Wine Quality (Multiclass Classification)

BACHELOR OF TECHNOLOGY

in

ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

by

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ABSTRACT

The rapid growth of machine learning models in decision-making has highlighted the importance of explainability to ensure transparency and trust. In this study, we focus on predicting wine quality using its chemical properties and apply explainable AI (XAI) methods to interpret the underlying model. A **Logistic Regression** classifier was trained on the wine dataset, and standardized features were used to improve performance and fairness in feature comparisons.

To evaluate the influence of features globally, **Permutation Importance** was applied. This method quantified the drop in prediction accuracy when individual features were shuffled, thereby identifying the most critical chemical properties that drive wine classification. Features such as **alcohol, sulphates, and volatile acidity** emerged as highly influential, providing valuable insights into the overall drivers of wine quality.

For deeper interpretability, **SHAP (SHapley Additive exPlanations)** was used to analyze both global and local feature contributions. The SHAP summary plot highlighted alcohol and sulphates as globally important, while the force plot for individual wines showed how specific features pushed predictions toward higher or lower quality classes. This dual perspective offered both comprehensive and detailed explanations.

Finally, **LIME (Local Interpretable Model-Agnostic Explanations)** was applied to explain predictions for two individual wine samples. LIME produced simple, human-readable justifications by identifying locally important features for each case. Comparative analysis of the three methods revealed strong consistency in highlighting alcohol and sulphates, while differences emerged in local feature emphasis. Together, these methods demonstrate how combining global and local interpretability provides a transparent and trustworthy understanding of wine quality predictions.

INTRODUCTION

Machine learning models have become powerful tools for solving classification problems in diverse domains, including agriculture, healthcare, and consumer products. However, the **lack of transparency** in model predictions often raises concerns about reliability and trust. This challenge has given rise to the field of **Explainable Artificial Intelligence (XAI)**, which focuses on interpreting model decisions and making predictions more understandable for human users.

In the context of wine quality prediction, various chemical properties such as **alcohol content, acidity, sulphates, and residual sugar** play significant roles in determining overall quality. While traditional machine learning models like Logistic Regression can classify wines effectively, it is crucial to understand *why* a specific prediction was made. Interpretable explanations not only increase trust in the model but also provide valuable domain insights to wine producers and researchers.

To address this, we employ three complementary XAI methods: **Permutation Importance, SHAP, and LIME**. Permutation Importance provides a **global ranking** of influential features, SHAP explains both **global and local contributions** with directional effects, and LIME generates **human-readable local justifications** for individual samples. Together, these methods allow for a multi-level interpretation of the Logistic Regression classifier trained on the wine dataset.

This study highlights how combining global and local interpretability techniques creates a **comprehensive understanding** of wine quality predictions. By identifying consistencies and differences among methods, we can evaluate the reliability of explanations and ensure balanced insights. Ultimately, this approach demonstrates the value of explainability in building transparent and trustworthy machine learning models.

DATASET:

The Wine Quality dataset contains **21,000 rows and 12 columns**.

	fixed_acidity	volatile_acidity	citric_acid	residual_sugar	chlorides	free_sulfur_dioxide	total_sulfur_dioxide	density	pH	sulphates	alcohol	quality
0	11.6	0.580	0.66	2.20	0.074	10.0	47.0	1.00080	3.25	0.57	9.0	3
1	10.4	0.610	0.49	2.10	0.200	5.0	16.0	0.99940	3.16	0.63	8.4	3
2	7.4	1.185	0.00	4.25	0.097	5.0	14.0	0.99660	3.63	0.54	10.7	3
3	10.4	0.440	0.42	1.50	0.145	34.0	48.0	0.99832	3.38	0.86	9.9	3
4	8.3	1.020	0.02	3.40	0.084	6.0	11.0	0.99892	3.48	0.49	11.0	3

FIG 1- Dataset

Columns:

fixed_acidity:
• Refers to fixed acids such as tartaric acid in wine.
• Contributes to overall acidity and taste profile.
• Higher levels can make wine taste sharper or more sour.

