the total acidity in wine. Acid, sugar, and alcohol content are the three most dominant qualities for wine evaluation for the consumer. When adding some information about chemical compounds, such as sulphur dioxide, ph and chloride, the machine can make pretty accurate predictions of a good or not good wine.

Feature distribution across the dataset



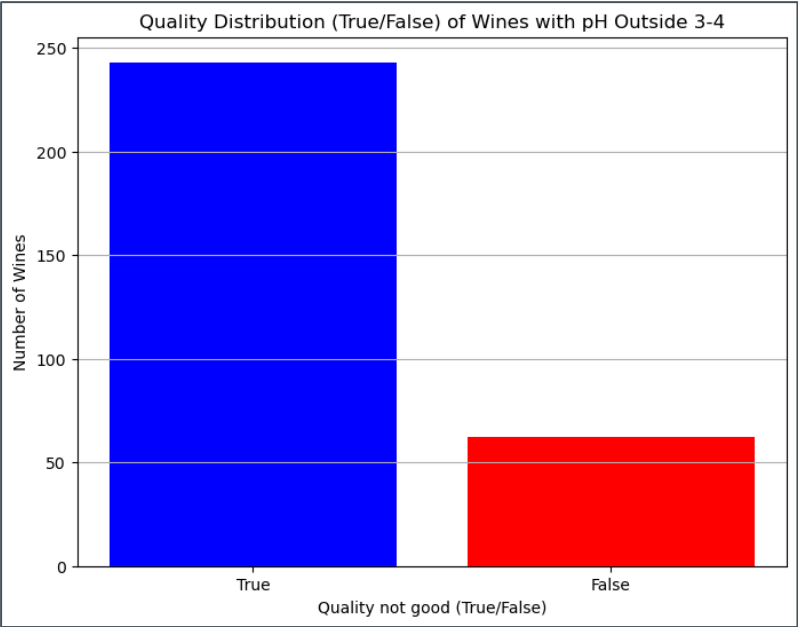
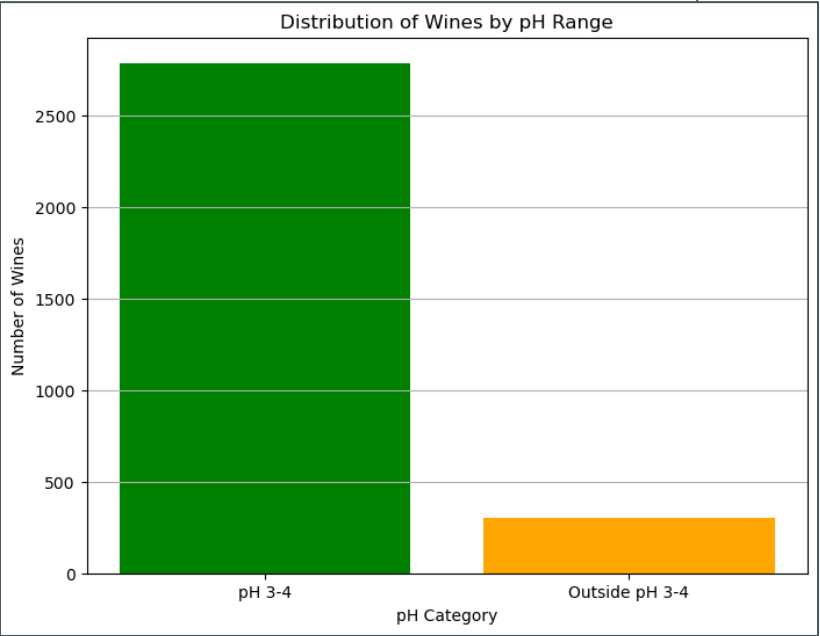
CHECK THE DATA AND PREPPING

