

Deliverable 2: Data Summarization and Visualization

Data Summarization:

Descriptive Statistics:

The dataset contains 1143 observations. Here's a summary of key statistical measures for numerical variables:

Fixed Acidity: Mean = 8.31, Std. Dev. = 1.75, Min = 4.6, Max = 15.9
Volatile Acidity: Mean = 0.53, Std. Dev. = 0.18, Min = 0.12, Max = 1.58
Citric Acid: Mean = 0.27, Std. Dev. = 0.20, Min = 0.0, Max = 1.0
Residual Sugar: Mean = 2.53, Std. Dev. = 1.36, Min = 0.9, Max = 15.5
Chlorides: Mean = 0.087, Std. Dev. = 0.047, Min = 0.012, Max = 0.611
Free Sulfur Dioxide: Mean = 15.62, Std. Dev. = 10.25, Min = 1, Max = 68
Total Sulfur Dioxide: Mean = 45.91, Std. Dev. = 32.78, Min = 6, Max = 289
Density: Mean = 0.997, Std. Dev. = 0.0019, Min = 0.990, Max = 1.004
pH: Mean = 3.31, Std. Dev. = 0.16, Min = 2.74, Max = 4.01
Sulphates: Mean = 0.66, Std. Dev. = 0.17, Min = 0.33, Max = 2.0
Alcohol: Mean = 10.44, Std. Dev. = 1.08, Min = 8.4, Max = 14.9
Quality (Target Variable): Mean = 5.66, Std. Dev. = 0.81, Min = 3, Max = 8

Data Summary	
Name	wine_dataset
Number of columns	13
Column type frequency:	
numeric	13
Group variables	
	None

	skim_variable <chr>	n_missing <int>	complete_rate <dbl>	mean <dbl>	sd <dbl>	p0 <dbl>	p25 <dbl>	p50 <dbl>	p75 <dbl>	p100 <dbl>	hist <chr>
1	fixed.acidity	0	1	8.31111111	1.747595e+00	4.60000	7.10000	7.90000	9.100000	15.90000	
2	volatile.acidity	0	1	0.53133858	1.796332e-01	0.12000	0.39250	0.52000	0.640000	1.58000	
3	citric.acid	0	1	0.26836395	1.966859e-01	0.00000	0.09000	0.25000	0.420000	1.00000	
4	residual.sugar	0	1	2.53215223	1.355917e+00	0.90000	1.90000	2.20000	2.600000	15.50000	
5	chlorides	0	1	0.08693263	4.726734e-02	0.01200	0.07000	0.07900	0.090000	0.61100	
6	free.sulfur.dioxide	0	1	15.61548556	1.025049e+01	1.00000	7.00000	13.00000	21.000000	68.00000	
7	total.sulfur.dioxide	0	1	45.91469816	3.278213e+01	6.00000	21.00000	37.00000	61.000000	289.00000	
8	density	0	1	0.99673041	1.925067e-03	0.99007	0.99557	0.99668	0.997845	1.00369	
9	pH	0	1	3.31101487	1.566641e-01	2.74000	3.20500	3.31000	3.400000	4.01000	
10	sulphates	0	1	0.65770779	1.703987e-01	0.33000	0.55000	0.62000	0.730000	2.00000	
11	alcohol	0	1	10.44211140	1.082196e+00	8.40000	9.50000	10.20000	11.100000	14.90000	
12	quality	0	1	5.65704287	8.058242e-01	3.00000	5.00000	6.00000	6.000000	8.00000	
13	id	0	1	804.96937883	4.639971e+02	0.00000	411.00000	794.00000	1209.500000	1597.00000	

13 rows

fixed.acidity	volatile.acidity	citric.acid	residual.sugar	chlorides	free.sulfur.dioxide
Min. : 4.600	Min. :0.1200	Min. :0.0000	Min. : 0.900	Min. : 1.00	
1st Qu.: 7.100	1st Qu.:0.3925	1st Qu.:0.0900	1st Qu.: 1.900	1st Qu.:0.07000	1st Qu.: 7.00
Median : 7.900	Median :0.5200	Median :0.2500	Median : 2.200	Median :0.07900	Median :13.00
Mean : 8.311	Mean :0.5313	Mean :0.2684	Mean : 2.532	Mean :0.08693	Mean :15.62
3rd Qu.: 9.100	3rd Qu.:0.6400	3rd Qu.:0.4200	3rd Qu.: 2.600	3rd Qu.:0.09000	3rd Qu.:21.00
Max. :15.900	Max. :1.5800	Max. :1.0000	Max. :15.500	Max. :0.61100	Max. :68.000
total.sulfur.dioxide	density	pH	sulphates	quality	
Min. : 6.00	Min. :0.9901	Min. :2.740	Min. :0.3300	Min. : 8.40	Min. :3.000
1st Qu.:21.00	1st Qu.:0.9956	1st Qu.:3.205	1st Qu.:0.5500	1st Qu.: 9.50	1st Qu.:5.000
Median :37.00	Median :0.9967	Median :3.310	Median :0.6200	Median :10.20	Median :6.000
Mean :45.91	Mean :0.9967	Mean :3.311	Mean :0.6577	Mean :10.44	Mean :5.657
3rd Qu.:61.00	3rd Qu.:0.9978	3rd Qu.:3.400	3rd Qu.:0.7300	3rd Qu.:11.10	3rd Qu.:6.000
Max. :289.00	Max. :1.0037	Max. :4.010	Max. :2.0000	Max. :14.900	Max. :8.000
id					
Min. : 0					
Median :794					
Mean :805					
3rd Qu.:1210					
Max. :1597					

Fixed.acidity:

Minimum: 4.6, Maximum: 15.9

Mean: 8.311, Median: 7.9

25th Percentile (1st Qu.): 7.1, 75th Percentile (3rd Qu.): 9.1

volatile.acidity:

Minimum: 0.12, Maximum: 1.58

Mean: 0.5313, Median: 0.52

25th Percentile (1st Qu.): 0.3925, 75th Percentile (3rd Qu.): 0.64

citric.acid:

Minimum: 0, Maximum: 1

Mean: 0.2684, Median: 0.25

25th Percentile (1st Qu.): 0.09, 75th Percentile (3rd Qu.): 0.42

residual.sugar:

Minimum: 0.9, Maximum: 15.5 Mean: 2.532, Median: 2.2

25th Percentile (1st Qu.): 1.9, 75th Percentile (3rd Qu.): 2.6

chlorides:

Minimum: 0.012, Maximum: 0.611

Mean: 0.08693, Median: 0.079

25th Percentile (1st Qu.): 0.07, 75th Percentile (3rd Qu.): 0.09

free.sulfur.dioxide:

Minimum: 1, Maximum: 68

Mean: 15.62, Median: 13

25th Percentile (1st Qu.): 7, 75th Percentile (3rd Qu.): 21

total.sulfur.dioxide:

Minimum: 6, Maximum: 289

Mean: 45.91, Median: 37

25th Percentile (1st Qu.): 21, 75th Percentile (3rd Qu.): 61

density:

Minimum: 0.9901, Maximum: 1.0037

Mean: 0.9967, Median: 0.9967 25th Percentile (1st Qu.): 0.9956, 75th Percentile (3rd Qu.): 0.9978

pH:

Minimum: 2.74, Maximum: 4.01

Mean: 3.311, Median: 3.31

25th Percentile (1st Qu.): 3.205, 75th Percentile (3rd Qu.): 3.4

sulphates:

Minimum: 0.33, Maximum: 2

Mean: 0.6577, Median: 0.62

25th Percentile (1st Qu.): 0.55, 75th Percentile (3rd Qu.): 0.73

alcohol:

Minimum: 8.4, Maximum: 14.9

Mean: 10.44, Median: 10.2

25th Percentile (1st Qu.): 9.5, 75th Percentile (3rd Qu.): 11.1

quality:

Minimum: 3, Maximum: 8

Mean: 5.657, Median: 6

25th Percentile (1st Qu.): 5, 75th Percentile (3rd Qu.): 6

Id:

Minimum: 0, Maximum: 1597

Mean: 805, Median: 794

25th Percentile (1st Qu.): 0, 75th Percentile (3rd Qu.): 1210

Note: -Please look for Quartiles and Median in the above screenshot.

Missing Data:

No missing data was identified in the dataset. Handling Missing Data: -

If there are missing values, here are common strategies to handle them:

- **Imputation:** Replace missing values with a meaningful estimate. This could be the mean, median, or mode of the respective variable.
- **Deletion:** Remove observations or variables with missing values. This should be done cautiously, as it may result in loss of valuable information.
- **Advanced Imputation Techniques:** For more complex datasets, consider using advanced imputation methods such as K-nearest neighbours (KNN) or regression imputation.

Data Preprocessing:

Based on the descriptive statistics, potential preprocessing steps could include normalization or standardization, especially for variables with high variance.

Scaling:

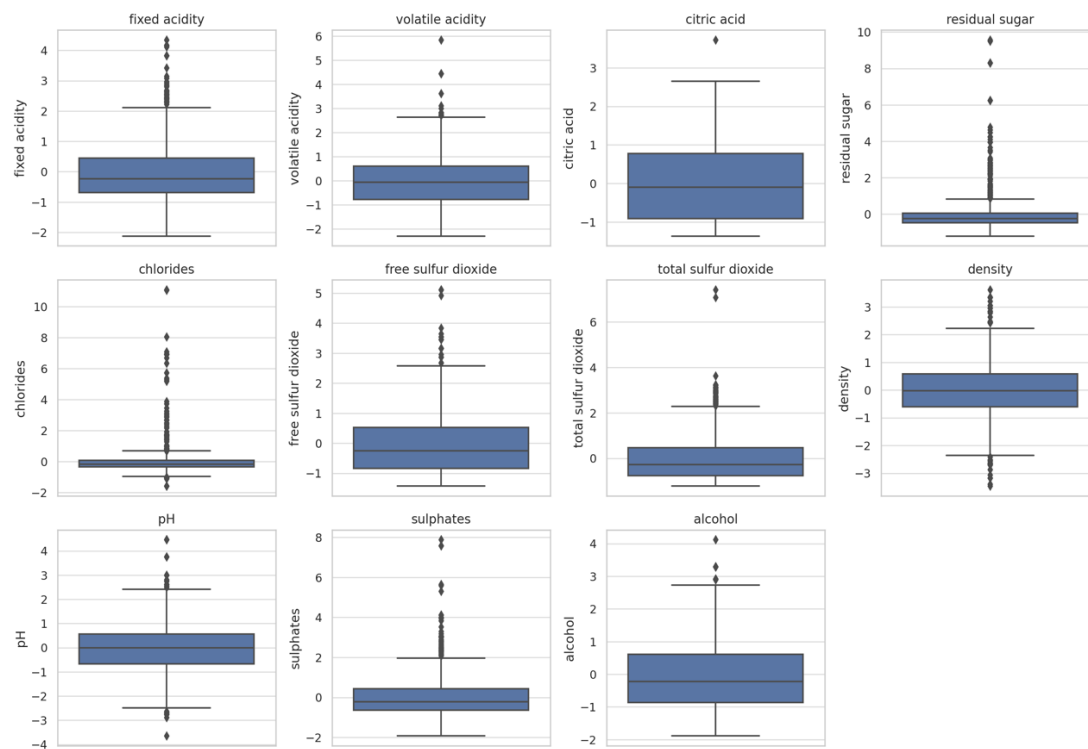
The preprocessing step of standardization has been applied to the wine dataset, excluding the target variable 'quality' and the non-relevant 'Id' column.

This process involved scaling the numerical features to have a mean of 0 and a standard deviation of 1, which is important for many machine learning algorithms that are sensitive to the scale of input features.

Standardization helps in dealing with features that have high variance and ensures that each feature contributes equally to the distance computations in models like K-Means or K-Nearest Neighbors, and in models where gradient descent is involved, like Logistic Regression or Neural Networks.

Handling Outliner:

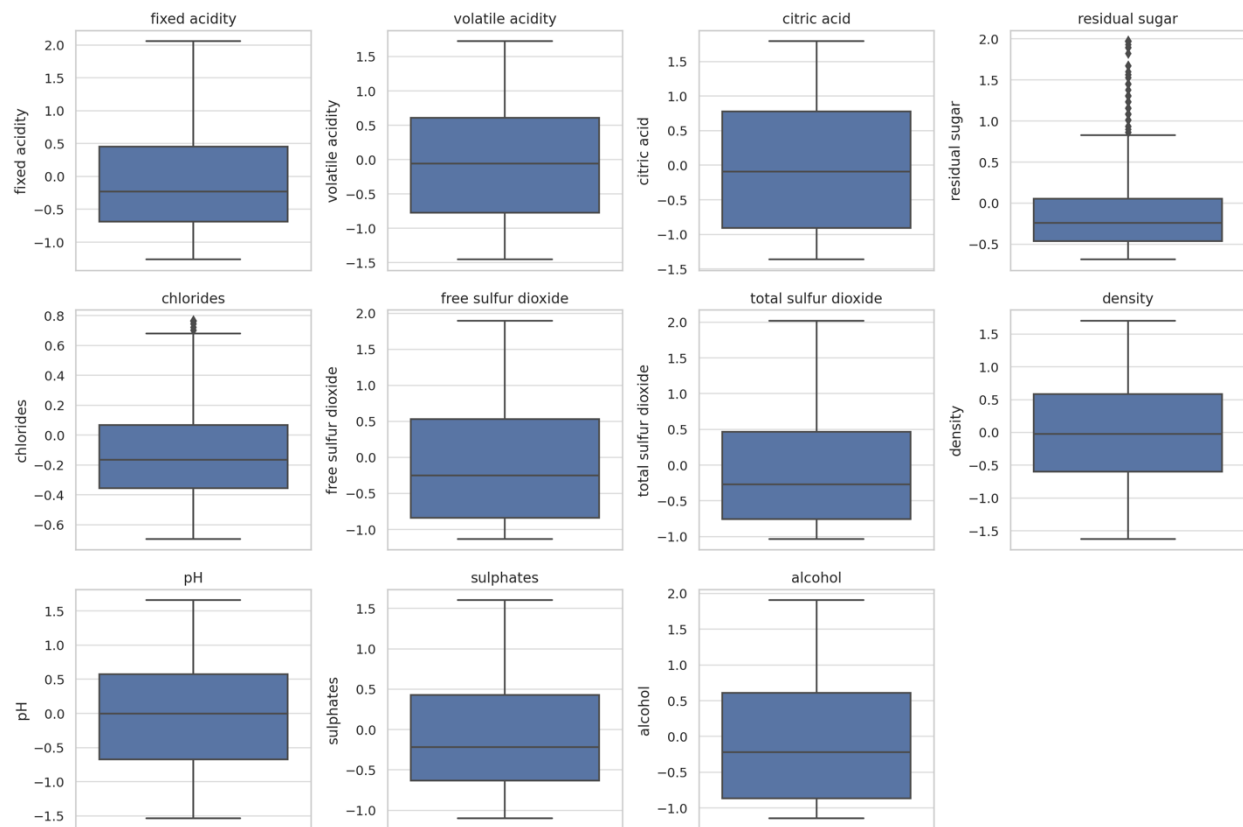
The dataset is preprocessed and ready for the next steps in our analysis or model building. This includes training machine learning models for regression (predicting wine quality) or classification (distinguishing between red and white wines), as previously discussed.



The box plots for each variable in the preprocessed dataset illustrate how standardization has transformed the data. After standardization, all variables now have a mean of 0 and a standard deviation of 1, as reflected in the scales of the box plots.

It's important to note that standardization does not eliminate outliers; it merely scales the data. This means that while the influence of outliers on the scale of the data is reduced, the outliers themselves are still present in the data, as indicated by the points beyond the whiskers in the box plots.

If outlier handling is a concern for our analysis or predictive modeling, we might consider additional steps such as trimming (removing outliers) or applying transformations (like log transformation) that can reduce the impact of outliers. However, the decision to modify or remove outliers should be made with caution and a good understanding of the data, as outliers can sometimes contain valuable information for certain types of analyses or models.



The box plots for the winsorized dataset show the effect of dealing with outliers. Winsorization has been applied to each numerical column by limiting the extreme values to the 5th and 95th percentiles. This method reduces the influence of outliers by replacing them with the nearest values within the specified percentiles.

After Winsorization: -

The range of each feature has been compressed, and extreme outliers have been significantly reduced.

The central tendency and spread of the data are now more representative of most of the data points.

This approach to handling outliers can be particularly useful for models sensitive to extreme values. However, it's important to consider the potential impact of altering the data in this way, as it might affect the interpretation of the results, especially if the outliers were meaningful or indicative of certain phenomena in the original data.

With the outliers addressed, the dataset is now in a more robust state for further analysis or predictive modeling.

Imputation:

```
{r}
wine_dataset <- wine_dataset[, !(names(wine_dataset) %in% c("Id"))]
str(wine_dataset)

'data.frame':  1143 obs. of  12 variables:
 $ fixed.acidity      : num  7.4 7.8 7.8 11.2 7.4 7.4 7.9 7.3 7.8 6.7 ...
 $ volatile.acidity   : num  0.7 0.88 0.76 0.28 0.7 0.66 0.6 0.65 0.58 0.58 ...
 $ citric.acid        : num  0 0 0.04 0.56 0 0 0.06 0 0.02 0.08 ...
 $ residual.sugar     : num  1.9 2.6 2.3 1.9 1.9 1.8 1.6 1.2 2 1.8 ...
 $ chlorides          : num  0.076 0.098 0.092 0.075 0.076 0.075 0.069 0.065
 0.073 0.097 ...
 $ free.sulfur.dioxide : num  11 25 15 17 11 13 15 15 9 15 ...
 $ total.sulfur.dioxide: num  34 67 54 60 34 40 59 21 18 65 ...
 $ density            : num  0.998 0.997 0.997 0.998 0.998 ...
 $ pH                 : num  3.51 3.2 3.26 3.16 3.51 3.51 3.3 3.39 3.36 3.28 ...
 $ sulphates          : num  0.56 0.68 0.65 0.58 0.56 0.56 0.46 0.47 0.57 0.54
 ...
 $ alcohol            : num  9.4 9.8 9.8 9.8 9.4 9.4 9.4 10 9.5 9.2 ...
 $ quality            : int  5 5 5 6 5 5 5 7 7 5 ...
```

No need to keep id column as not needed for analysis.

Data Visualization:

Answering business question from deliverable 1

Answer 1:

Our approach to predict wine quality using regression techniques, such as linear regression, is well-founded. Given the Wine Quality dataset, focusing on the chemical attributes listed will be instrumental in building a predictive model. Here's a brief overview of how each of these variables can be crucial for the prediction model: -

Fixed Acidity: Critical for taste and stability. High acidity can make wine taste tart, while low acidity might result in flat-tasting wines.

Volatile Acidity: Elevated levels can lead to unpleasant vinegar-like flavors. It's a key factor in the overall balance of the wine.

Citric Acid: Adds freshness and flavor. It's a significant component of the wine's acid profile and can influence the wine's freshness and flavor profile.

Residual Sugar: Determines sweetness level. This is particularly important in the context of the wine style, as different styles (dry, semi-sweet, sweet) have varying sugar levels.

Chlorides: Affects taste, particularly in terms of saltiness. Excessive chloride levels can negatively affect the taste profile.