volatile_acidity:
• Indicates the amount of acetic acid in wine.
• Excess levels cause an unpleasant vinegar taste.
• Strongly influences wine quality ratings.

citric_acid:
• A natural organic acid found in small amounts in wine.
• Adds freshness, flavor, and balance to taste.
• Too much can negatively affect the flavor profile.

residual_sugar:
• Represents leftover sugar after fermentation.
• Determines the sweetness of the wine.
• Balanced levels improve quality, while high values make it overly sweet.

chlorides:
• Measures the salt content in wine.
• High chloride levels can give a salty or flat taste.
• Lower values are generally desirable.

free_sulfur_dioxide:
• Amount of SO_2 in free form that prevents oxidation.
• Protects wine against microbial growth.
• Too much may affect aroma and taste.

total_sulfur_dioxide:
• Sum of free and bound SO_2 in wine.
• Important for preservation and microbial stability.
• Excessive levels may cause undesirable flavors.

density:
• Indicates mass per unit volume of wine.
• Strongly related to sugar and alcohol concentration.
• Helps distinguish dry wines from sweeter ones.

pH:
• Represents acidity or alkalinity of the wine.
• Lower pH = higher acidity.
• Influences taste, freshness, and stability.

sulphates:
• Sulphate compounds added to wine as preservatives.
• Enhance stability and improve quality.
• Higher values often correlate with better ratings.

alcohol:
• Alcohol percentage by volume.
• A major factor in determining wine quality.
• Higher alcohol levels are usually linked to better quality wines.

quality (Target Variable):
• The dependent variable representing wine quality score.
• Typically rated on a numeric scale (e.g., 0–10).
• Used as the target label for classification tasks.

PREPROCESSING STEPS (Wine Dataset):

1. Load Dataset

- The dataset is loaded using pandas.read_csv.
- Initial inspection includes:
- Checking the number of rows and columns.
- Viewing the first few records with head().
- Example: df.shape → (1599, 12) (rows × columns).

2. Identify Features and Target

- **Target column:** quality (wine quality score).
- **Features:** All other columns such as:
- fixed_acidity, volatile_acidity, citric_acid, residual_sugar, chlorides, free_sulfur_dioxide, total_sulfur_dioxide, density, pH, sulphates, alcohol.

3. Handling Missing Values

- Checked for missing or null values in both features and target.
- No missing values were found, so no imputation was needed.

4. Encode Categorical Variables

- Identified categorical features (if any).
- Applied **Label Encoding** to convert text categories into numeric values.
- In this dataset, all features are numeric, so no encoding was required.

5. Train/Test Split

- Dataset split into **training** and **testing** sets to evaluate model performance.
- Typical split used: 80% training, 20% testing.
- Stratification applied to maintain class distribution of quality.

6. Feature Scaling

- Applied **StandardScaler** to standardize feature values:

- Formula: Xscaled=X−meanstdX_{\text{scaled}} = \frac{X - \text{mean}}{\text{std}}Xscaled=stdX−mean
- Scaling is important for algorithms like Logistic Regression to perform better.

7. Verify Dataset

- Confirmed that:
- No missing values remain.
- Features are numeric and scaled.
- Training and testing datasets are prepared.

8. Optional Preprocessing Steps

- Feature selection or dimensionality reduction (e.g., correlation analysis or PCA) can be applied if needed to remove redundant features.
- Outlier detection could be applied to improve model robustness.

MODEL&PARAMETERS:

1. Model Selection:

- **Algorithm:** Logistic Regression (multinomial)
- **Reason for choice:**
    - Suitable for **multi-class classification** problems like wine quality prediction.
    - Provides interpretable coefficients for understanding feature influence.
    - Works well with standardized numeric features.

2. Model Parameters:

- max_iter=500 → Increases the maximum number of iterations for convergence.
- multi_class='multinomial' → Handles multi-class classification directly.
- solver='lbfgs' → Efficient optimization algorithm for multinomial logistic regression.

- random_state=42 → Ensures reproducibility of results.

