Predicting Red Wine Quality Report

1. Introduction

The wine industry is highly competitive and saturated with many different varieties and blends for the consumer to choose from. As such, many wine rating websites have popped up such as Wine Enthusiast and Vivino, which help customers separate the gems from the chaff. For a winery, it's important for them to invest in wines that are going to get high ratings so that they can recoup their investments. This project will use Red Wine Quality Data Set, available on the UCI machine learning repository https://archive.ics.uci.edu/ml/datasets/wine+quality/winequality-red.csv to perform binary classification for wine quality using ML Algorithm .
In this report, we summarized the findings and insights gained from analyzing the red wine dataset from UCI machine learning repository.
In this project we used Logistic Regression and Random Forest Classifier to predict red wine quality. We also showed each models' performance on the test data.

2. Dataset Analysis and Preprocessing

Dataset Description:

Wine Quality dataset is publicly available for research in the University of California, Irvine Machine Learning repository created by Paulo Cortez (Univ. Minho), Antonio Cerdeira, Fernando Almeida, Telmo Matos and Jose Reis (CVRVV) in 2009. This repository has two datasets of red and white wine samples which consists of inputs including objective tests (e.g. PH values) and the output is based on sensory data (median of at least 3 evaluations made by wine experts). Each expert graded the wine quality between 0 (very bad) and 10 (very excellent).

The original data set has 1599 rows and 12 columns. The dataset is clean, with no missing values, no duplicates.

Input variables (based on physicochemical tests):

1. Alcohol: the amount of alcohol in wine
2. Volatile acidity: are high acetic acid in wine which leads to an unpleasant vinegar taste
3. Sulphates: a wine additive that contributes to SO2 levels and acts as an antimicrobial and antioxidant
4. Citric Acid: acts as a preservative to increase acidity (small quantities add freshness and flavor to wines)
5. Total Sulfur Dioxide: is the amount of free + bound forms of SO2
6. Density: sweeter wines have a higher density
7. Chlorides: the amount of salt in the wine

8. Fixed acidity: are non-volatile acids that do not evaporate readily
9. pH: the level of acidity
10. Free Sulfur Dioxide: it prevents microbial growth and the oxidation of wine
11. Residual sugar: is the amount of sugar remaining after fermentation stops. The key is to have a perfect balance between sweetness and sourness

Output variable (based on sensory data): 12 - quality (score between 0 and 10)

We performed some transformation to the target variable "quality" in order to perform binary classification.

We categorized wines with score higher than 6 as high quality (hi_quality = 1) and wines with score less than 6 were categorized as low grade(hi_quality =0). And we rename the column from "quality" to hi_quality"

It is important to note that there is an imbalance in the dataset with only 13.57% of the data were high quality red wines, and 86.43% were low quality. This class imbalance is taken into consideration when splitting the data into training and testing data by using stratification. We also relied more on the metrics that are not heavily skewed by class imbalance, like F1-score, precision, and recall.

Data Exploration:

We explored the dataset to understand its structure, features, and distribution. This involved examining descriptive statistics, checking for missing values, and visualizing relationships between variables. Fortunately, our small dataset is pretty clean with no duplicates or missing values.

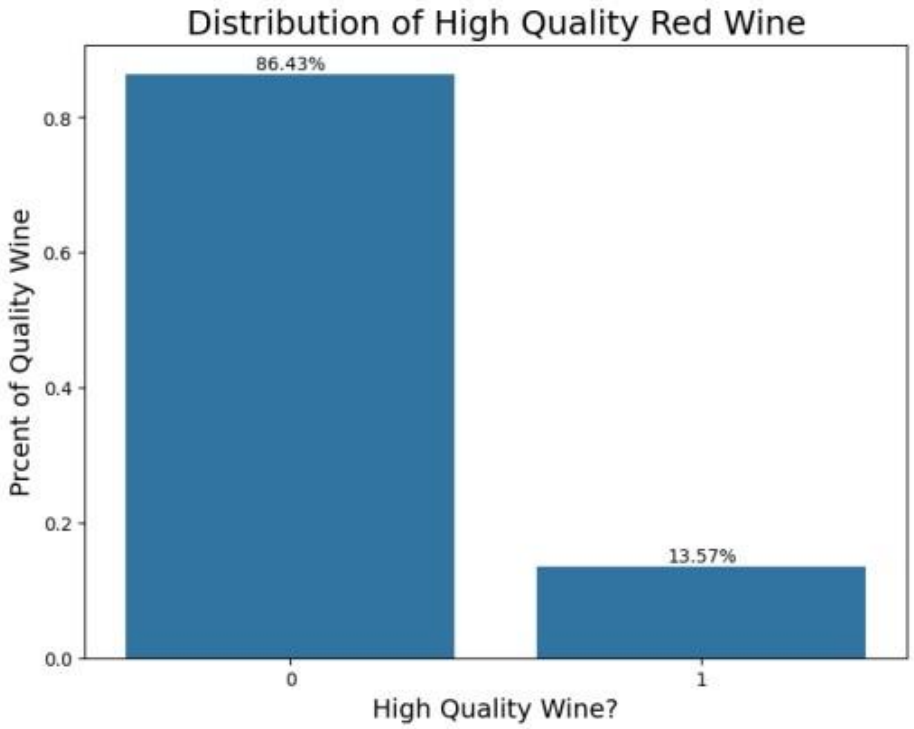
Preprocessing Steps:

We handled missing values, encoded categorical variables using one-hot encoding, and split the dataset into training and testing sets for model development.

2.1 Exploratory Data Analysis (EDA) and Discovery

First, we created a univariate chart of our target variable, Quality, to look at its distribution.
Our dataset consists mostly of mediocre wine quality.

We will create 2 bins for the quality column. Originally the score was from 3 to 8. Instead we will categorize wines with score higher than 6 as high quality (hi_quality = 1) and wines with score less than 6 will be categorized as low grade(hi_quality =0). And we rename the column from "quality" to hi_quality" Then let's look at the distribution again.

