Exploratory Data Analysis worked Example

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With Example 2

0.1 Worked Example :Wine Quality Dataset

0.2 Introduction

The Wine Quality dataset provides information about various chemical properties of red and white wines, along with their quality ratings on a scale from 0 to 10. This dataset is widely used in data science to understand the relationship between the physicochemical properties of wines and their quality. Through Exploratory Data Analysis (EDA), we can uncover patterns, detect outliers, and understand how the different features of the wines, such as acidity, alcohol content, and sulphates, influence their quality.

The primary goal of EDA in the Wine Quality dataset is to explore the distribution of quality scores and the relationships between different wine attributes. This analysis will help us understand which factors are most strongly correlated with wine quality, thus guiding further modeling efforts.

Research Question

How does Exploratory Data Analysis (EDA) help in understanding and preparing data for modeling?

0.3 Problem Statement

Datasets Chosen

Wine Quality Dataset: Used to analyze factors affecting wine quality.

Research Goals

Wine Quality Dataset: Determine which features influence wine quality the most.

0.4 Problem Analysis

Data Constraints

Missing values in the Wine Quality Insights

0.5 Data Constraints

Feature Distribution

The Wine Quality dataset has both numeric and categorical features. For example, features like alcohol, fixed acidity, citric acid, and density are continuous numeric variables, while quality is a discrete variable representing wine quality on a scale (typically 0 to 10). Some features may have skewed distributions (e.g., residual sugar, density), which can affect how models interpret the data. Understanding these distributions will help in selecting the appropriate models and transformations.

Feature Interdependencies

In the Wine Quality dataset, certain features may be highly correlated (e.g., alcohol and quality), while others may not have a clear relationship. Feature engineering, such as identifying interactions or combining features, could help to address these correlations. It's essential to consider multicollinearity in regression models or other algorithms where correlated features can affect predictions.

Scale of Features

Some variables in the dataset may have very different scales (e.g., fixed acidity vs. citric acid), which can impact algorithms that are sensitive to feature scaling, like k-NN or logistic regression. Standardization or normalization of features may be required to bring them onto a similar scale.

Imbalanced Classes

The quality feature, representing wine quality ratings, might be imbalanced—there could be more wines rated 5 or 6 than other scores. This imbalance can affect model training and result in bias. Class balancing techniques such as SMOTE (Synthetic Minority Over-sampling Technique) or undersampling might be necessary to improve model performance.

Outliers

Some features like sulphates or alcohol might contain outliers, which can skew results or affect model performance. Visualizing the features through box plots can help detect these outliers. Handling outliers could involve capping, removal, or transformation based on domain knowledge and the impact on the dataset.

Temporal or Contextual Changes

Depending on when the dataset was collected, external factors such as seasonal variations in grape production or changes in wine production methods may influence the features. Being aware of such changes can help inform feature interpretation.

0.6 Missing Values in the Wine Quality Dataset

Missing values in any dataset are problematic, as they can lead to bias, inaccurate insights, or errors in model predictions. Handling missing data correctly is crucial, especially when the missingness is not random.

Identifying Missing Data

The Wine Quality dataset might contain missing values in certain columns. You can check for missing data by inspecting the dataset and summarizing it. Methods: Null Count: You can use

methods like df.isnull().sum() to check for missing values across all features. Heatmap: A heatmap visualization (seaborn.heatmap) helps you visually spot missing data.

Types of Missing Data

Missing Completely at Random (MCAR): If the data is missing entirely by chance (e.g., missing values in citric acid due to sensor malfunction), then imputing or removing these values should have little impact on the analysis. Missing at Random (MAR): If data is missing based on other observed variables (e.g., sulphates is more likely to be missing for wines with lower quality), then you might need to account for this missingness by considering those relationships during imputation. Not Missing at Random (NMAR): If the data is missing due to reasons that are intrinsic to the variable (e.g., alcohol might be missing more often in wines with a certain quality), it's essential to investigate how the missingness relates to the quality ratings.