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	6
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	6
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	6
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6

check for nulls (no nulls), and data type
df.info()

```
<class 'pandas.core.frame.DataFrame'>  
RangeIndex: 4898 entries, 0 to 4897  
Data columns (total 12 columns):  
#   Column              Non-Null Count  Dtype  
---  -  
0   fixed acidity        4898 non-null   float64  
1   volatile acidity     4898 non-null   float64  
2   citric acid          4898 non-null   float64  
3   residual sugar       4898 non-null   float64  
4   chlorides            4898 non-null   float64  
5   free sulfur dioxide  4898 non-null   float64  
6   total sulfur dioxide 4898 non-null   float64  
7   density              4898 non-null   float64  
8   pH                   4898 non-null   float64  
9   sulphates            4898 non-null   float64  
10  alcohol              4898 non-null   float64  
11  quality              4898 non-null   int64  
dtypes: float64(11), int64(1)  
memory usage: 459.3 KB
```

anything over 150 is likely data entry error, so we are dropping those values
df = df[df['total sulfur dioxide'] <= 150]

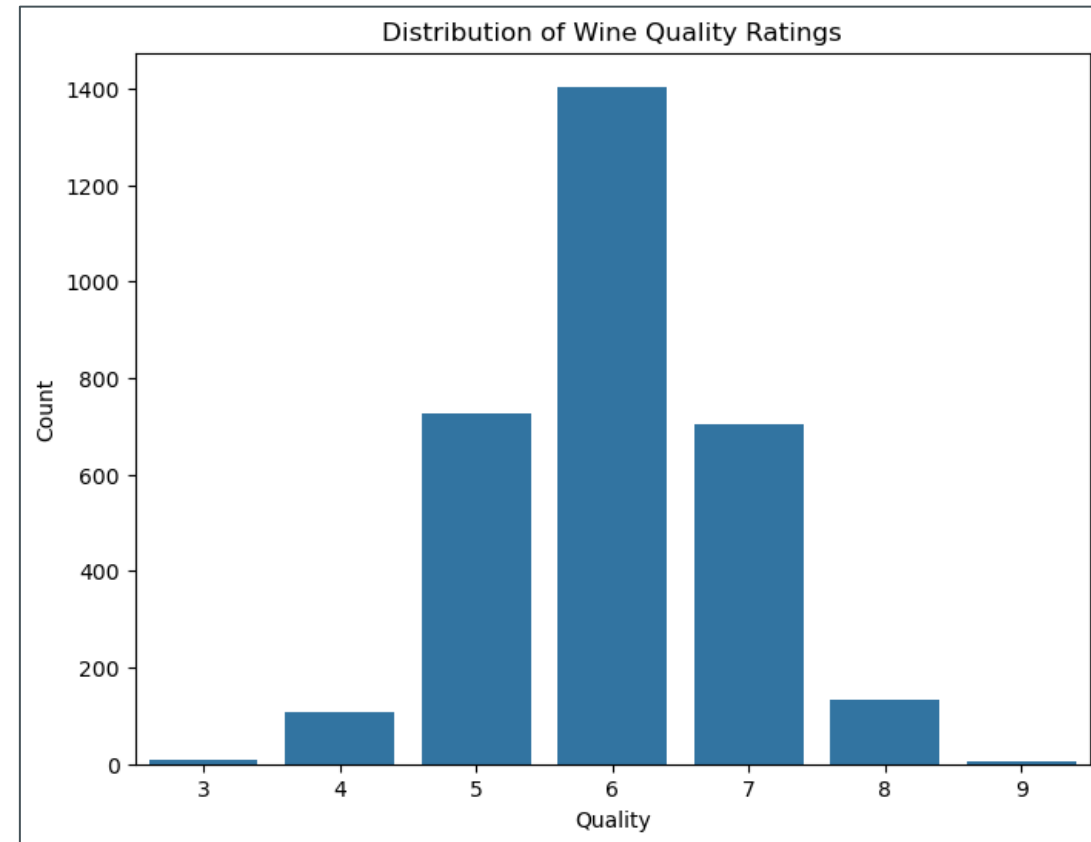


CREATING OUR CLASSIFICATIONS

```
# The scale for wine quality is 1-10, so we create a binary classification to use for our ML models
df['quality_label'] = np.where(df['quality'] >= 7, 'good', 'not good')
df.drop('quality', axis=1, inplace=True)
```