Free Sulfur Dioxide and Total Sulfur Dioxide: Used as preservatives, they can influence both aroma and taste. Balancing sulfur dioxide is crucial to prevent microbial growth while maintaining taste.

Density: Related to alcohol and sugar concentration. It can provide insights into the wine's body and mouthfeel, which are important quality parameters.

pH: Influences stability and taste. It affects the color, stability, and taste of the wine. Wines typically have a pH between 3 and 4.

Alcohol: A significant factor in wine quality. It affects the body, flavor, and overall balance of the wine.

Sulfates (Sulphates): Act as antioxidants and antimicrobial agents. They can impact both the shelf life and the flavor profile of the wine.

Given these variables, it's important to analyze the relationships between them and the quality score. We might want to use correlation analysis or feature importance tools within the regression modeling to identify which variables are most predictive of wine quality. It's also important to consider interactions between variables, as the quality of wine is often the result of complex interactions between its chemical components.

When building the regression model, we should be mindful of potential multicollinearity, as some of these variables might be highly correlated with each other. This could affect the interpretability of the model. Regularization techniques in linear regression, like Ridge or Lasso, can be useful in such scenarios.

Finally, validating the model with a separate test dataset and using metrics like RMSE (Root Mean Square Error) or R^2 (Coefficient of Determination) will be key to ensuring the robustness and reliability of our predictions.

Answer 2:

Employing classification algorithms such as logistic regression to categorize wines into red or white based on their characteristics is a practical approach. The variables we've identified are indeed relevant in differentiating between red and white wines. Here's a breakdown of how each variable can contribute to the classification:

Fixed Acidity: Red wines often have higher fixed acidity compared to white wines. This difference in acidity levels can be a significant indicator for classification, as it affects the wine's body and structure.

Citric Acid: White wines generally have higher citric acid content, which contributes to their freshness and flavor profile. This variable can be a key differentiator, as it influences the wine's overall taste and aroma.

Residual Sugar: White wines typically contain more residual sugar, leading to a sweeter profile. This characteristic can be a crucial distinguishing factor, as the sugar level directly impacts the taste and style of the wine.

Chlorides: The level of chlorides, which can impact the saltiness and overall flavor of the wine, often differs between red and white wines. Red wines usually have higher chloride levels, which can be used as a feature for classification.

When developing our classification model, it would be beneficial to:

Perform Exploratory Data Analysis (EDA): To visualize and understand the distribution and relationship of these features with the wine type. This can include plotting histograms, box plots, or violin plots for each variable, segmented by wine type.

Feature Engineering: Consider creating new features or transforming existing ones to improve model performance. For example, interactions between variables or polynomial features could capture more complex relationships.

Model Selection: While logistic regression is a good starting point, exploring other classification algorithms like decision trees, random forests, or support vector machines might yield better results, depending on the dataset's characteristics.

Model Evaluation: Use appropriate metrics like accuracy, precision, recall, F1-score, and ROC-AUC to evaluate the model's performance. Cross-validation can help in assessing the model's robustness.

Handle Imbalanced Classes: If there's a significant imbalance in the number of red and white wine samples, techniques like oversampling, under sampling, or using algorithms that handle imbalances natively might be necessary.

Finally, the success of our model will largely depend on the quality and nature of the data, as well as the appropriateness of the features selected for the classification task.

Visualizing the data set:

Given the nature of the dataset, the following visualizations are recommended to gain insights relevant to the business question:

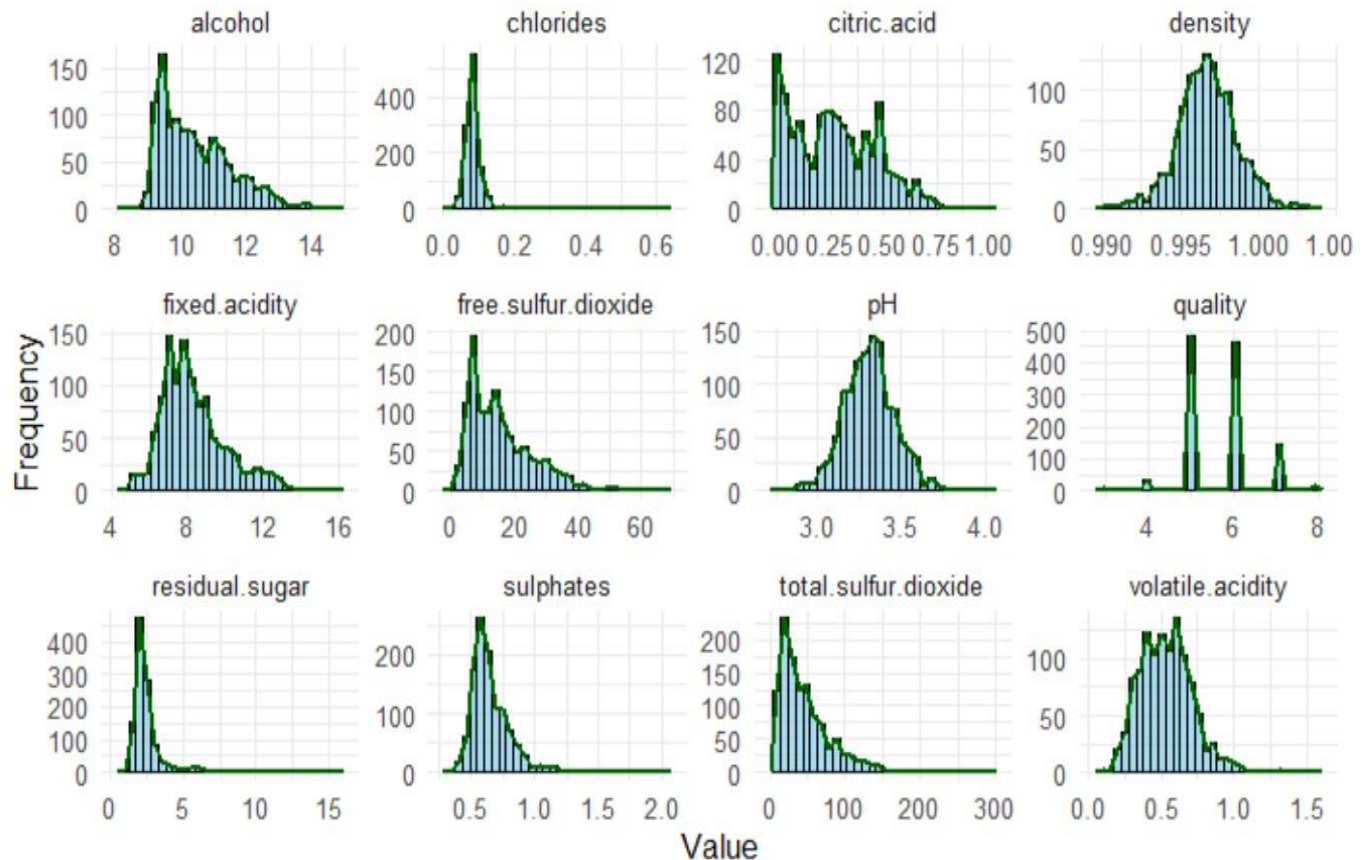
Histograms: For variables like alcohol content, pH, and quality to understand their distribution.