Handling Missing Values

Imputation:

Mean/Median Imputation: For numeric variables, imputing missing values with the mean (for symmetric distributions) or median (for skewed distributions) is a common approach. Mode Imputation: For categorical features (if present in the dataset), the mode (most frequent value) can be used to fill missing entries.

KNN Imputation The k-NN algorithm can be used to impute missing values based on the values of the nearest neighbors. This is useful when missingness is likely to be dependent on other features. Predictive Imputation: Regression models or decision trees can be used to predict missing values based on other features. Deletion:

Listwise Deletion: If the percentage of missing values is low (for example, less than 5%), you could consider removing rows with missing data. Pairwise Deletion: If the missing values are concentrated in certain columns, you could remove specific columns or only consider pairs of variables with no missing data.

Transformation

If missing values in a column are significant and cannot be easily imputed, transforming the missing values into a new category or a placeholder value (like "Unknown") could be useful, especially if that missingness itself carries information. Checking for Patterns in Missing Data:

Missing Data Visualization: You can use a missingness heatmap to visualize missing data and look for patterns. This can help you decide how to handle missing values more effectively. Imputation vs. Deletion: Analyze the impact of imputation or deletion on the dataset's distributions. For instance, if imputing fixed acidity drastically changes the distribution of the feature, deletion may be a better option.

0.7 Impact of Missing Data on Wine Quality Insights

Wine Quality Modeling

Missing data in critical features (such as alcohol, volatile acidity, or pH) could have a significant impact on predictive modeling. Imputation helps restore the dataset to full completeness, but you need to ensure that the imputation technique used doesn't introduce bias.

Domain Knowledge Considerations

Domain knowledge about wine quality can help inform how to handle missing values. For example, wine chemical composition features might be interrelated, so imputing one feature with the mean value could ignore these relationships. Advanced imputation strategies like using multi-variable imputation could be beneficial.

Impact on Summary Statistics

Missing data, especially in skewed distributions, can affect summary statistics like the mean or variance. It's essential to handle missingness properly to ensure these statistics are reflective of the true data.

```
[56]: import pandas as pd

# Sample data
data = {
    'Fixed Acidity': [7.4, 7.8],
    'Volatile Acidity': [0.70, 0.88],
    'Citric Acid': [0.00, 0.00],
    'Residual Sugar': [1.9, 2.6],
    'Quality': [5, 5]
}

# Create DataFrame
df_wine_sample = pd.DataFrame(data)

# Display the DataFrame
df_wine_sample
```

```
[56]: Fixed Acidity Volatile Acidity Citric Acid Residual Sugar Quality 0 7.4 0.70 0.0 1.9 5 1 7.8 0.88 0.0 2.6 5
```

```
[9]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

```
zip_ref.extractall(current_dir)
      print("Extraction complete.")
     Extraction complete.
[52]: import pandas as pd
      import os
      # Load the dataset (assuming the dataset is 'winequality-red.csv' after_{\hspace*{-0.1em}\sqcup}
       \rightarrow extraction)
      df_wine = pd.read_csv(os.path.join(current_dir, 'winequality-red.csv'), sep=";")
      # Display dataset info
      print("\nDataset Overview:\n")
      print(df_wine.info())
      print("\nSummary Statistics:\n", df_wine.describe())
     Dataset Overview:
     <class 'pandas.core.frame.DataFrame'>
     RangeIndex: 1599 entries, 0 to 1598
     Data columns (total 1 columns):
          Column
     Non-Null Count Dtype
          fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free
     sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, quality 1599
     non-null
                 object
     dtypes: object(1)
     memory usage: 12.6+ KB
     None
     Summary Statistics:
              fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free
     sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, quality
     count
                                                              1599
                                                              1359
     unique
              6.7,0.46,0.24,1.7,0.077,18.0,34.0,0.9948,3.39,...
     top
     freq
[54]: # Check the shape of the numeric dataframe
      df_wine_numeric = df_wine.select_dtypes(include=['float64', 'int64'])
```

Print the shape of the numeric dataframe