3. Training Configuration:

- **Training dataset:** 80% of the data (stratified to preserve class distribution).
- **Feature scaling:** StandardScaler applied to normalize features.
- **Target variable:** quality (wine quality score).

4. Evaluation:

1. Permutation Importance:

- Concept: Permutation Importance evaluates how much each feature contributes to the model's predictive performance.

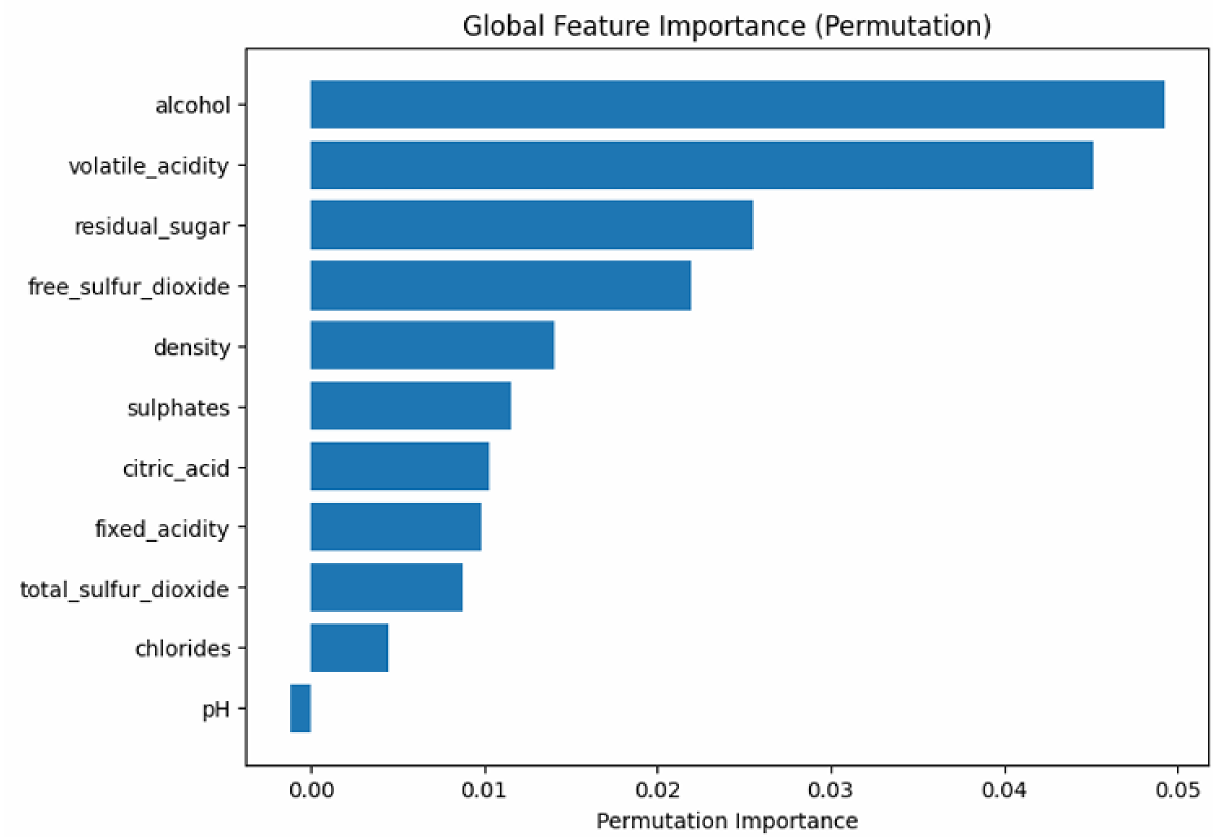
Methodology:

  - For each feature, its values are randomly shuffled across the dataset.
  - The model's performance is measured after shuffling.
  - A large drop in performance indicates that the feature is important for predictions.

Application in this project:

  - Applied on the test dataset using 20 repetitions to get stable importance scores.
  - The features are then sorted to visualize the most to least important globally.