Scatter Plots: To explore relationships between variables like quality and other features.

Box Plots: To visualize the spread and identify outliers in variables such as fixed acidity and volatile acidity.

Heatmap: To illustrate the correlation between different variables.

Each visualization will include clear labels, titles, and legends for easy interpretation, and will be accompanied by a narrative explaining its relevance to the business question. Let's proceed with generating these visualizations.

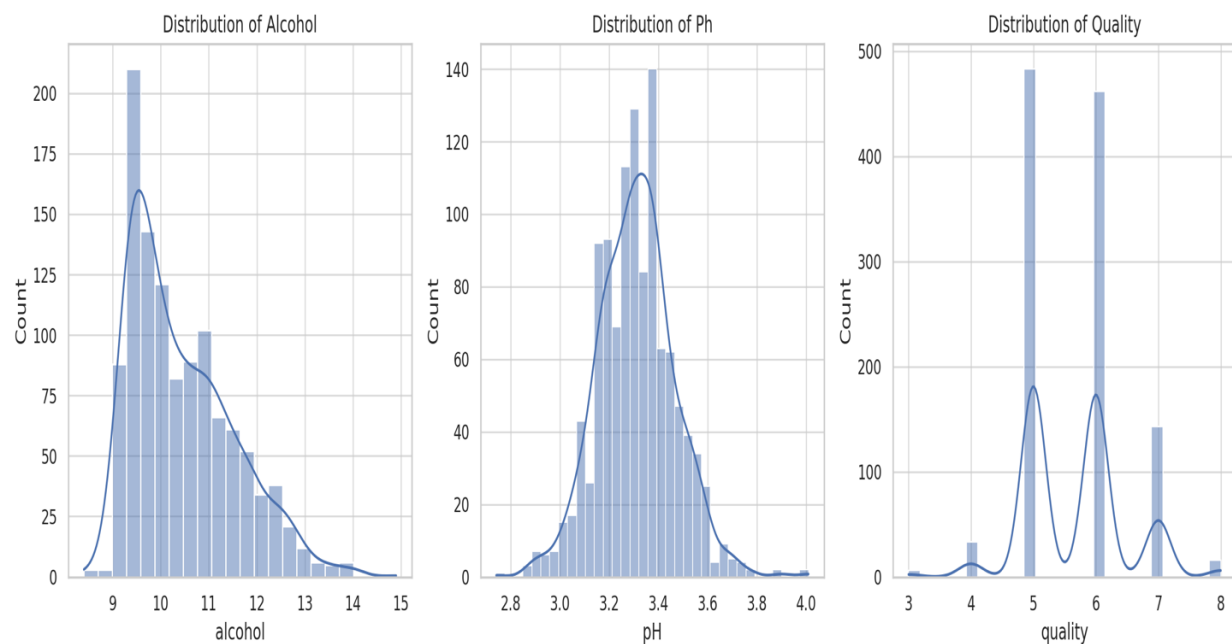


Histogram 1 for the given dataset:

The image displays a series of histograms, each representing the distribution of different variables from a dataset presumably related to wine characteristics. Here's a description for each histogram:

- **Alcohol:** The distribution is slightly right skewed, showing that most of the wine samples have an alcohol percentage around 9-10%, with fewer wines having higher alcohol content.
- **Chlorides:** This histogram is heavily right skewed, with most wines having low chloride levels, suggesting that high chloride content is less common in this dataset.
- **Citric Acid:** The distribution has multiple peaks, indicating variability in citric acid content across different wine samples.
- **Density:** Appears normally distributed, centering around 0.996-0.998, indicating a consistent density in most of the wine samples.
- **Fixed Acidity:** This histogram is right-skewed, with most wines having lower fixed acidity, while a few have significantly higher values.
- **Free Sulfur Dioxide:** Also right-skewed, showing that a majority of the wines have lower levels of free sulfur dioxide.
- **pH:** The distribution looks approximately normal, centered around a pH of 3.2-3.3.

- **Quality:** The quality ratings are discrete, with most wines rated around 5 or 6. There are fewer instances of very low (3-4) or high (7-8) quality ratings.
- **Residual Sugar:** Heavily right skewed, most wines have low residual sugar levels, with a long tail indicating a small number of wines with high sugar content.
- **Sulphates:** Right-skewed distribution, with the bulk of wine samples having lower sulphates content.
- **Total Sulfur Dioxide:** Another right-skewed histogram, like free sulfur dioxide, showing that most wines have a lower concentration of total sulfur dioxide.
- **Volatile Acidity:** Shows a slightly right-skewed distribution, where most wines have lower levels of volatile acidity.

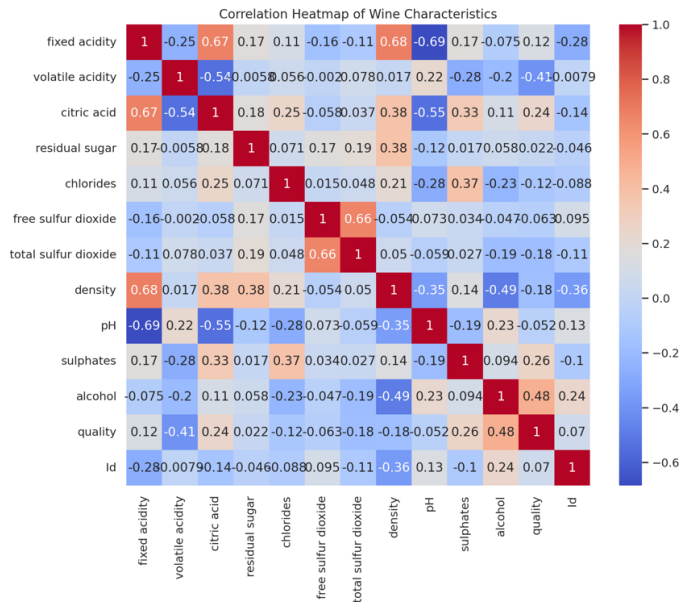


Histograms 2: Distribution of Key Variables

Alcohol Content: Shows a slightly right-skewed distribution, indicating most wines have moderate alcohol content.