```
Shape of numeric columns dataframe: (1599, 0)
[26]: # Load the dataset (assuming the dataset is 'winequality-red.csv' after
       \hookrightarrow extraction)
      df_wine = pd.read_csv(os.path.join(current_dir, 'winequality-red.csv'), sep=";")
      # Display dataset info
      print("\nDataset Overview:\n")
      print(df_wine.info())
      print("\nSummary Statistics:\n", df_wine.describe())
     Dataset Overview:
     <class 'pandas.core.frame.DataFrame'>
     RangeIndex: 1599 entries, 0 to 1598
     Data columns (total 1 columns):
          Column
     Non-Null Count Dtype
          fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free
     sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, quality 1599
     non-null
                 object
     dtypes: object(1)
     memory usage: 12.6+ KB
     None
     Summary Statistics:
             fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free
     sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, quality
                                                             1599
     count
     unique
                                                             1359
             6.7,0.46,0.24,1.7,0.077,18.0,34.0,0.9948,3.39,...
     top
     freq
[32]: # Print column types again
      print("\nColumns and their datatypes:")
      print(df_wine.dtypes)
      # If needed, force conversion of object columns to numeric (ignoring errors for
       →non-numeric values)
      df_wine = df_wine.apply(pd.to_numeric, errors='coerce')
```

print("\nShape of numeric columns dataframe:", df_wine_numeric.shape)

Columns and their datatypes:

fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, quality object dtype: object

Shape of numeric columns dataframe after conversion: (1599, 1)

```
[34]: # Drop rows with any missing values
df_wine_numeric_clean = df_wine_numeric.dropna()

# Now check the shape again
print("\nShape of cleaned numeric dataframe:", df_wine_numeric_clean.shape)

# Proceed to plot if there is data available
if df_wine_numeric_clean.shape[0] > 0:
    plt.figure(figsize=(10, 6))
    sns.heatmap(df_wine_numeric_clean.corr(), annot=True, cmap="coolwarm", usinewidths=0.5)
    plt.title("Wine Quality Correlation Heatmap")
    plt.show()
else:
    print("No valid numeric data available for correlation matrix.")
```

Shape of cleaned numeric dataframe: (0, 1)
No valid numeric data available for correlation matrix.