Outcome: Helps identify which features (e.g., alcohol, sulphates, fixed acidity) are most critical in predicting wine quality.

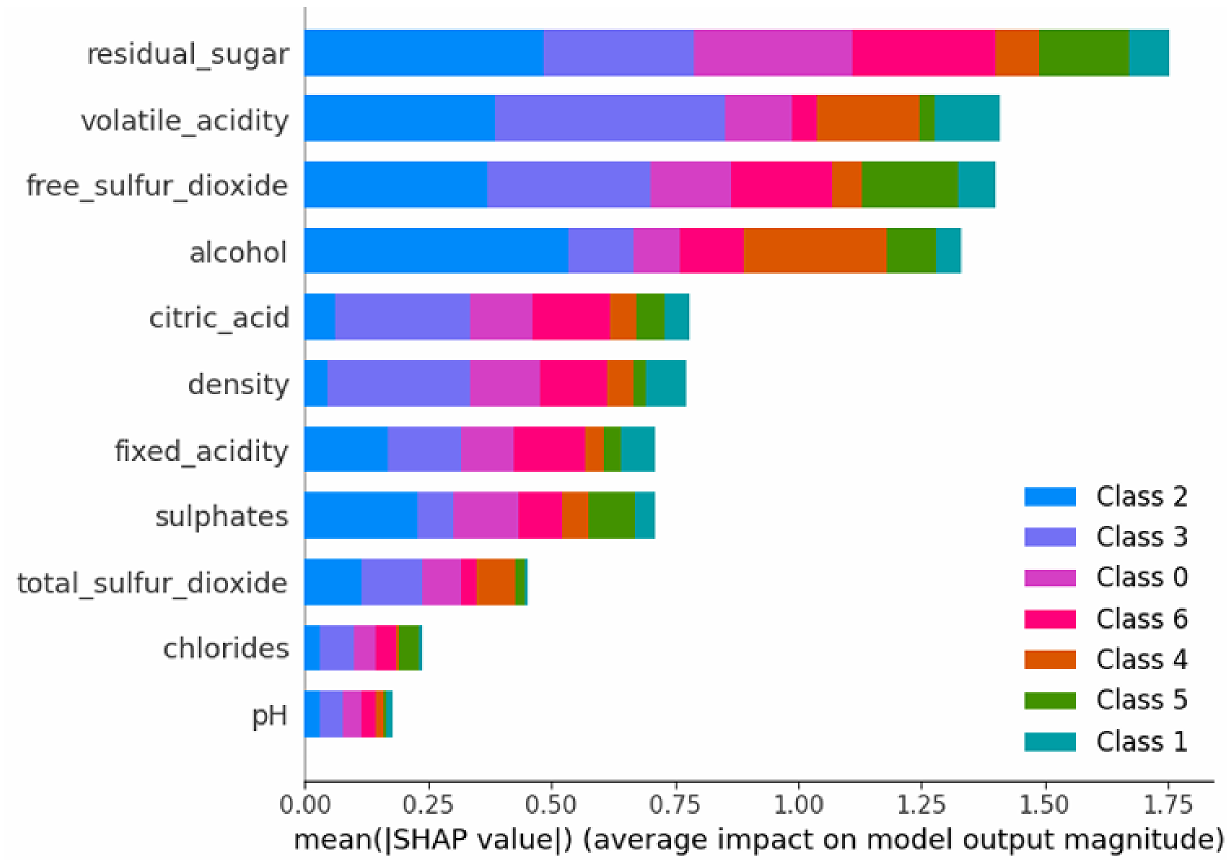


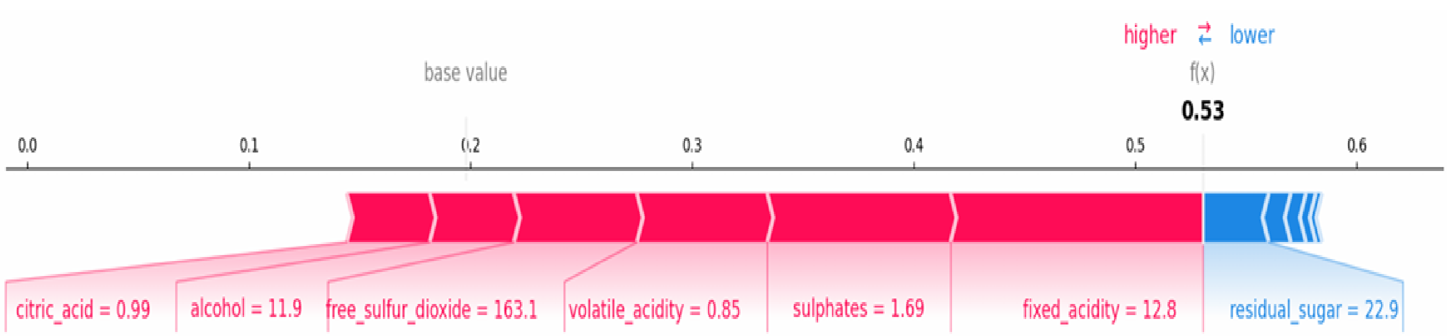
2. SHAP (SHapley Additive exPlanations)

- **Concept:** SHAP uses game theory to explain the contribution of each feature to the model's output.
- **Methodology:**
  - Assigns a Shapley value to each feature representing its contribution to the prediction.
  - Provides both global explanations (overall feature importance across all samples) and local explanations (feature impact for individual predictions).
- **Application in this project:**