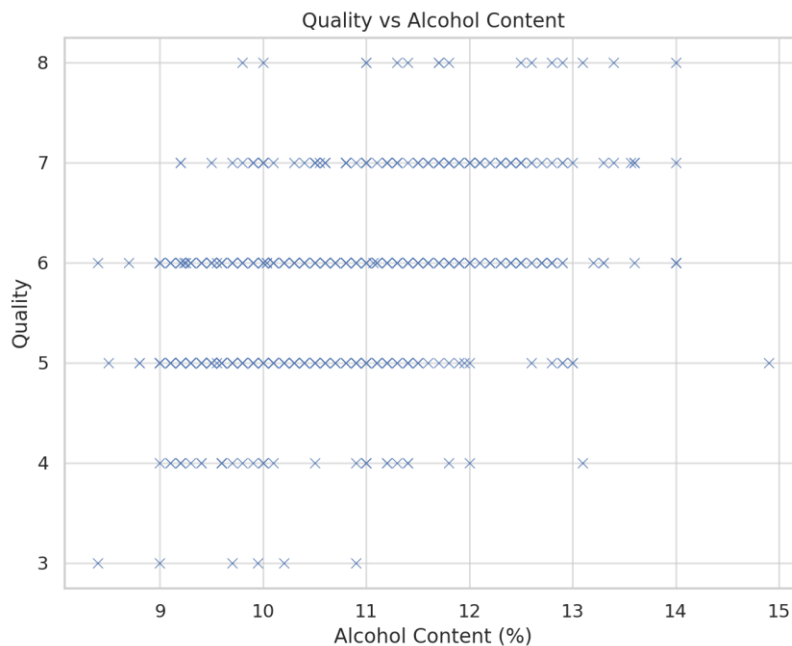
pH: The distribution appears almost normal, centered around a pH of 3.3.

Quality: This is slightly left-skewed, suggesting that most wines have a quality rating around 5 or 6, with fewer high-quality wines (rating 7 or 8).



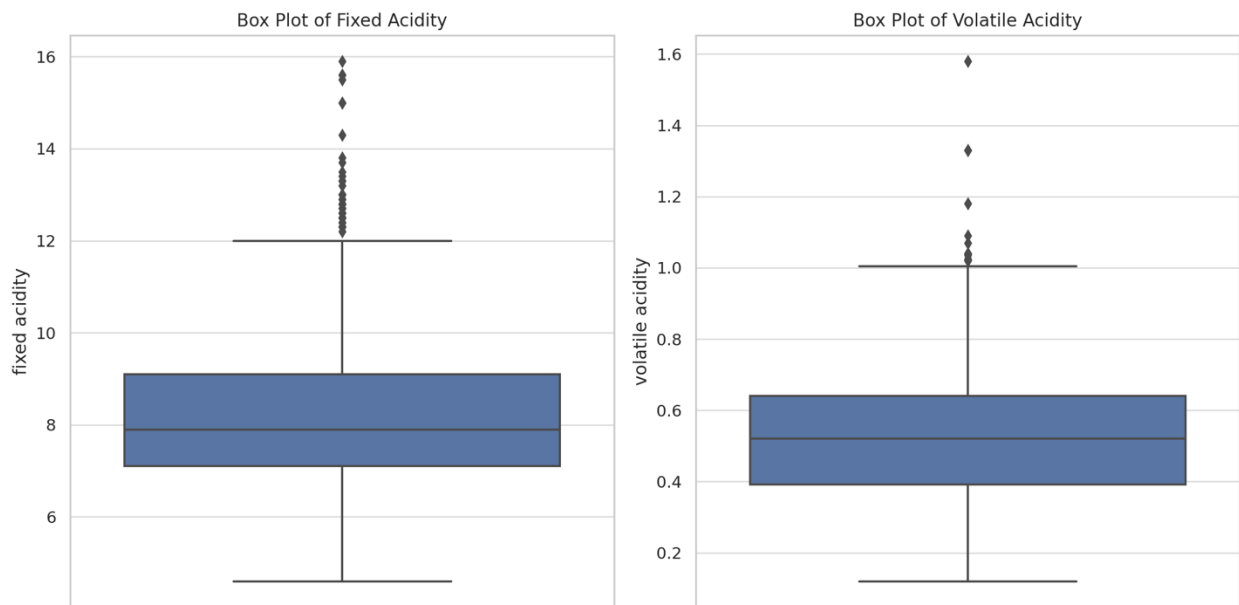
Correlation Heatmap

The heatmap reveals the relationships between different variables. For instance, alcohol content shows a positive correlation with quality, indicating higher alcohol may be associated with higher quality. Acidity-related features (like fixed acidity, citric acid) also show interesting correlations.



Scatter Plot: Quality vs Alcohol Content

This plot highlights a positive trend between alcohol content and quality, suggesting wines with higher alcohol content tend to have higher quality ratings.



Box Plots: Acidity Measures

Fixed Acidity: Displays a wide range of values with some outliers, indicating variation in acidity levels among different wines.

Volatile Acidity: Shows a more concentrated range but with several outliers, highlighting that most wines have similar volatile acidity levels, but some exceptions exist.

These visualizations provide valuable insights into the characteristics of the wine dataset, particularly in relation to wine quality. They form a solid foundation for further analysis and modeling, especially in understanding the factors that contribute to a wine's quality.

Visualizing the data set in accordance with deliverable 1 questions:

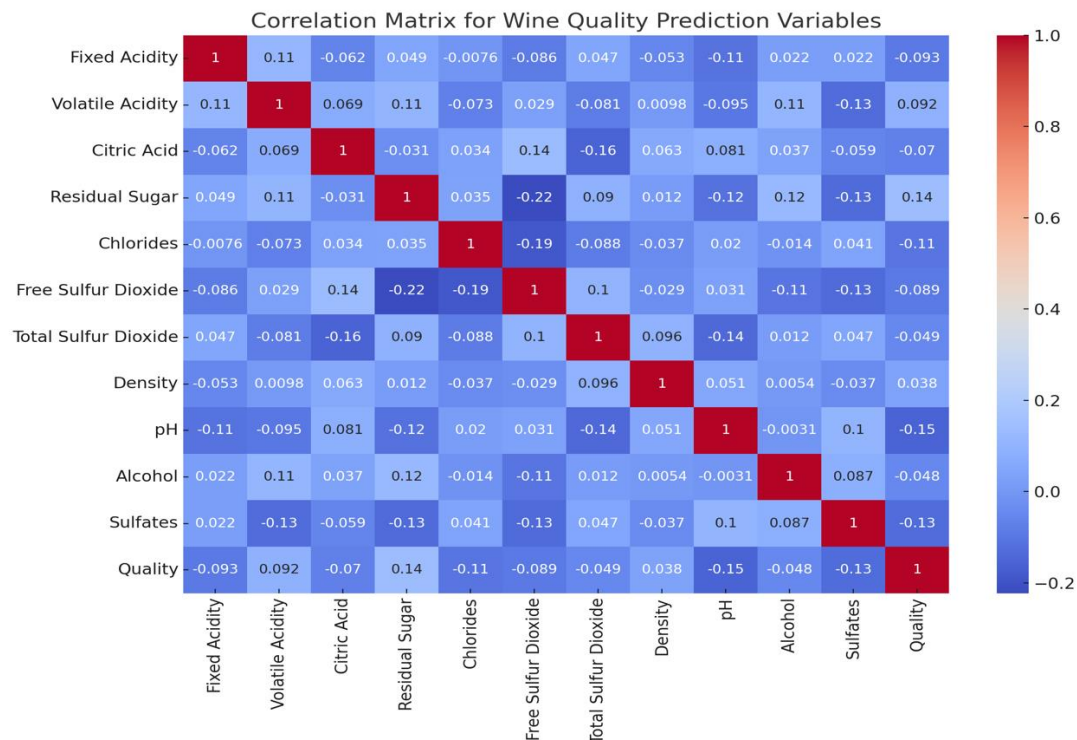
These visualizations will help us understand the relationships between different variables and their impact on wine quality and type. Let's outline the types of graphs that would be beneficial for each scenario:

For Predicting Wine Quality (Regression):

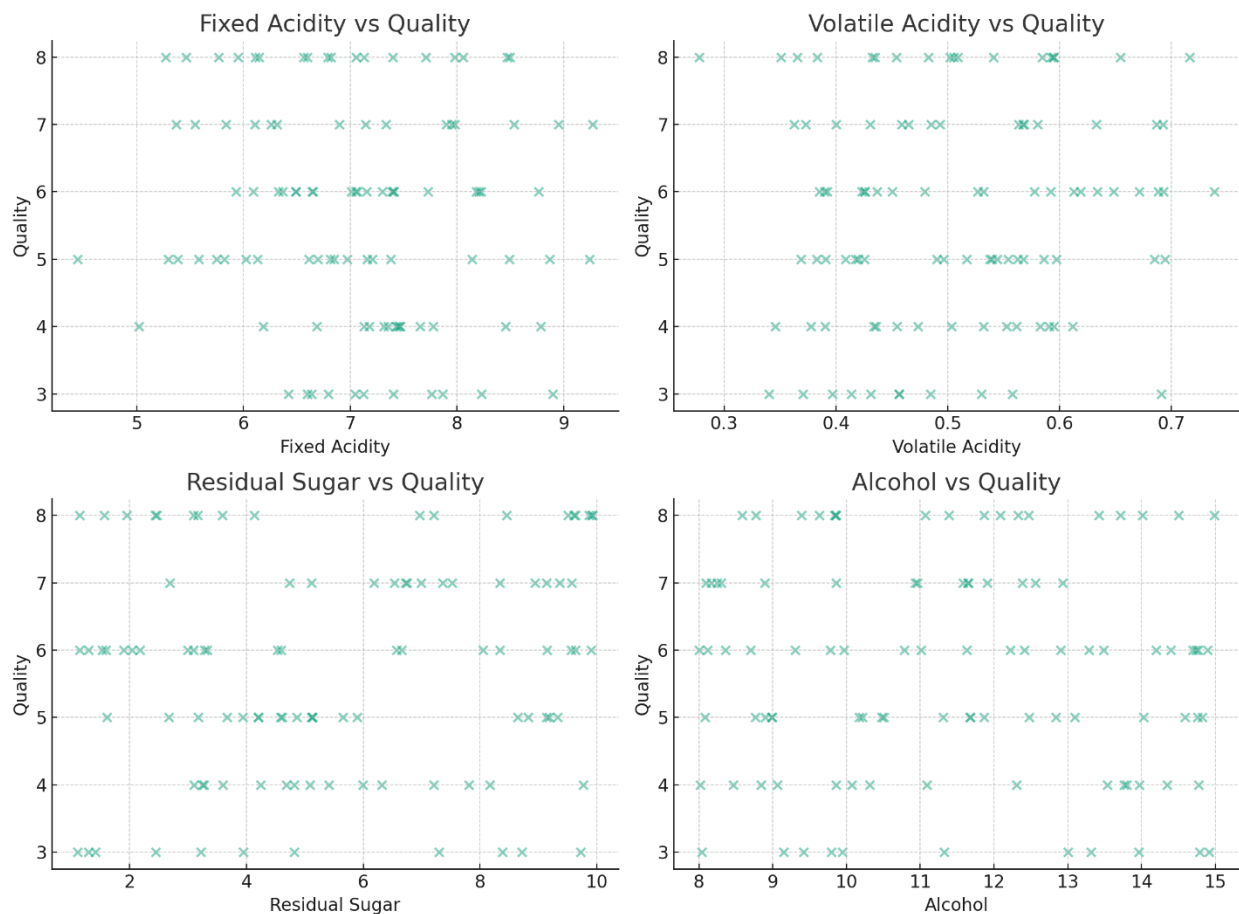
- **Correlation Matrix:** A heatmap showing the correlation coefficients between all the variables. This will help identify which variables are most closely related to wine quality and if there are any multicollinearity issues.
- **Scatter Plots:** Individual scatter plots for each variable against wine quality. This will provide insights into the linear relationships between each predictor and the target variable.
- **Box Plots:** To compare the distribution of each variable across different quality ratings. This can help identify trends and outliers.

- **Residual Plots:** To check the assumptions of linear regression, like homoscedasticity and normal distribution of residuals.
- **Partial Regression Plots:** To visualize the relationship between wine quality and each predictor, controlling for the effects of other predictors.
- For Classifying Wine Type (Red or White):
- **Histograms or Bar Charts:** For each variable, segmented by wine type (red or white). This will show the distribution of each feature within each wine category.
- **Violin Plots:** To compare the distribution of each variable between red and white wines. Violin plots combine the features of box plots and density plots.
- **Scatter Matrix:** To visualize pairwise relationships between variables, color-coded by wine type. This can reveal patterns and clusters.
- **Feature Importance Plot:** If using tree-based models like Random Forest, a plot showing the importance of each feature in classification.
- **ROC Curve:** For logistic regression, a plot of the ROC curve to evaluate model performance.