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 3090 entries, 1 to 4897
Data columns (total 12 columns):
 #   Column                Non-Null Count  Dtype  
---  -
 0   fixed acidity          3090 non-null   float64
 1   volatile acidity       3090 non-null   float64
 2   citric acid            3090 non-null   float64
 3   residual sugar         3090 non-null   float64
 4   chlorides              3090 non-null   float64
 5   free sulfur dioxide    3090 non-null   float64
 6   total sulfur dioxide   3090 non-null   float64
 7   density                3090 non-null   float64
 8   pH                    3090 non-null   float64
 9   sulphates              3090 non-null   float64
10   alcohol                3090 non-null   float64
11   quality_label          3090 non-null   object  
dtypes: float64(11), object(1)
memory usage: 313.8+ KB
```



ENCODING AND SCALING

```
: # separate features from target
y=df['quality_label_not good']
X=df.drop(columns='quality_label_not good')
```

```
# clean it up, scale it etc
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)
X_scaled_df = pd.DataFrame(X_scaled, columns=X.columns)
```

```
# convert categorical variables into numerical ones using one-hot encoding to use in our model
df = pd.get_dummies(df, columns=['quality_label'], drop_first=True)
```

```
df.head()
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality_label_not good
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	True
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	True
5	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	True
6	6.2	0.32	0.16	7.0	0.045	30.0	136.0	0.9949	3.18	0.47	9.6	True
8	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	True

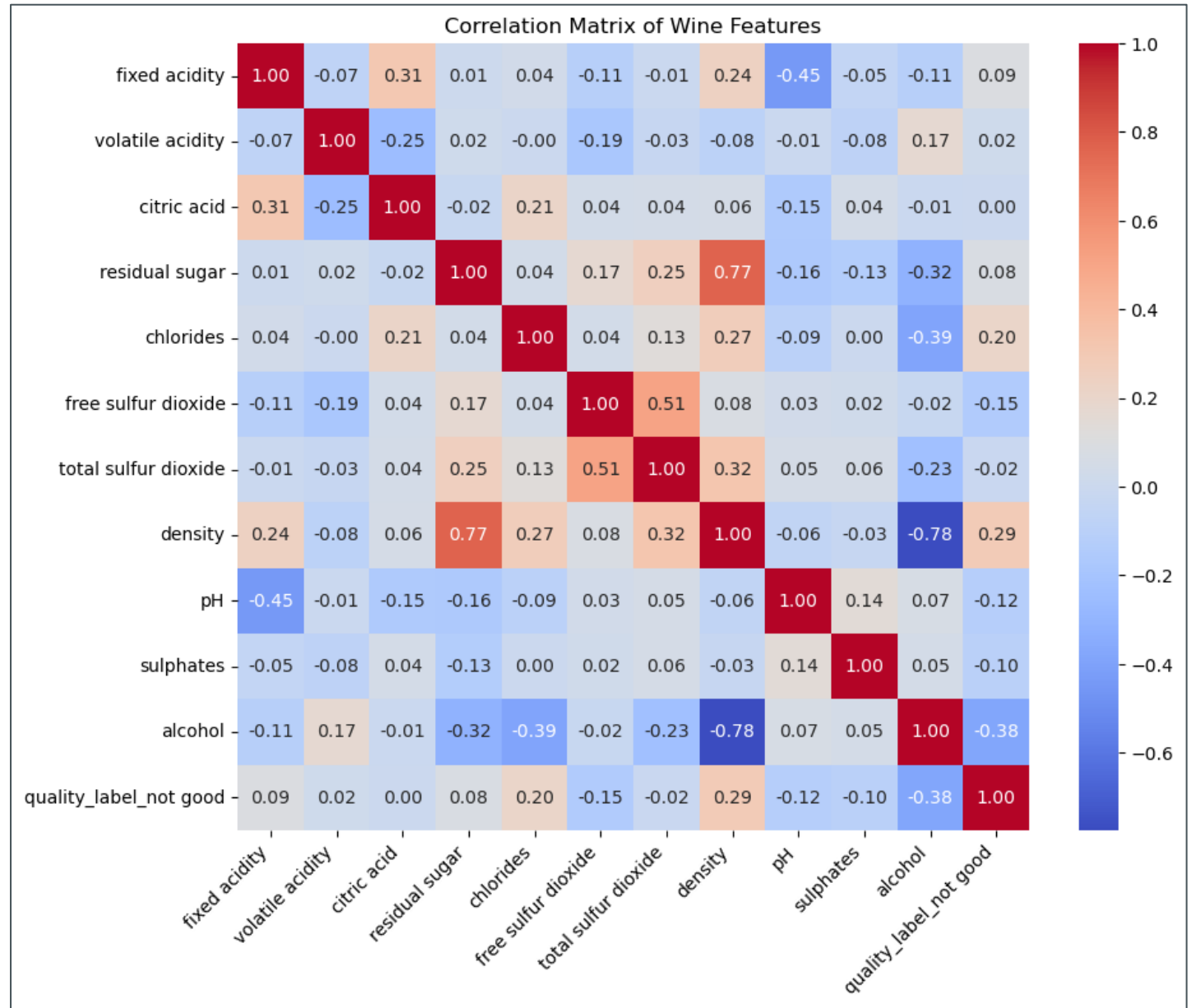
```
# check that shape
df.shape
```

```
(3090, 12)
```