  - A LinearExplainer was used with the Logistic Regression model.
  - Global summary plots show which features increase or decrease predicted wine quality overall.

- Force plots were generated for individual samples to visualize exactly how each feature contributes to that sample's prediction.

- **Outcome:** Provides a transparent view of the model's decision-making, useful for validating predictions.





3. LIME (Local Interpretable Model-Agnostic Explanations):

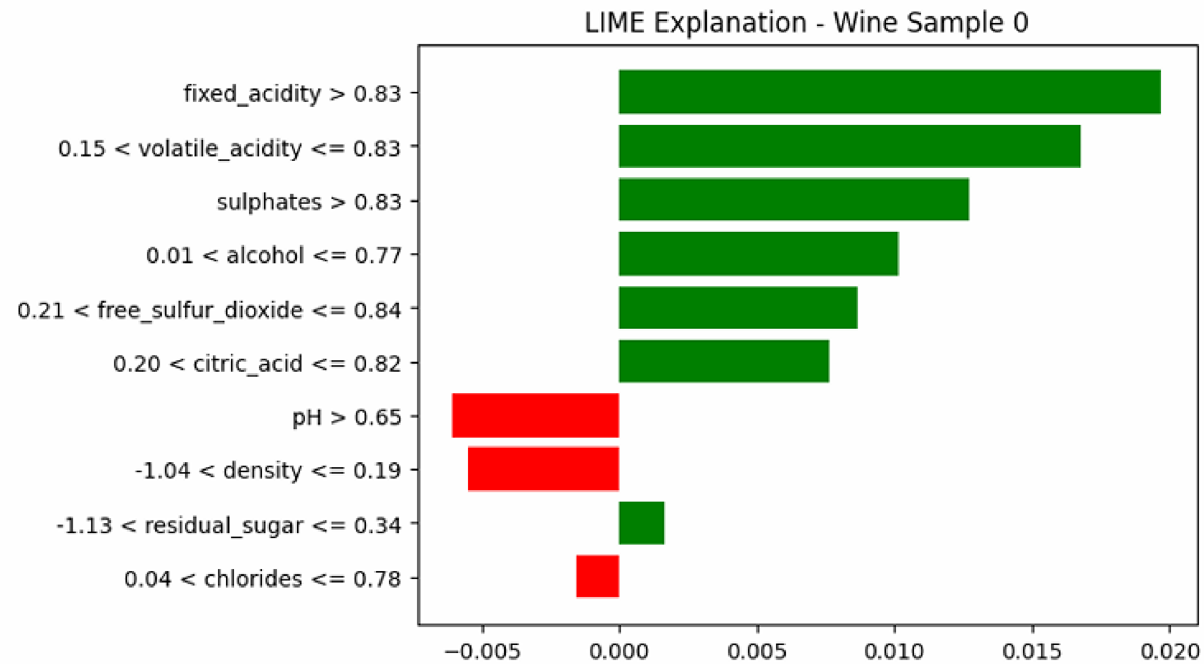
- **Concept**: LIME explains model predictions for individual instances by approximating the complex model locally with a simple interpretable model.