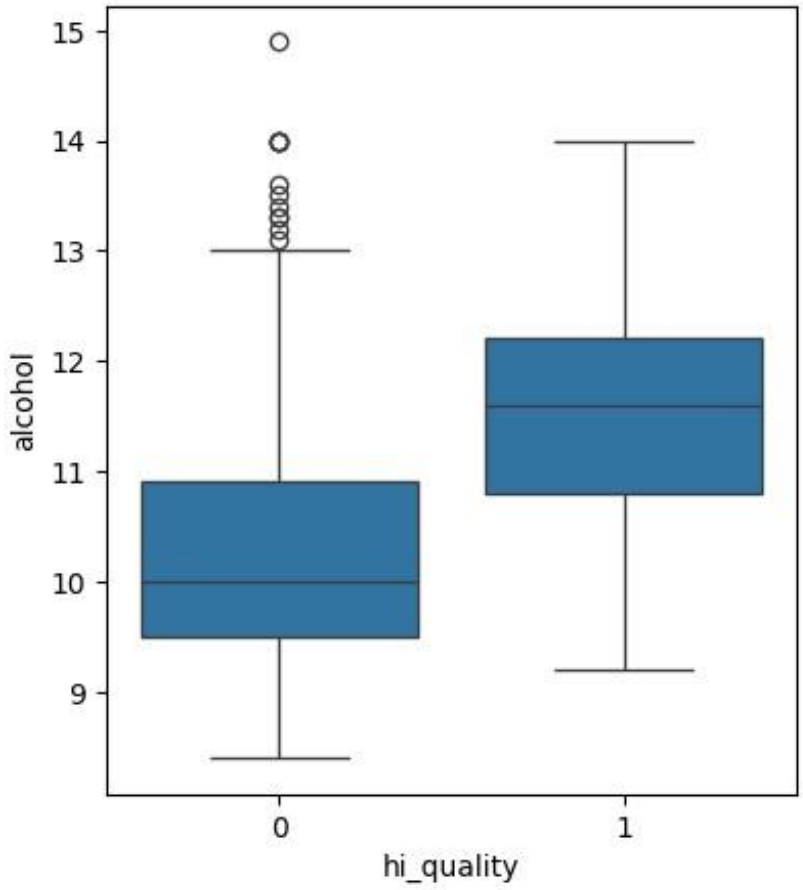


As can be seen above, only 13.57% of our wines are high quality. We have an imbalance dataset here.

Then we created various bivariate and multivariate charts to see how each feature relates to the target variable, hi_quality.

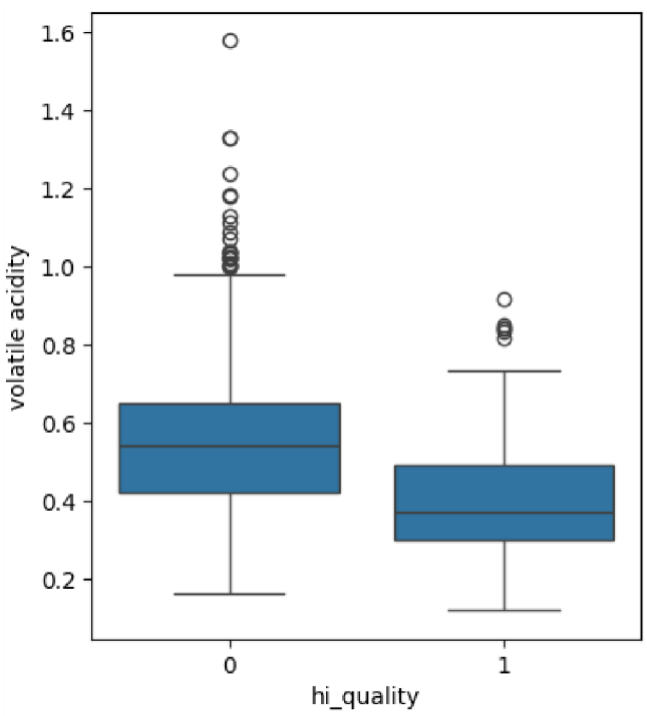
Let's look at some boxplots to see how each feature related to target variable "hi_quality"

2a: **High Quality vs Alcohol**



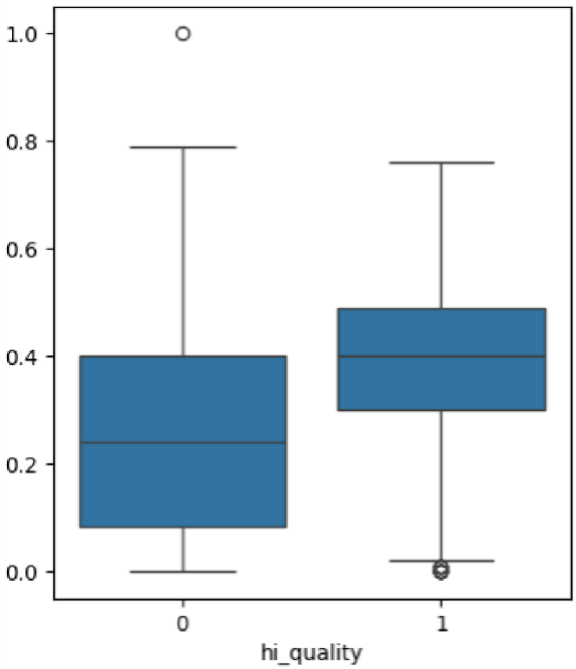
High quality wines have about 1.5% more alcohol on average than low quality wines. While it's unclear exactly why this might be the case, it may simply be due to general taste preferences of the raters lean more towards wine that is alcoholic. This was shown to be statistically significant via a t test (p-value < .005)

Figure 2b: High Quality vs volatile acidity



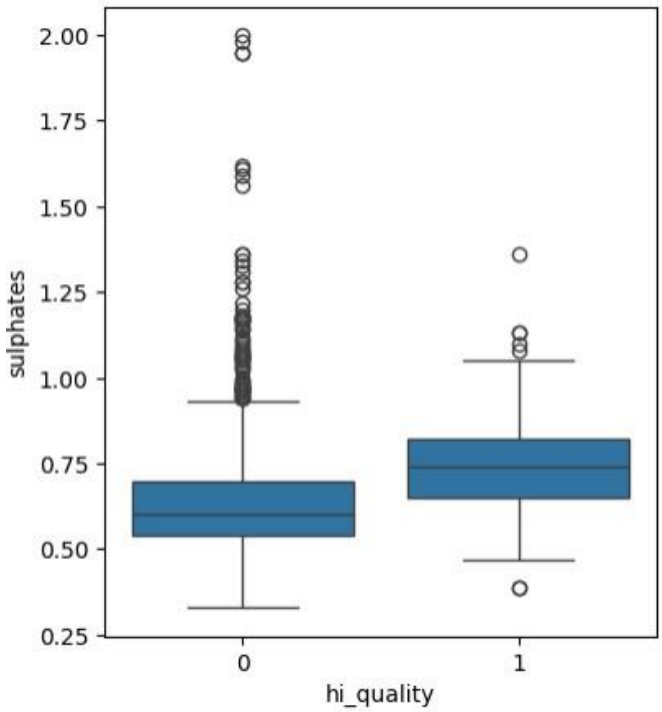
There is an inverse relationship between volatile acidity and wine quality: higher quality wine tends to have a lower level of volatile acidity. Volatile acids, similar to acetic acid, give a sour taste to our wine, degrading its quality. This relationship was shown to be statistically significant via a t-test (p-value < 0.05)

