Wine Quality Prediction

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1 Summary

This project aims to analyze patterns in wine data through exploratory data analysis (EDA) and develop predictive models to classify wines or predict their quality. The analysis includes

Figure 1: Such an adorable couple

uncovering relationships between key features and their influence on wine quality, visualizing distributions and correlations, and identifying significant predictors. Predictive models such as logistic regression and random forests are developed and optimized using cross-validation and hyperparameter tuning.

By leveraging machine learning techniques, we evaluated model performance with metrics like accuracy and F1-score, providing actionable insights for enhancing wine quality. The results offer a data-driven approach to understanding wine characteristics and their impact on quality, benefiting decision-making in winemaking and marketing.

2 Introduction

2.1 Background Information

The quality of wine plays a crucial role in the wine industry, as it directly affects consumer satisfaction, pricing, and demand. Traditionally, wine quality is determined through sensory analysis by trained experts, who evaluate factors such as taste, aroma, and texture. However, these evaluations are inherently subjective, costly, and time-consuming.

With advancements in data analysis and machine learning, it is now possible to model and predict wine quality using objective, measurable features. These features include chemical and physical attributes such as acidity, sugar levels, alcohol content, and more, which directly influence the sensory properties of wine.

2.2 Dataset

The data was downloaded from UCI Machine Learning Repository. - **Quality**: This is the target variable, is a score between 0 and 10 assigned by wine tasters based on sensory evaluations with blind tastes. 0-"very bad" 10-"excellent" - **Fixed Acidity(g/dm^3):** Measures non-volatile acids that do not evaporate. The higher the value the more the acidity of the sample. - **Volatile Acidity(g/dm^3):** Measures volatile acids that can impact wine aroma. When present in moderation, it adds complexity, but in excess, it can produce vinegar-like or pungent odors, becoming a flaw. - **Citric Acid(g/dm^3):** A component that can add freshness and complex flavor to wine. - **Residual Sugar(g/dm^3):** The sugar content left after fermentation. Wine taste sweeter with higher residual sugar. - **Chlorides($g(sodium chloride)/dm^3$):** Indicates salt content. More salty with higher chlorides. - **Free Sulfur Dioxide and Total Sulfur Dioxide(mg/dm^3):** Measures preservatives that can affect taste, stability and longevity. - **Density(mg/dm^3):** Relates to sugar and alcohol content. The weight of wine per unit volume. - **pH:** Measures acidity/alkalinity. Related to the color and shelf life of wine. - **Sulphates:** Amount of Sulphates contained in the wine. - **Alcohol:** This is the amount of alcohol contained in the sample.

2.3 Research Question

The primary question we sought to answer in this project is: "Can the quality of wine be effectively predicted based on its measurable physicochemical properties? Additionally, which features are most influential in determining wine quality?"

This project aimed to explore whether measurable data about wine's chemical and physical properties could provide a reliable means of assessing its quality. By identifying the most important predictors of wine quality, we can gain insights into the production processes that have the greatest impact on consumer satisfaction.

2.4 Methodology Overview

We utilized the Wine Quality Dataset from the UCI Machine Learning Repository, which contains information about Portuguese "Vinho Verde" wine. (Cortez et al. 2009)

Our analysis involved: - Data cleaning and preprocessing - Exploratory data analysis - Classification modeling using Decision Tree - Hyperparameter tuning - Model evaluation and feature importance analysis

2.5 Tools and Libraries Used

The analysis and model building for this report were conducted using the Python programming language. Specifically, the following libraries and packages were utilized:

- scikit-learn(Pedregosa et al. 2011): For implementing the decision tree classifier and conducting hyperparameter tuning with GridSearchCV.
- NumPy(Harris et al. 2020): For numerical computations and handling arrays.
- Pandas(McKinney et al. 2011): For data manipulation and preprocessing.
- Pandera(Bantilan 2020): For validating dataframes and ensuring data quality during preprocessing.

3 Data Preparation and Exploration

3.1 Dataset Characteristics

Our dataset contains 5318 wine samples where

- 4,898 observations are of white wines
- 1,599 observations are of red wines
- 11 numerical input features representing physicochemical attributes

Figure 2 shows the distribution of various features in our dataset.

4 Model Development

To develop the decision tree classifier, we initialized a base model using `DecisionTreeClassifier` with a fixed random seed (`random_state=16`) to ensure reproducibility. A hyperparameter tuning process was conducted using `GridSearchCV` to identify the optimal configuration. The grid search evaluated various combinations of hyperparameters, including `max_depth`, `max_features`, `min_samples_leaf`, and `min_samples_split`, over a 5-fold cross-validation.