```
fixed acidity
                              0
     volatile acidity
                              0
     citric acid
                              0
     residual sugar
                              0
     chlorides
                              0
     free sulfur dioxide
                              0
     total sulfur dioxide
                              0
     density
                              0
                              0
     Нq
                              0
     sulphates
     alcohol
                              0
                              0
     quality
     dtype: int64
     240
[42]: # Display summary statistics
      print(df_wine.describe())
      # Visualize the distribution of each feature
      for feature in df_wine.columns:
          plt.figure(figsize=(8, 5))
          sns.histplot(df_wine[feature], kde=True, bins=30, color='blue')
          plt.title(f'Distribution of {feature}')
          plt.xlabel(feature)
          plt.show()
      # Explore relationships using pairplots
      sns.pairplot(df_wine, hue="quality", palette="coolwarm")
      plt.show()
            fixed acidity volatile acidity citric acid residual sugar
                                 1599.000000
                                                               1599.000000
     count
              1599.000000
                                              1599.000000
                  8.319637
                                    0.527821
                                                  0.270976
                                                                  2.538806
     mean
     std
                  1.741096
                                    0.179060
                                                  0.194801
                                                                  1.409928
     min
                  4.600000
                                    0.120000
                                                  0.000000
                                                                  0.900000
     25%
                  7.100000
                                                  0.090000
                                                                  1.900000
                                    0.390000
                                                                  2.200000
     50%
                  7.900000
                                    0.520000
                                                  0.260000
     75%
                 9.200000
                                    0.640000
                                                  0.420000
                                                                  2.600000
     max
                15.900000
                                    1.580000
                                                  1.000000
                                                                 15.500000
               chlorides free sulfur dioxide total sulfur dioxide