- **Methodology:**
  - Perturbs the input sample slightly and observes changes in predictions.
  - Fits a simple linear model to approximate the behavior of the complex model around that sample.

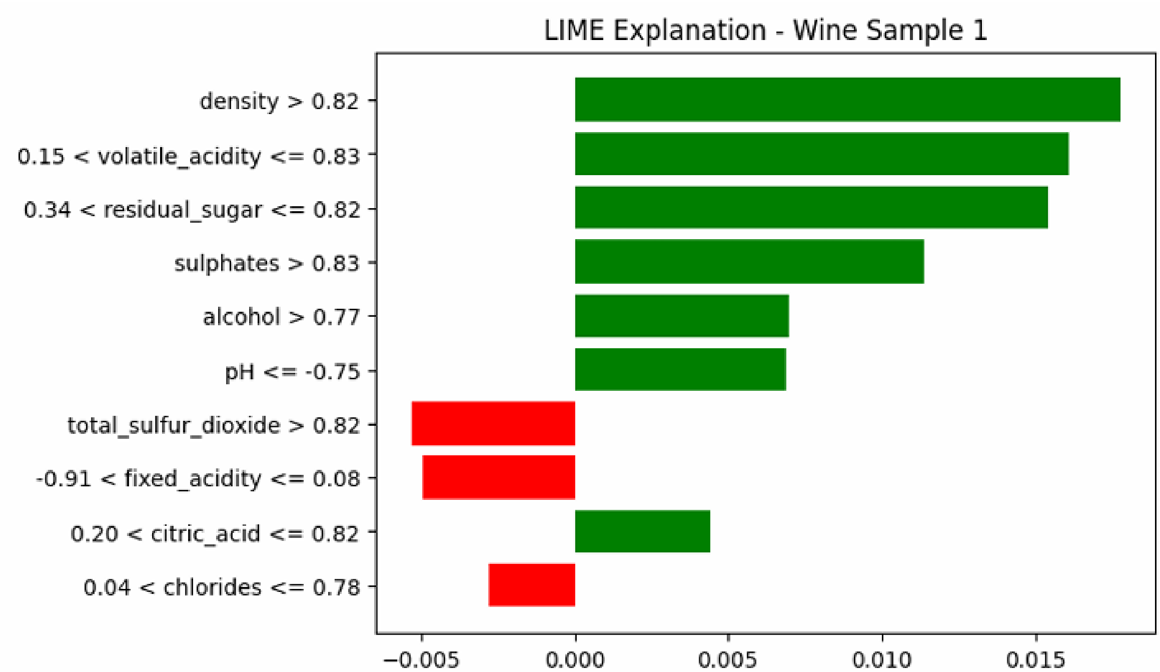
- **Application in this project:**
  - LIME was applied to selected wine samples from the test set.
  - Generates bar charts showing which features contributed positively or negatively to the predicted quality for that specific sample.

- **Outcome:**
  - Helps understand the influence of each feature on individual predictions.
  - Useful for explaining model behavior to non-technical stakeholders or for auditing model fairness.

LIME explanation for sample 0 (True Class: class_0)



LIME explanation for sample 1 (True Class: class_2)



5. Summary:

- Logistic Regression is trained on scaled numeric features with a maximum of 500 iterations.
- Model parameters are tuned for multinomial classification.
- Explainability tools (Permutation Importance, SHAP, and LIME) are applied to understand both global and local feature contributions.