The best-performing hyperparameters identified were:
- `max_depth`: 5
- `max_features`: None
- `min_samples_leaf`: 1
- `min_samples_split`: 2

The model was optimized using the accuracy metric (`scoring='accuracy'`) and leveraged parallel processing for efficiency (`n_jobs=-1`).
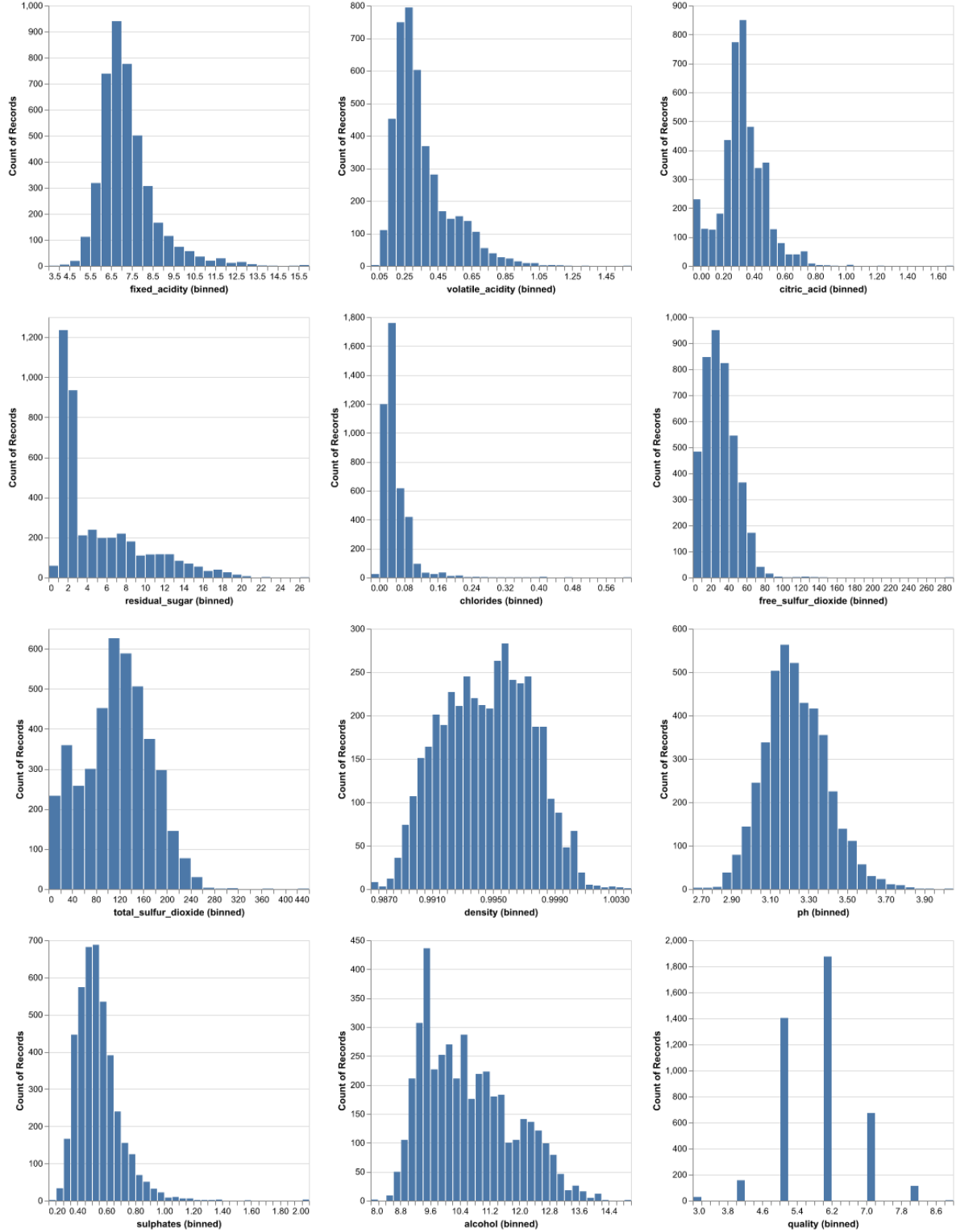
Figure 2: Distribution of all the features

4.1 Model Performance

The Decision Tree model (Boulesteix and Strimmer 2007) achieved a test accuracy of 52.44% .