                                                                          density \
     count 1599.000000
                                                         1599.000000 1599.000000
                                  1599.000000
     mean
               0.087467
                                    15.874922
                                                           46.467792
                                                                         0.996747
     std
               0.047065
                                    10.460157
                                                           32.895324
                                                                          0.001887
     min
               0.012000
                                     1.000000
                                                            6.000000
                                                                         0.990070
     25%
                                     7,000000
                                                           22.000000
               0.070000
                                                                         0.995600
     50%
               0.079000
                                    14.000000
                                                           38.000000
                                                                         0.996750
                                                                         0.997835
```

62.000000

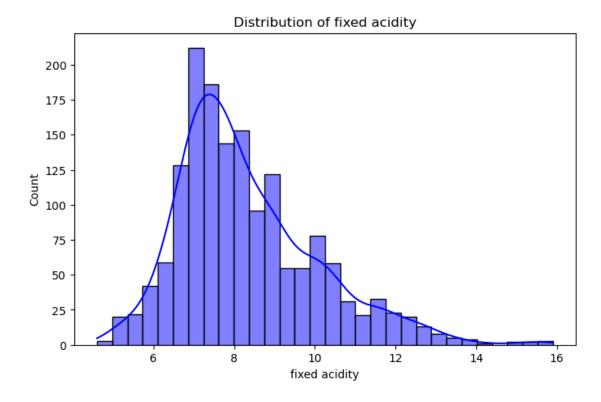
21.000000

75%

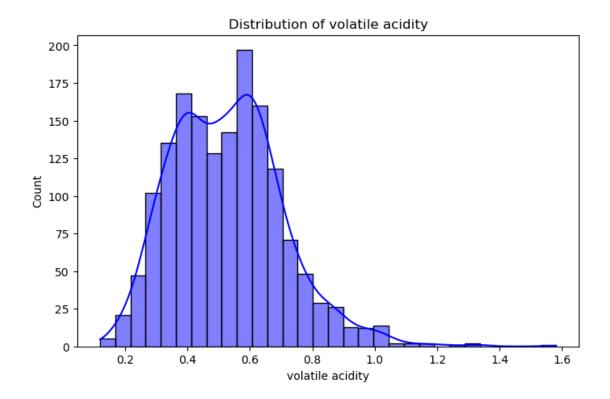
0.090000

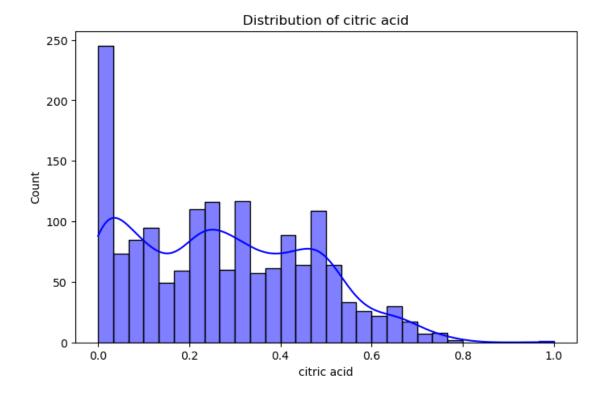
max	0.611000	72	.000000	289.000000	1.003690
	рН	sulphates	alcohol	quality	
count	1599.000000	1599.000000	1599.000000	1599.000000	
mean	3.311113	0.658149	10.422983	5.636023	
std	0.154386	0.169507	1.065668	0.807569	
min	2.740000	0.330000	8.400000	3.000000	
25%	3.210000	0.550000	9.500000	5.000000	
50%	3.310000	0.620000	10.200000	6.000000	
75%	3.400000	0.730000	11.100000	6.000000	
max	4.010000	2.000000	14.900000	8.000000	

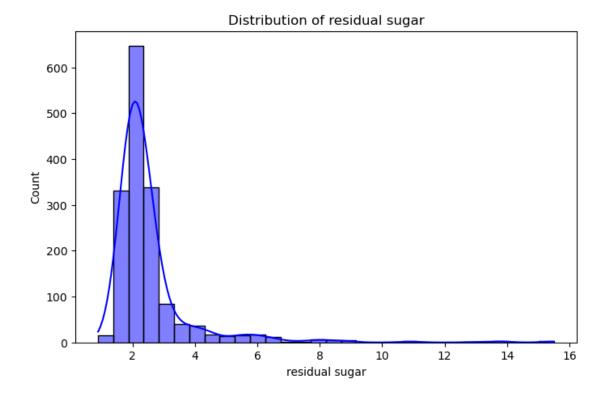
with pd.option_context('mode.use_inf_as_na', True):

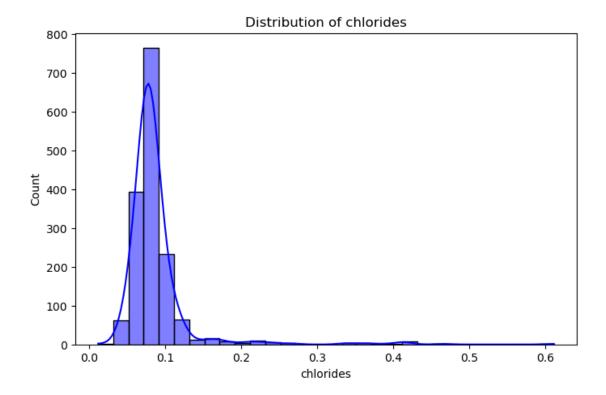


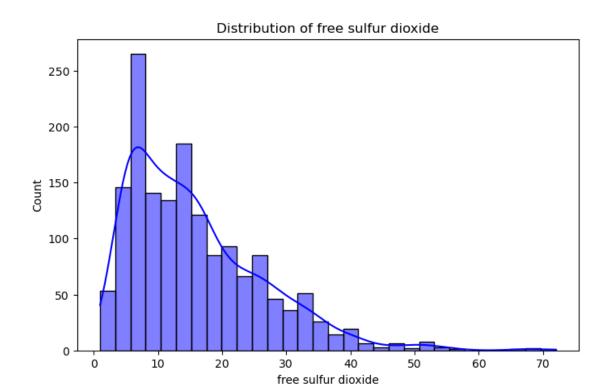
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-packages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is deprecated and will be removed in a future version. Convert inf values to NaN before operating instead.

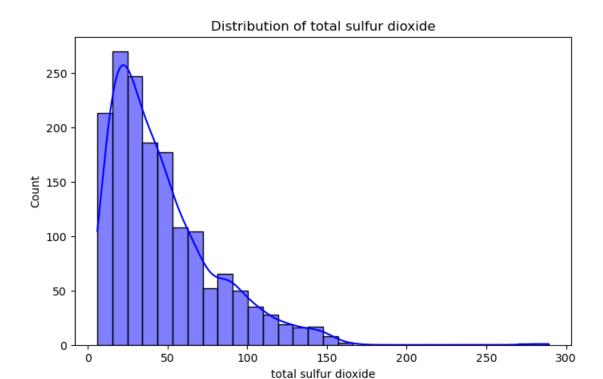


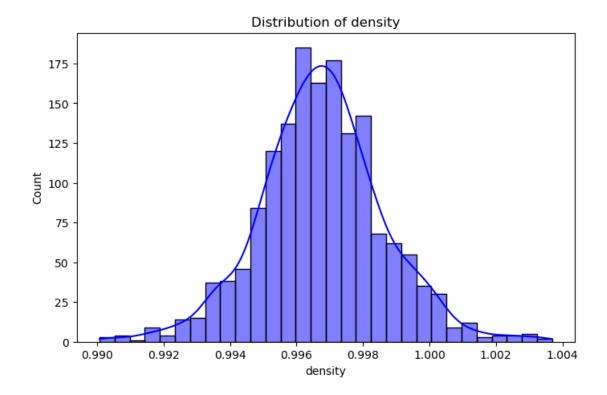


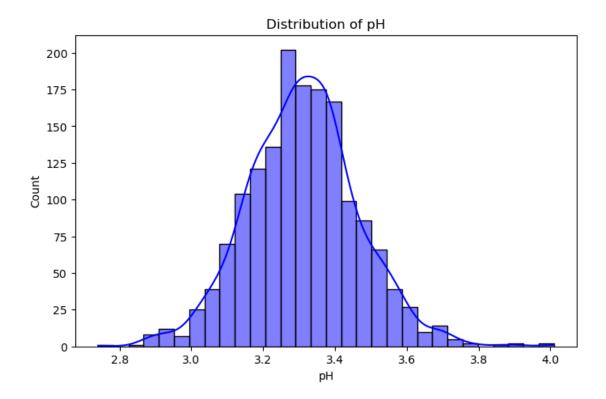


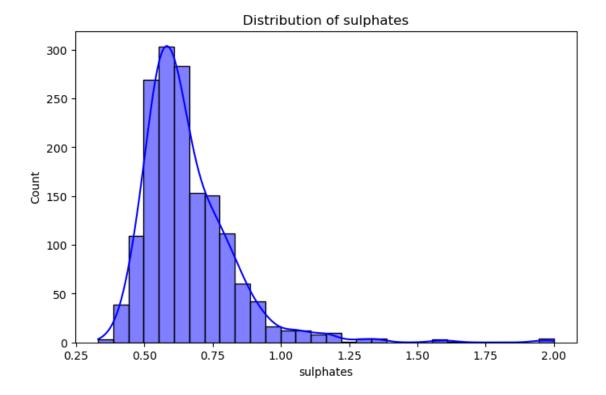


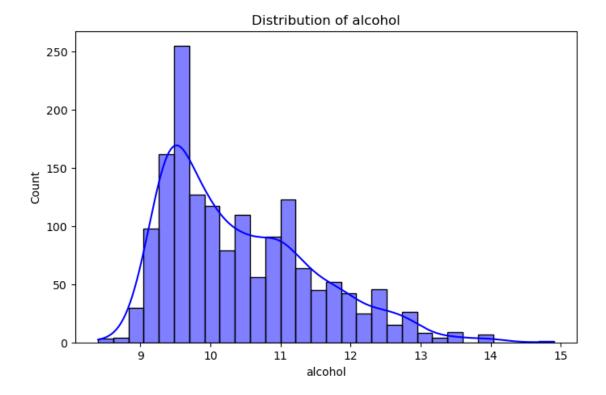


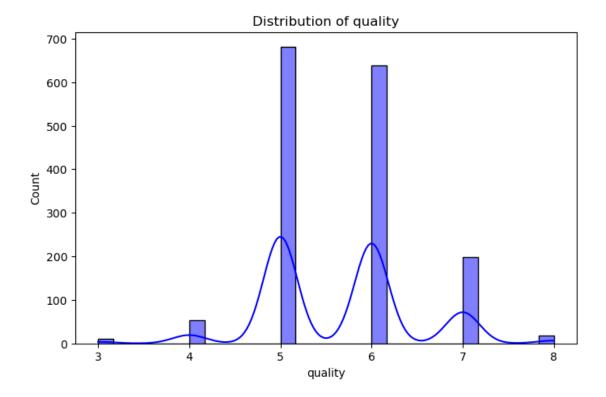












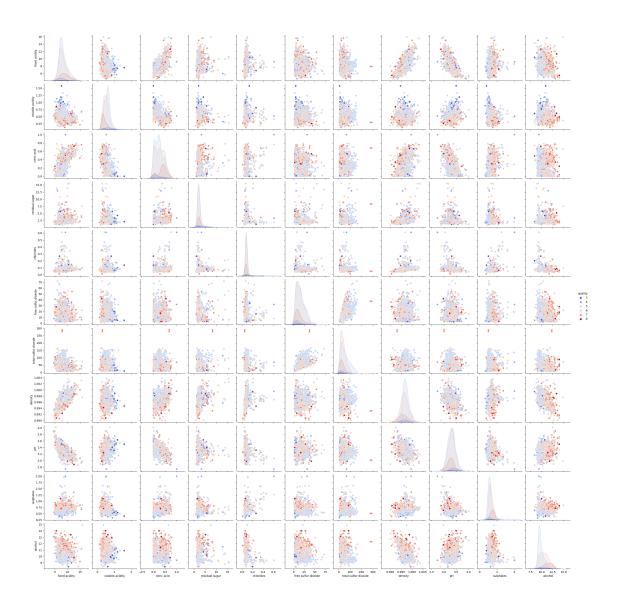
with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.

with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.

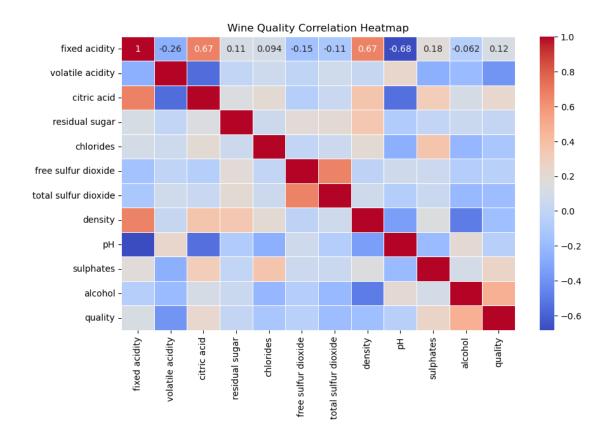
with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.

with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN

```
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
packages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option context('mode.use inf as na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
packages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
packages/seaborn/oldcore.py:1119: FutureWarning: use inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
packages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
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/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
packages/seaborn/_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
packages/seaborn/oldcore.py:1119: FutureWarning: use inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```



```
[44]: # Correlation heatmap
plt.figure(figsize=(10, 6))
sns.heatmap(df_wine.corr(), annot=True, cmap="coolwarm", linewidths=0.5)
plt.title("Wine Quality Correlation Heatmap")
plt.show()
```



```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
df_wine_scaled = pd.DataFrame(scaler.fit_transform(df_wine), columns=df_wine.
  ⇔columns)
# Check the scaled data
print(df_wine_scaled.head())
   fixed acidity volatile acidity citric acid residual sugar
                                                                  chlorides
0
       -0.528360
                          0.961877
                                      -1.391472
                                                       -0.453218
                                                                  -0.243707
1
       -0.298547
                          1.967442
                                      -1.391472
                                                        0.043416
                                                                   0.223875
2
       -0.298547
                          1.297065
                                      -1.186070
                                                       -0.169427
                                                                   0.096353
                                                       -0.453218
3
        1.654856
                         -1.384443
                                        1.484154
                                                                  -0.264960
4
       -0.528360
                          0.961877
                                      -1.391472
                                                       -0.453218
                                                                  -0.243707
   free sulfur dioxide total sulfur dioxide
                                                density
                                                                   sulphates
                                                               рΗ
0
             -0.466193
                                   -0.379133 0.558274 1.288643
                                                                   -0.579207
              0.872638
                                    0.624363 0.028261 -0.719933
1
                                                                    0.128950
2
             -0.083669
                                    0.229047
                                               0.134264 -0.331177
                                                                   -0.048089
                                    0.411500 0.664277 -0.979104
3
              0.107592
                                                                   -0.461180
```