Figure 2c: **High Quality vs citric acid**



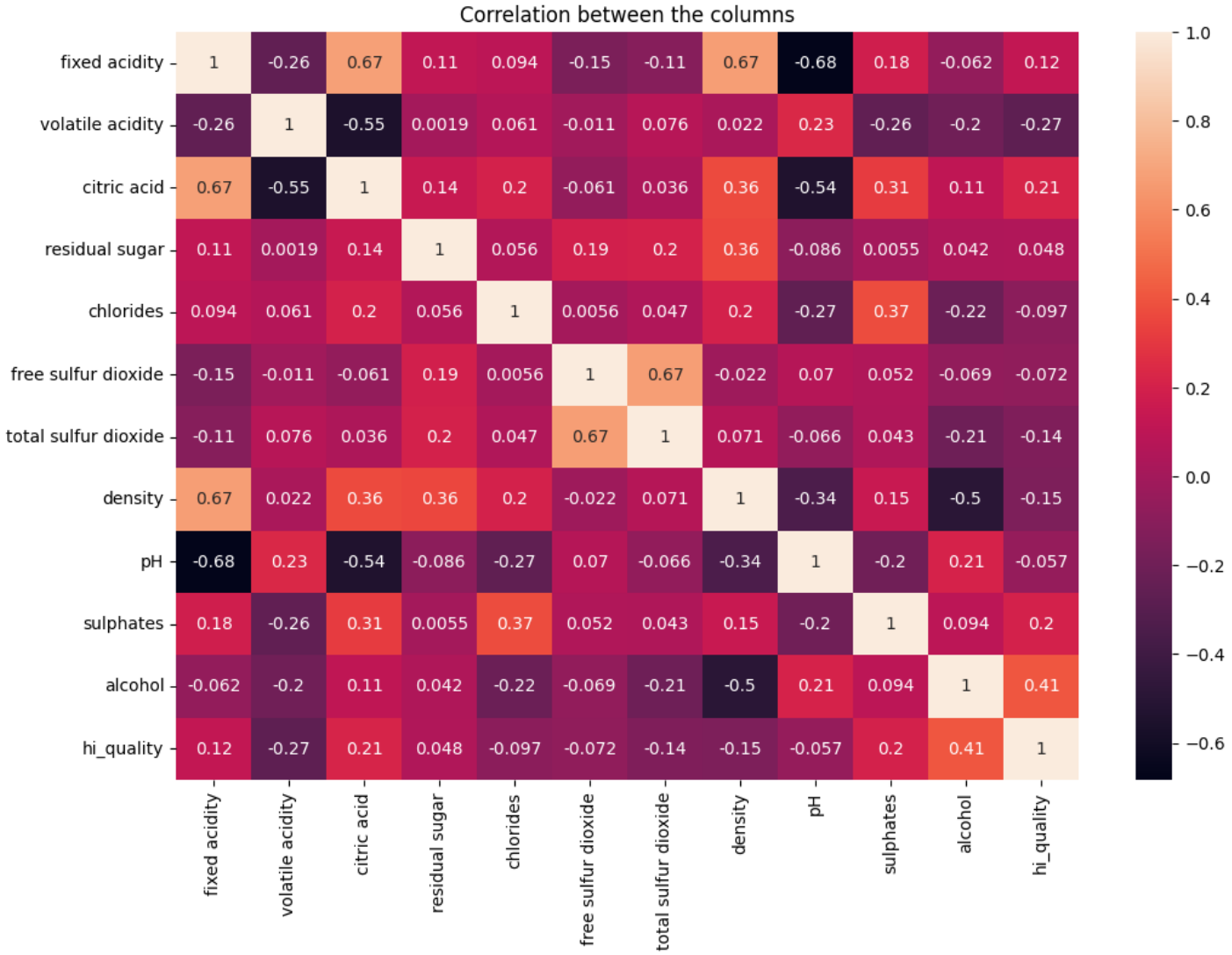
Higher quality wines tend to have more citric acid. Citric acid can give the wine a "fresh" taste, enhancing its flavor. Citric acid is often used as a stabilizer in food and beverages. This relationship was shown to be statistically significant via a t-test (p-value < 0.05)

Figure 2d: **High Quality vs sulphates**



High quality wines have more sulphates than low quality wine. This relationship was shown to be statistically significant via a t-test (p-value < 0.05)

Dependent Correlation: We created a correlation matrix heatmap to see how the dependent variables relate to our target variable "hi_quality". This relationship was shown to be statistically significant via a t-test (p-value < 0.01)