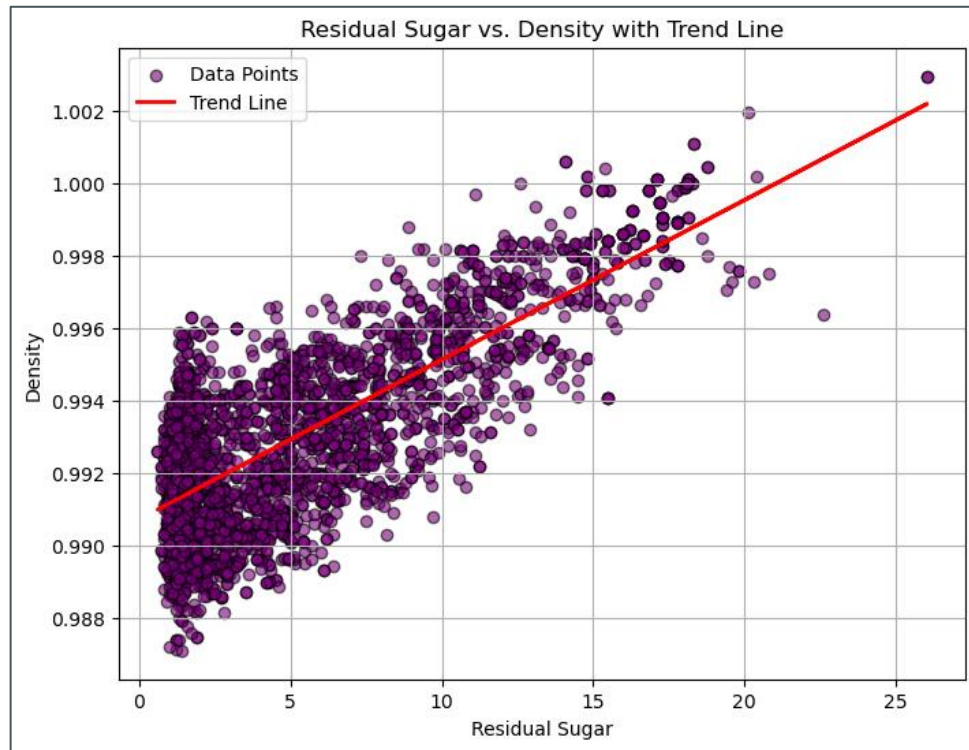
CHECKING CORRELATIONS ACROSS THE FEATURES

We found 2 interesting relations

- The sugar amounts and density have a high positive correlation
- Density and alcohol have a high negative correlation