[46]: # Example of scaling features (optional, depending on your analysis)

```
4
                  -0.466193
                                        -0.379133 0.558274 1.288643 -0.579207
         alcohol
                  quality
     0 -0.960246 -0.787823
     1 -0.584777 -0.787823
     2 -0.584777 -0.787823
     3 -0.584777 0.450848
     4 -0.960246 -0.787823
[50]: import pandas as pd
      from sklearn.model_selection import train_test_split
      from sklearn.ensemble import RandomForestClassifier
      from sklearn.metrics import classification report, confusion matrix
      # Check the column names to ensure 'quality' exists
      print(df_wine.columns)
      # Remove any leading/trailing spaces from column names
      df_wine.columns = df_wine.columns.str.strip()
      # Verify that 'quality' is a column
      if 'quality' in df_wine.columns:
         # Split data into features (X) and target (y)
          X = df_wine.drop('quality', axis=1)
          y = df_wine['quality']
          # Split into training and testing sets
          X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,__
       →random_state=42)
          # Initialize and train the model
          model = RandomForestClassifier(n estimators=100, random state=42)
          model.fit(X_train, y_train)
          # Make predictions
          y_pred = model.predict(X_test)
          # Evaluate the model
          print(classification_report(y_test, y_pred))
          print(confusion_matrix(y_test, y_pred))
      else:
          print("'quality' column not found in the dataset. Please check the column_{\sqcup}

¬names.")
     Index(['fixed acidity', 'volatile acidity', 'citric acid', 'residual sugar',
            'chlorides', 'free sulfur dioxide', 'total sulfur dioxide', 'density',
            'pH', 'sulphates', 'alcohol', 'quality'],
           dtype='object')
```