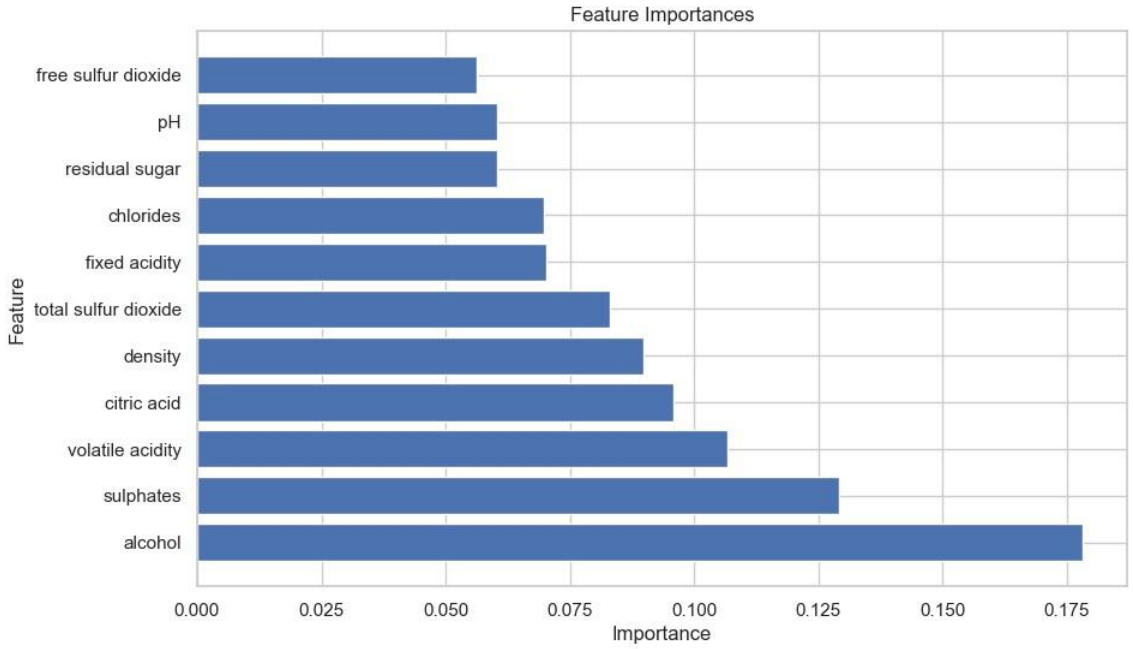
The heatmap shows that pH and volatile acidity have inverse correlation with hi_quality, as well as chlorides, density, total sulfur dioxide and free sulfur dioxide.

Multicollinearity: There is a strong positive correlation between fixed acidity and density (0.67). Also a strong positive correlation between total sulfur dioxide and free sulfur dioxide (0.67)
We will keep an eye on this going forward but for now will not drop any columns from the dataset

Some columns like citric acid, alcohol, sulphates are strongly and positively correlated whereas a lot of columns like pH, volatile acidity, chlorides, density, total sulfur dioxide and free sulfur dioxide have a negative correlation. Highest correlation: alcohol. Smallest correlation: residual sugar

Feature importances: The top 10 most important feature according to Random Forest Classifier

The top 10 most important feature according to Random Forest Classifier:



The top 10 most important feature according to Random Forest Classifier:
Alcohol, sulphates, volatile acidity, citric acid, density, total sulfur dioxide, fixed acidity, chlorides, residual sugar, pH, free sulfur dioxide

Data Preprocessing

We scale our data using Standard Scaler, which applies a linear transformation to our features such that their mean is zero and their variance is one. This is especially useful since the data has varying scales and it prevents the algorithms like linear regression from making assumptions that the data has a Gaussian distribution.

3. Model Development

We experimented with two machine learning algorithms for discrete binary classification, including Logistic Regression and Random Forest. We evaluated each model's performance using metrics such as accuracy, precision, recall, F1-score as well as AUC-ROC score on the test data. Optimization techniques like hyperparameter tuning were applied to improve model performance.

Model Performance Metrics: Model performance metrics are used to evaluate the performance of a machine learning model. Because the dataset appears to be imbalanced, with positive class (hi_quality=1) as low as 13.57%%, selecting the right model performance measure is critical. As a

result, model accuracy alone cannot determine the robustness of a machine learning model. Based on a confusion matrix created for training dataset predictions:

- **Accuracy** is defined as the number of correct predictions made by the machine learning model divided by the total number of datapoints. The best accuracy is 100 percent, which indicates that all predictions are correct. Given our dataset only has 13.57% positive class, accuracy is not a valid measure of model performance. Even if all of our predictions are incorrect, our model's accuracy would still be 86.43%. As a result, additional model performance measures are included. (precision, recall, f1 score, and AUC-ROC score)
- **Precision:** the proportion of positive predictions made by a model that are actually correct, essentially measuring the quality of a model's positive predictions by dividing the number of true positives by the total number of predicted positives (including false positives). A high precision indicates that when the model predicts something as positive, it is likely to be correct. In our scenario, especially for small wine breweries we want high precision and minimize false positives as much as possible. But we also do not want to classify most wines as low quality either.
- **Recall:** recall is a metric that measures how well a model can identify all relevant positive instances within a dataset, essentially answering the question: "Out of all the actual positive cases, how many did the model correctly predict as positive?". It is also known as "sensitivity" or "true positive rate" and is calculated by dividing the number of true positives by the sum of true positives and false negatives. Recall prioritizes catching all relevant positive cases, even if it means potentially including some false positives. Recall is important when: Missing a positive case has severe consequences, like in medical diagnosis where a false negative could be life-threatening which does not apply in our scenario
- **F1 score:** F1 score is a metric used to evaluate the performance of a classification model, particularly in scenarios with imbalanced classes, by combining the precision and recall of a model into a single value, essentially representing a balanced average of how well the model identifies positive cases while minimizing false positives and false negatives; it is calculated as the harmonic mean of precision and recall, with a higher F1 score indicating better performance. Unlike accuracy, which can be misleading in imbalanced datasets, the F1 score takes both precision (correct positive predictions divided by total positive predictions) and recall (correct positive predictions divided by all actual positive cases) into account, providing a more comprehensive evaluation. The F1 score is calculated using the harmonic mean of precision and recall, which gives more weight to lower values, meaning a model needs to perform well on both precision and recall to achieve a high F1 score. F1 score is useful for our imbalanced dataset because one class is significantly outnumbered by another. TheF1 score is a valuable metric as it doesn't prioritize the majority class.
- **AUC-ROC score: a**n AUC ROC score (Area Under the Receiver Operating Characteristic Curve) is a metric used to evaluate the performance of a binary classification model, representing the probability that the model will rank a randomly chosen positive example higher than a randomly chosen negative example, essentially indicating how well the model can distinguish between positive and negative classes across different classification thresholds; a higher AUC score signifies better model performance, with a perfect model achieving an AUC of 1.0. It measures the area under the ROC curve, which is a graph plotting the True Positive Rate (TPR) against the False Positive Rate (FPR) at different classification thresholds.

AUC of 0.5 indicates the model performs no better than random guessing.