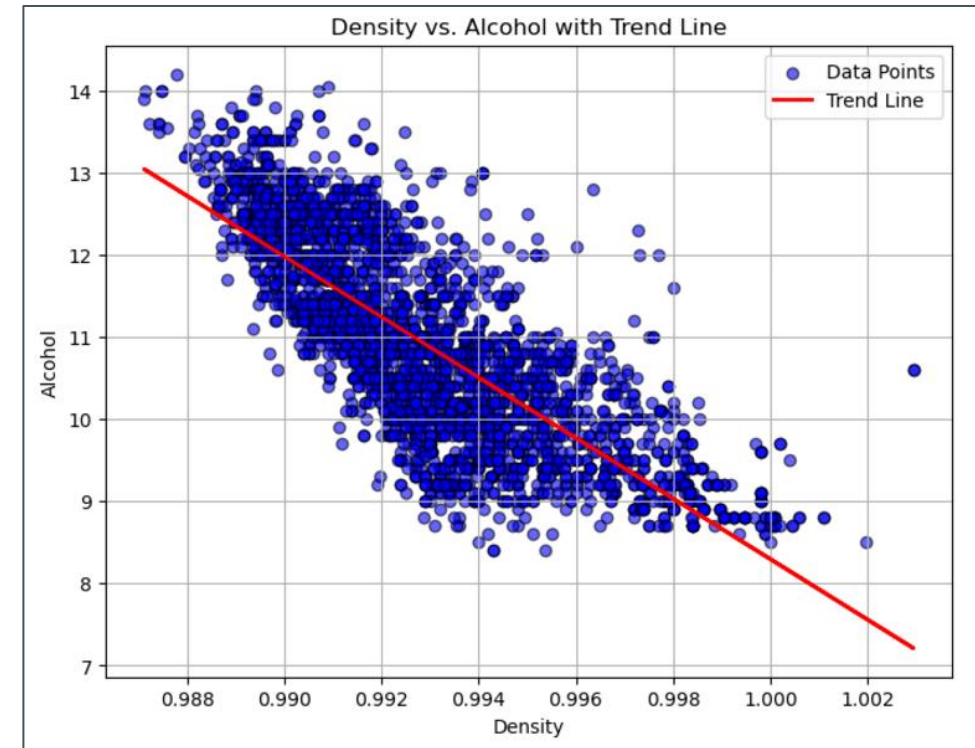


CHECKING CORRELATIONS



Correlation coefficient: 0.7657848803711766

- Higher sugar content creates a denser wine. Since these two have a strong correlation, we tested our accuracy numbers after dropping 'Sugar' or 'Density'. Surprisingly, both these actions led to lower accuracy numbers.



Correlation coefficient: -0.3170400981344824

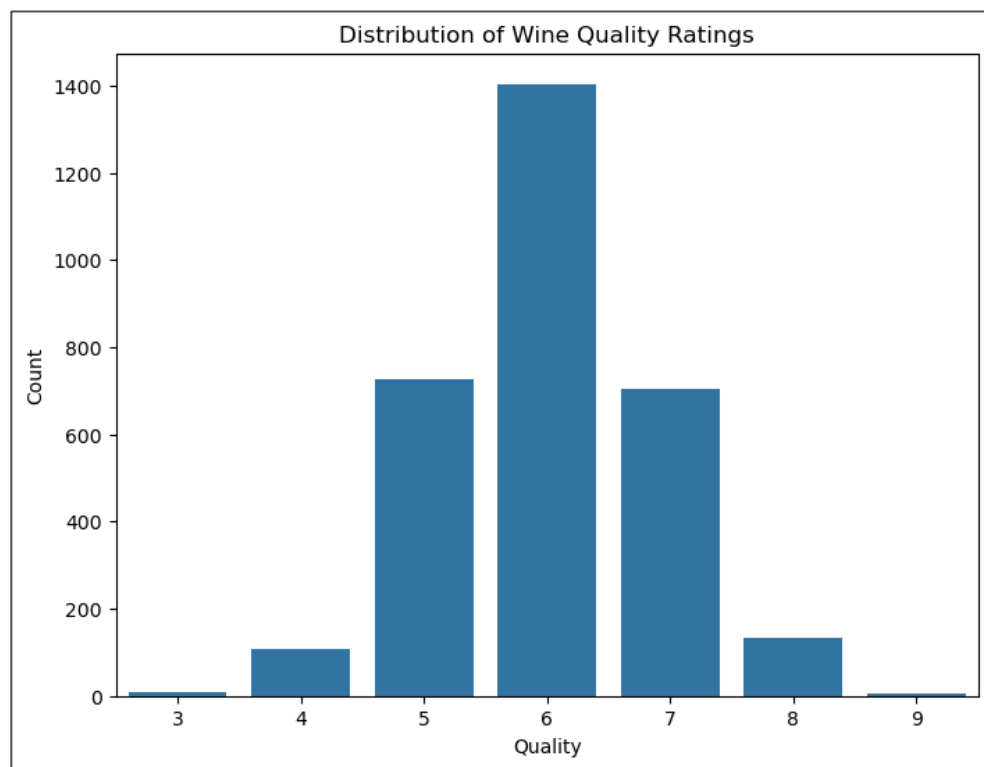
- The higher alcohol wines have a lower density. Alcohol inherently creates a less dense, less viscous drink.