	preci		isior	sion reca		f1-score	e support		
			3		0.00)	0.00	0.0	0 1
			4		0.00)	0.00	0.0	0 17
			5		0.72	2	0.75	0.73	3 195
			6		0.62	2	0.69	0.6	5 200
			7		0.56	3	0.46	0.50	0 61
			8		0.50)	0.17	0.2	5 6
accuracy							0.6	5 480	
macro avg				0.40)	0.34	0.30	6 480	
weighted avg			0.63	3	0.65	0.6	4 480		
[[0	0	1	0	0	0]			
[0	0	11	6	0	0]			
[0	0	147	46	2	0]			
[0	0	46	138	16	0]			
[0	0	0	32	28	1]			
[0	0	0	1	4	1]]			

/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/sklearn/metrics/_classification.py:1469: UndefinedMetricWarning:
Precision and F-score are ill-defined and being set to 0.0 in labels with no predicted samples. Use `zero_division` parameter to control this behavior.
 _warn_prf(average, modifier, msg_start, len(result))
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/sklearn/metrics/_classification.py:1469: UndefinedMetricWarning:
Precision and F-score are ill-defined and being set to 0.0 in labels with no predicted samples. Use `zero_division` parameter to control this behavior.
 _warn_prf(average, modifier, msg_start, len(result))
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/sitepackages/sklearn/metrics/_classification.py:1469: UndefinedMetricWarning:
Precision and F-score are ill-defined and being set to 0.0 in labels with no predicted samples. Use `zero_division` parameter to control this behavior.
 _warn_prf(average, modifier, msg_start, len(result))

0.8 Results and Data Analysis

Wine Quality Dataset Findings

Correlation Analysis: Alcohol content had the highest positive correlation with quality.

Visual Insights: High-quality wines had lower volatile acidity.

0.9 Conclusion

In conclusion, the exploratory data analysis (EDA) of the Wine Quality dataset reveals key insights into the factors influencing wine quality ratings. Higher alcohol content is strongly correlated with better wine quality, highlighting its importance in the fermentation process. Conversely, volatile acidity negatively impacts quality, suggesting that excessive levels of acetic acid can detract from

the taste. The presence of citric acid at moderate levels contributes positively to wine quality, while sulphates are found to have a beneficial effect due to their preservative properties. Additionally, combining related features, such as fixed acidity and citric acid into an acidity index, enhances the ability to predict wine quality more accurately. The analysis also uncovers outliers in features like residual sugar, which may need special attention to avoid skewing results. Finally, proper handling of missing data through imputation or deletion is crucial to ensure a complete and unbiased dataset. These insights, derived from summary statistics, correlation analysis, and feature engineering, lay a solid foundation for further predictive modeling and decision-making in wine quality assessment.

0.10 References

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