AUC close to 1 indicates the model performs well in distinguishing between positive and negative classes

Logistic Regression: A logistic regression model is used for predicting classes using the probability of the target variable. Unlike linear regression, which uses expected values of the response model, logistic regression

uses the probability or odds of the response variable to model based on the combination of values taken by the predictors. This model uses the sigmoid function that maps predicted values to probabilities. It works well on linearly separable classes with easy implementation, making it a popular choice for classification problems. There are two types of logistic regression models for classification: binary and multinomial. Binary logistic regression requires a dependent variable with only two possible outcomes whereas a multinomial requires three or more outcomes. In this case, the dataset is working with binary logistic regression since the target variable is binary (1 or 0). Logistic regression is applicable to this problem since we want to predict the probabilities and classify the red wine quality into two categories based on the explanatory variables. For the solver in the logistic regression model, liblinear is picked since it supports both L1 and L2 regularization. We first tried to build a logistic regression model, which is specifically designed for binary classification problems and is the most straightforward model in our case. And we also performed hyperparameter tuning via GridSearchCV to improve the result of our model. In addition, we adjusted the threshold to achieve a higher F1 score.

```
Best Parameters for Logistic Regression: {'C': 0.01, 'penalty': 'l2'}

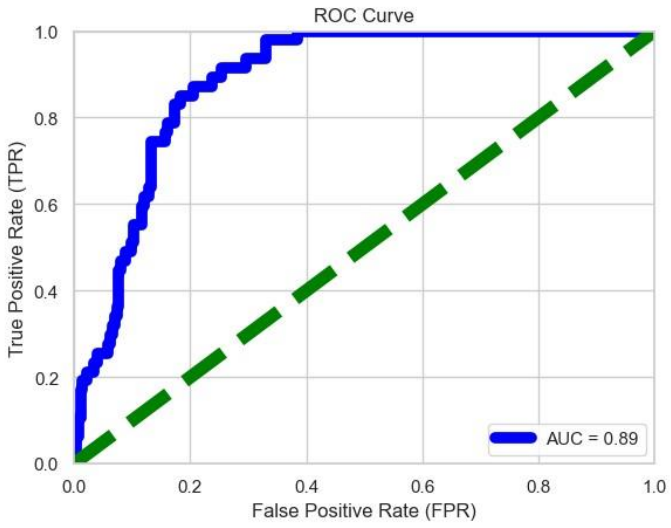
Accuracy Tuned for Logistic Regression: 0.846875

Confusion Matrix Tuned for Logistic Regression:
 [[245  28]
 [ 21  26]]

Classification Report Tuned for Logistic Regression:
              precision    recall  f1-score   support

           0       0.92      0.90      0.91       273
           1       0.48      0.55      0.51        47

    accuracy                           0.85       320
   macro avg       0.70      0.73      0.71       320
weighted avg       0.86      0.85      0.85       320
```




```
AUC-ROC Score: 0.8871483126802275
```

Best Parameters for Logistic Regression: {'C': 0.01, 'penalty': 'l2'}

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Classification Report Tuned for Logistic Regression:
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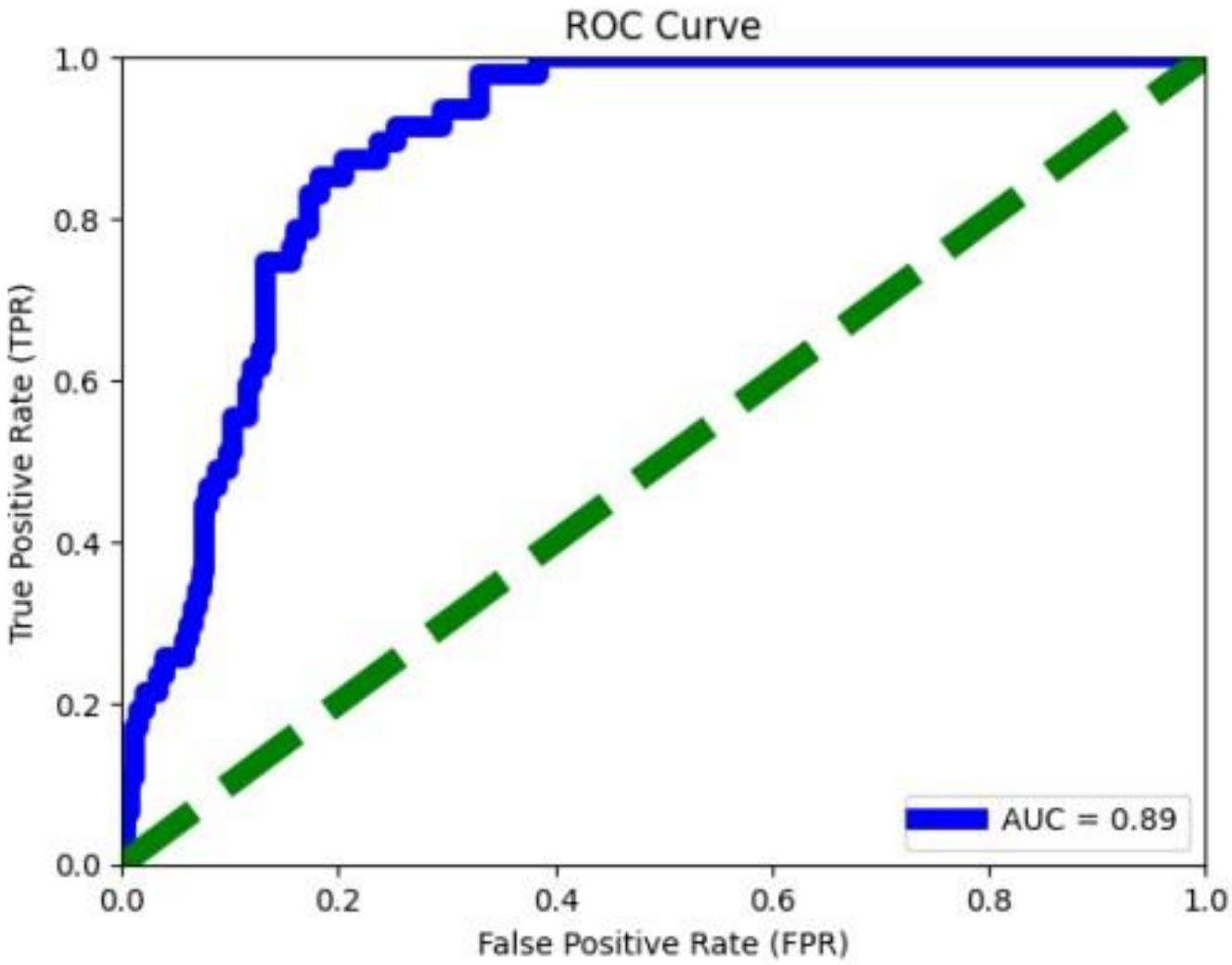
0 0.92 0.90 0.91 273
1 0.48 0.55 0.51 47