We'll create a correlation matrix heatmap and some scatter plots for the regression scenario, and histograms or bar charts for the classification scenario. Let's begin with the regression scenario.



Scatter Plots of Selected Features vs Wine Quality

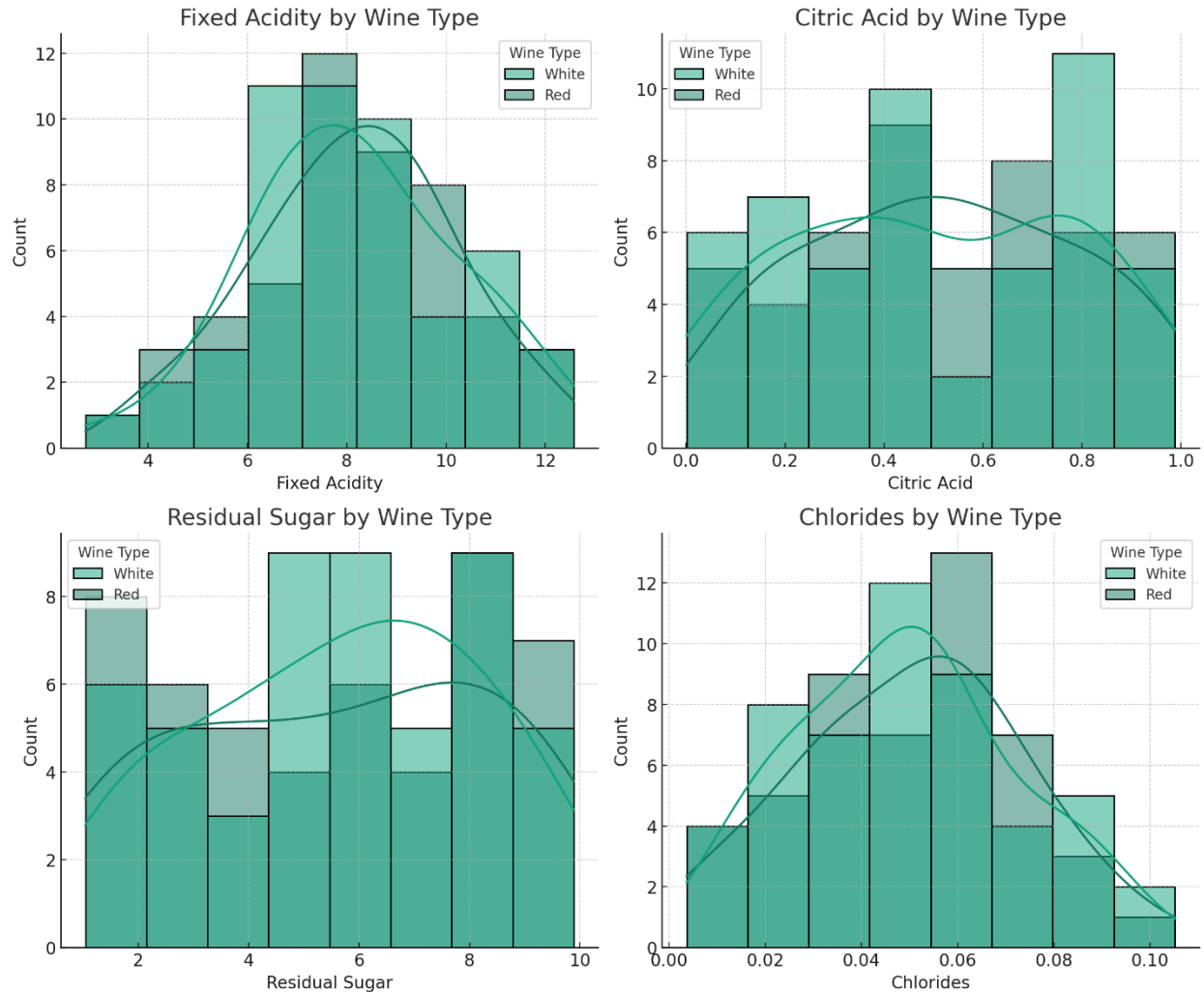


The visualizations for the wine quality prediction scenario show interesting insights:

Correlation Matrix: This heatmap reveals how each variable is correlated with wine quality and with each other. Strong colors (both red and blue) indicate stronger correlations. This helps in identifying which factors might be more influential in predicting wine quality and detecting any potential multicollinearity issues.

Scatter Plots: The scatter plots for selected features (Fixed Acidity, Volatile Acidity, Residual Sugar, and Alcohol) against wine quality offer a visual representation of their individual relationships with wine quality. These plots can give an initial sense of whether linear relationships exist between these variables and the wine quality.

Next, let's create some visualizations for the classification scenario, where we aim to differentiate between red and white wines based on their characteristics. We'll generate histograms or bar charts for each variable, segmented by wine type. This will help in understanding how each feature's distribution differs between red and white wines.



The histograms for the wine type classification scenario provide useful insights into how the distributions of various chemical attributes differ between red and white wines:

Fixed Acidity: This graph shows the distribution of fixed acidity levels across red and white wines. The overlap and distinct peaks can indicate how this variable may help in distinguishing between the two wine types.

Citric Acid: The distribution of citric acid content is plotted for both red and white wines. Differences in the spread and central tendency could be indicative of how citric acid contributes to the wine's profile and its classification.

Residual Sugar: This chart illustrates the varying levels of residual sugar in red and white wines. Since sugar content significantly impacts the taste and style of wine, this feature could be a key differentiator.

Chlorides: The chlorides graph displays the saltiness and flavor impact on red and white wines. Variations in chloride levels might be characteristic of each wine type.

These visualizations are crucial for both understanding the data and guiding the feature selection and model building process in machine learning tasks. For the regression task, they help assess the strength and nature of relationships between predictors and wine quality. For the classification task, they assist in understanding how different features can distinguish between red and white wines.

Conclusion:

The Wine Quality dataset presents a comprehensive view of the chemical makeup of wines and their quality ratings. Through data summarization, visualization, and outlier handling, several key insights emerged:

Alcohol Content: A strong influencer of quality, with higher alcohol often indicating higher quality.

Acidity and Sugar Balance: Critical in determining the overall flavor profile and quality of the wine.

Complex Interplay: Wine quality is the result of a complex interplay of various chemical properties.

The dataset is well-suited for predictive modeling, such as using regression techniques to predict quality scores or classification algorithms to differentiate between red and white wines. The insights gained from this analysis can guide further detailed analytical studies and predictive modeling to better understand and predict wine quality.