Table 1: Classification report

precision	recall	f1-score	support
0	0	0	2
0	0	0	50
0.59	0.59	0.59	347
0.51	0.66	0.57	448
0.43	0.31	0.36	181
0	0	0	35
0	0	0	1
0.52	0.52	0.52	0.52
0.22	0.22	0.22	1064
0.48	0.52	0.5	1064

Figure 3 provides the confusion matrix of the model.

The classification report in Table Table 1 provides a summary of the model's performance across different classes. Notably, the highest F1-scores are observed for classes 5 and 6, indicating the model performs well in these categories. However, performance is poor for class 3 and class 9, with precision, recall, and F1-scores all registering as zero. This suggests potential issues with class imbalance or inadequate representation in the dataset. Overall accuracy is 62%, with weighted averages for precision, recall, and F1-score also at 62%.

4.2 Feature Importance

The feature importance plot highlights the relative significance of each feature in the model. The most influential feature is `alcohol`, followed by `volatile_acidity` and `sulphates`. These features contribute significantly to the predictive performance of the model, while other features like `fixed_acidity` and `pH` have minimal impact. This information can be used to focus on the most important variables for further analysis or model refinement.
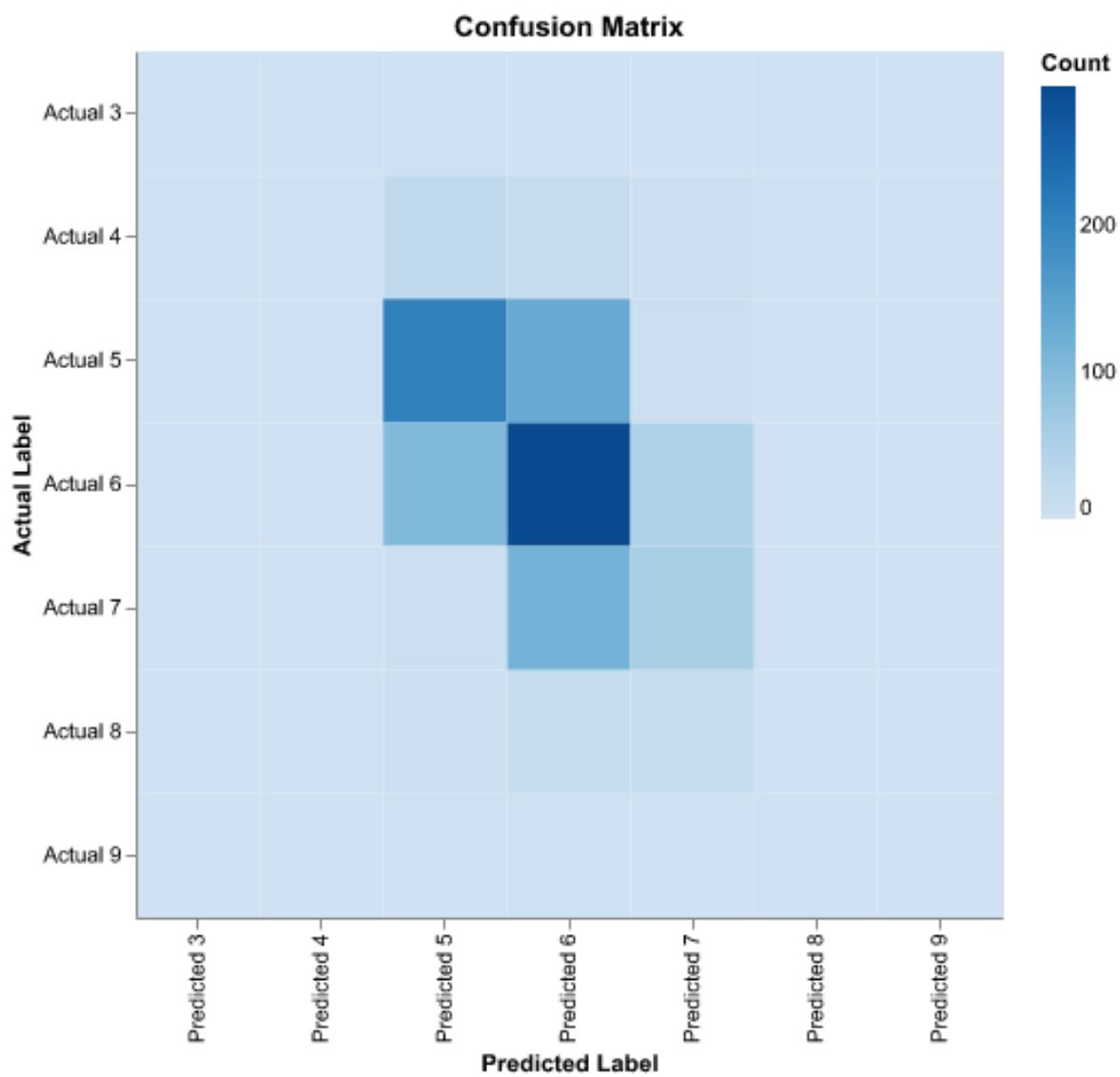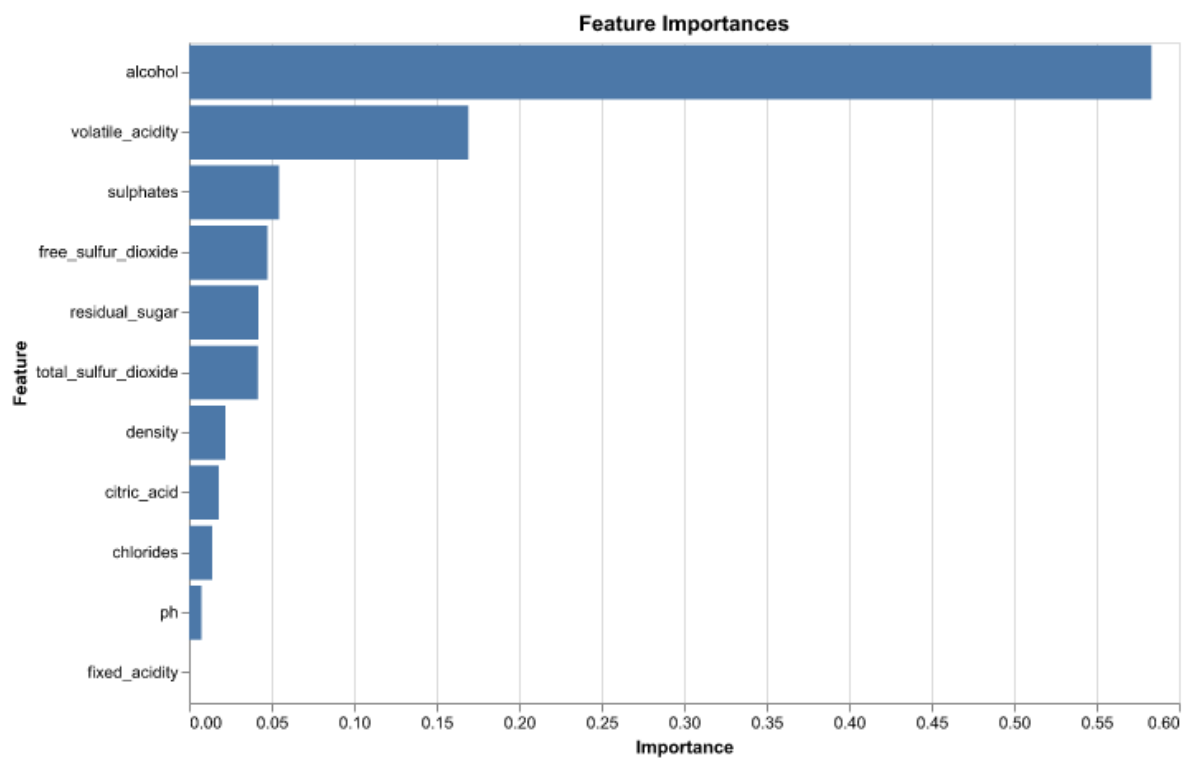
Figure 3: Confusion Matrix

Figure 4: The most important features

5 Discussion

5.1 Key Findings

Our analysis revealed that: - Top predictive features include `density`, `volatile acidity`, and `alcohol` content as seen in Figure 4. - The model achieved moderate predictive performance - Physicochemical properties provide insights into wine quality

5.2 Limitations and Future Work

Future research could explore:

1. Ensemble methods for improved accuracy
2. Incorporating sensory attributes
3. Investigating additional domain-specific features

6 Conclusion

This project demonstrates the potential of machine learning in understanding wine quality through objective, data-driven analysis. While our model provides valuable insights, there remains significant opportunity for refinement and deeper exploration.

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