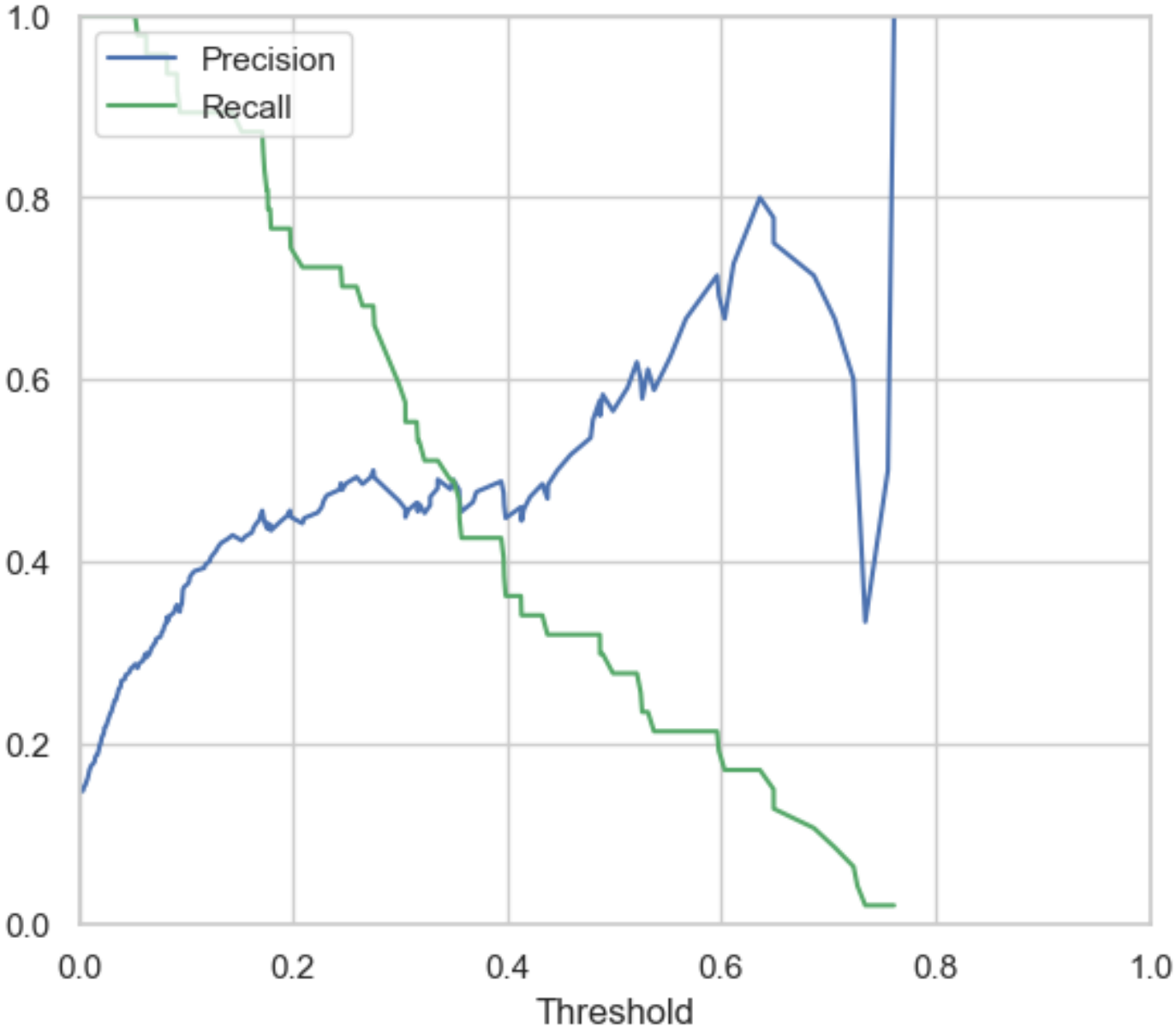
 accuracy 0.85 320   macro avg
0.70 0.73 0.71 320  weighted
avg 0.86 0.85 0.85 320
```