SPLITTING AND FITTING AND CLASSIFYING....OH MY

```
# train test module on our standard data
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X_scaled,
                                                    y,
                                                    random_state=1776,
                                                    stratify=y)
```

X_train.shape

(2317, 11)



```
# Logistic regress
from sklearn.linear_model import LogisticRegression
classifier = LogisticRegression(solver='lbfgs',
                               max_iter=200,
                               random_state=1776)
classifier.fit(X_train, y_train)
```

LogisticRegression

LogisticRegression(max_iter=200, random_state=1776)

```
# predictions and confusion matrix
testing_predictions = classifier.predict(X_test)
test_matrix = confusion_matrix(y_test, testing_predictions)
print(test_matrix)
```

```
[[ 78 133]
 [ 56 506]]
```

```
# classification report for our standard data
test_report = classification_report(y_test, testing_predictions)
print(test_report)
```

	precision	recall	f1-score	support
False	0.58	0.37	0.45	211
True	0.79	0.90	0.84	562
accuracy			0.76	773
macro avg	0.69	0.64	0.65	773
weighted avg	0.73	0.76	0.74	773

MODEL SELECTION

Extreme Gradient Boosting was our highest performing model

```
# xgboost model - our best performing model
from xgboost import XGBClassifier
|
xgb_clf = XGBClassifier(random_state=1776, scale_pos_weight=len(y_train[y_train == 0]) / len(y_train[y_train == 1]))
xgb_clf.fit(X_train, y_train)
predictions = xgb_clf.predict(X_test)
print(classification_report(y_test, predictions))
```

	precision	recall	f1-score	support
False	0.71	0.68	0.69	211
True	0.88	0.90	0.89	562
accuracy			0.84	773
macro avg	0.80	0.79	0.79	773
weighted avg	0.83	0.84	0.84	773

- SVM had the lowest overall accuracy and RandomForest was slightly less than XGBoost
- XGBoost can often outperform Random Forest due to its ability to learn from mistakes to prevent overfitting and optimize for efficiency.
- Each new tree focuses on correcting errors from the previous trees. So, each new tree contributes to improving performance.

VINOVISTA WINE ANALYSIS

- Our dataset comes from the food industry, where quality ratings from tasters are inherently subjective. Despite this, we believe our model's results are very strong. Additionally, the relatively small size of our dataset may contribute to a slight loss in accuracy. The overrepresentation of bad wines in the data has also led to an accuracy imbalance, particularly when predicting good wines.
- This model could also be leveraged for rapid, small-batch research and development.
- It could also be used to efficiently allocate for different wine groups. For example, delivering high-quality wine to upscale market sectors or average-quality wines to value-driven markets.
- We believe this model could also be used for quick packaging and customer decision-making, saving time and money on the identifying and packaging process, which addresses both marketing and production strategies.
- Quality ratings from tasters can take time to receive, but our model allows for swift detection and prediction of bad wines, which are most likely to receive a rating of 6. These wines could then be allocated as table wine batches, targeting high-volume clients or customers seeking affordable wines more efficiently.