```
AUC-ROC Score: 0.8871483126802275
```

The tuned Logistic Regression model has an F1-score of 0.51 and AUC=0.89 for hi_quality= 1. Considering only a small percentage of red wines are high quality, the Linear Regression model is doing a good job in predicting attrition. We have an imbalanced dataset. The F1 score is generally better than the area under the curve (AUC) for imbalanced datasets when the minority class is of interest. The F1 score is the harmonic mean of precision and recall, which balances the importance of both metrics. It's a more robust evaluation metric than accuracy because it gives a fair representation of a model's performance despite class imbalance.

The AUC is a single value that summarizes a model's overall performance. It's useful for comparing the performance of multiple models. However, the AUC and ROC curve may not be well-suited for imbalanced problems because they may be biased toward the majority class. The accuracy score may also be less useful here as there is less emphasis on the minority class (hi_quality = 0) with better results in the majority class. With the relatively small sample and lack of longitudinal data, these scores are pretty decent in aiding the company to predict red wine quality



Next, we examined the data through a different model - Random Forest. Considering the numerous correlations across the features, the low F1 score in the logistic regression may be attributed to more non-linear and complex relationships across features and Attrition. There may also be more noisy data in this case as our hyperparameter tuning did not pose much benefit to the linear regression. This prompted us to utilize the Random Forest model to see if we can deal better with the possible presence of complex relationships and noisy data.

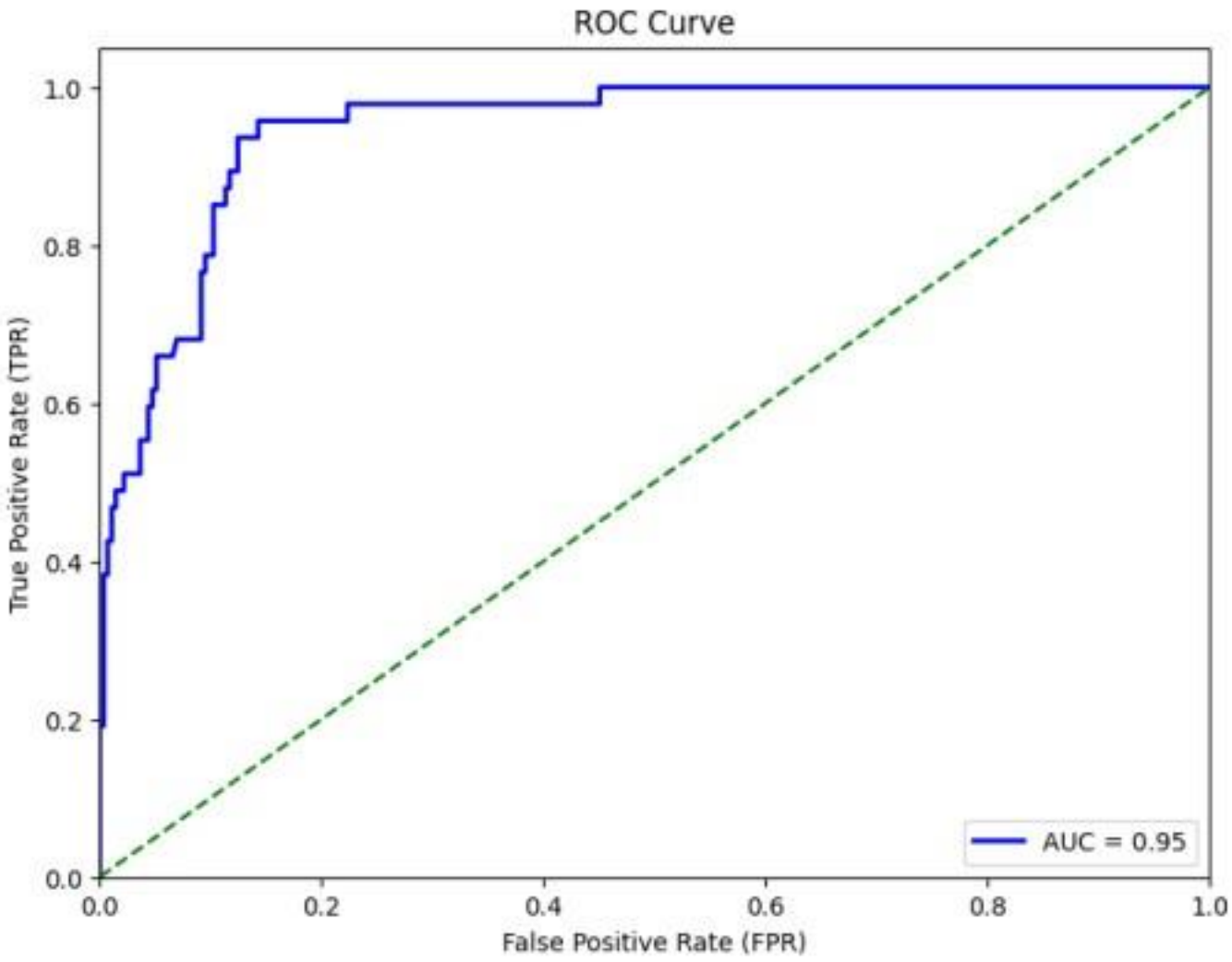
RANDOM FOREST: A Random Forest Classifier model is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. Trees in the forest use the best split strategy, i.e.,

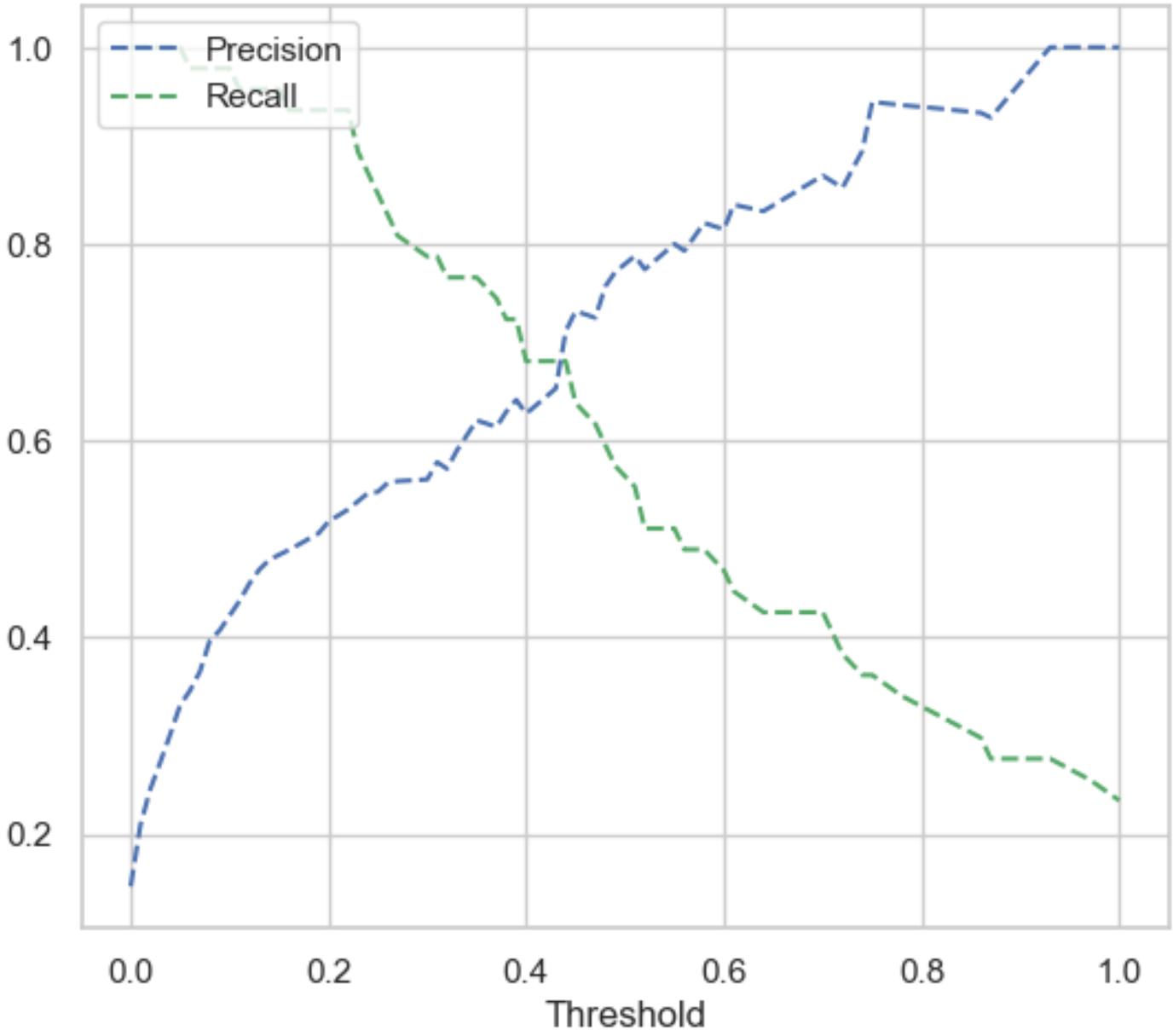
equivalent to passing splitter="best" to the underlying DecisionTreeRegressor. The sub-sample size is controlled with the max_samples parameter if bootstrap=True (default), otherwise, the whole dataset is used to build each tree. Here we went straight to tune the model by performing hyperparameter tuning via GridSearchCV to improve the result. We also adjust the threshold to achieve a higher F1 score.

```
Fitting 3 folds for each of 81 candidates, totalling 243 fits
Best Parameters (Random Forest): {'max_depth': 15, 'min_samples_leaf': 1,
'min_sampl es_split': 2, 'n_estimators': 500}  Accuracy (Tuned Random Forest):
0.89375  Confusion Matrix (Tuned Random Forest):
  [[255 18]
  [ 16 31]]
Classification Report (Tuned Random Forest):
precision recall f1-score support

 0 0.94 0.93 0.94 273
1 0.63 0.66 0.65 47

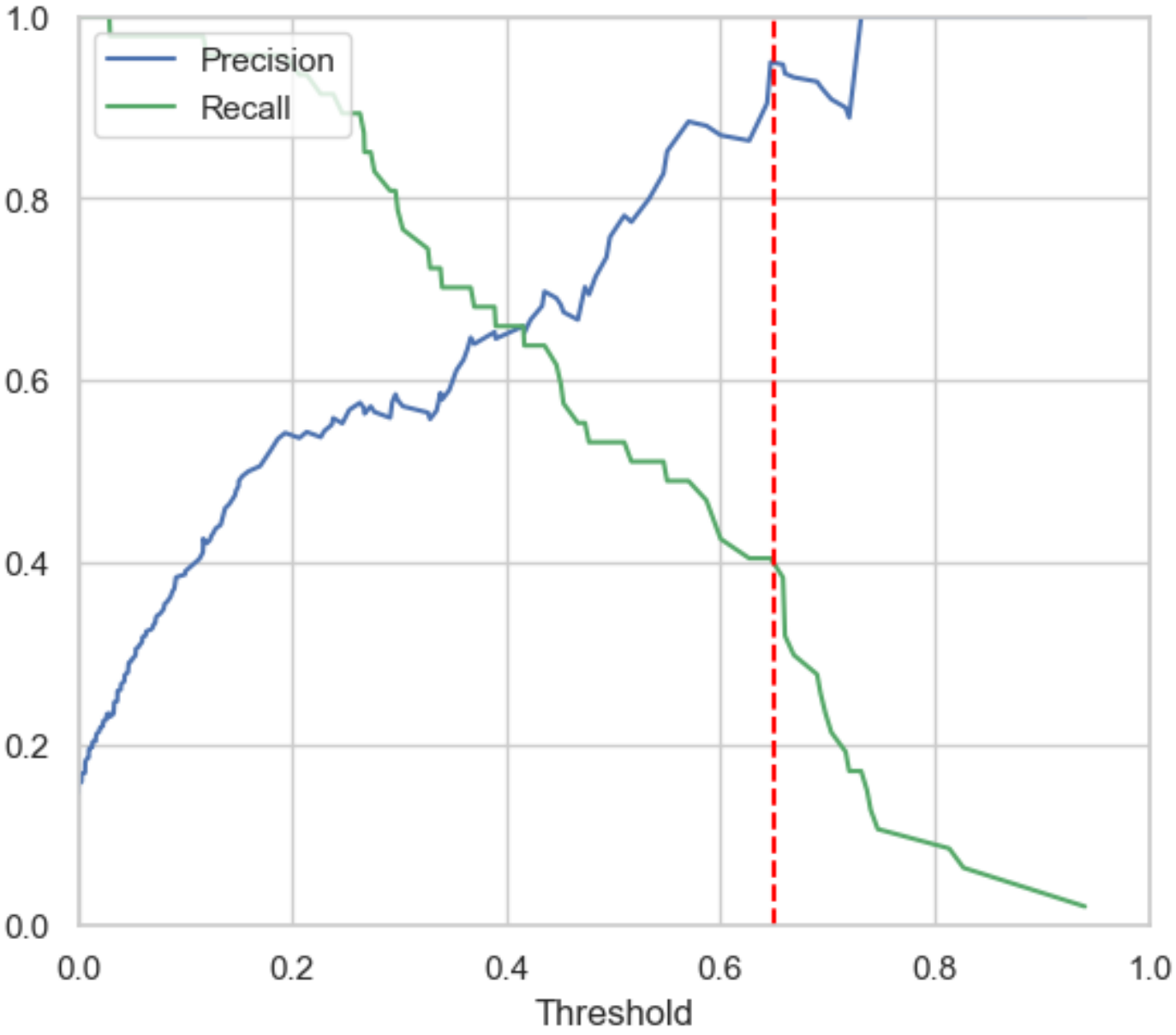
accuracy 0.89 320   macro
avg 0.79 0.80 0.79 320
weighted avg 0.90 0.89 0.89
320
```


ROC Curve
True Positive Rate (TPR)
False Positive Rate (FPR)
0.0
0.2
0.4
0.6
0.8
1.0
AUC = 0.95



The tuned Random Forest model (with GridSearchCV) has an F1-score of 0.65 and the AUC-ROC score of 0.95. The hyperparameter tuned Random Forest model has higher F1-score of 0.65 (the regular RF has F1-score of 0.62) and the AUC-ROC score is about the same 0.9485620762216507 vs 0.9457174031642117

Precision Recall Curve of tuned Random Forest: the sweet spot if we want to maximize precision is at threshold around 0.65

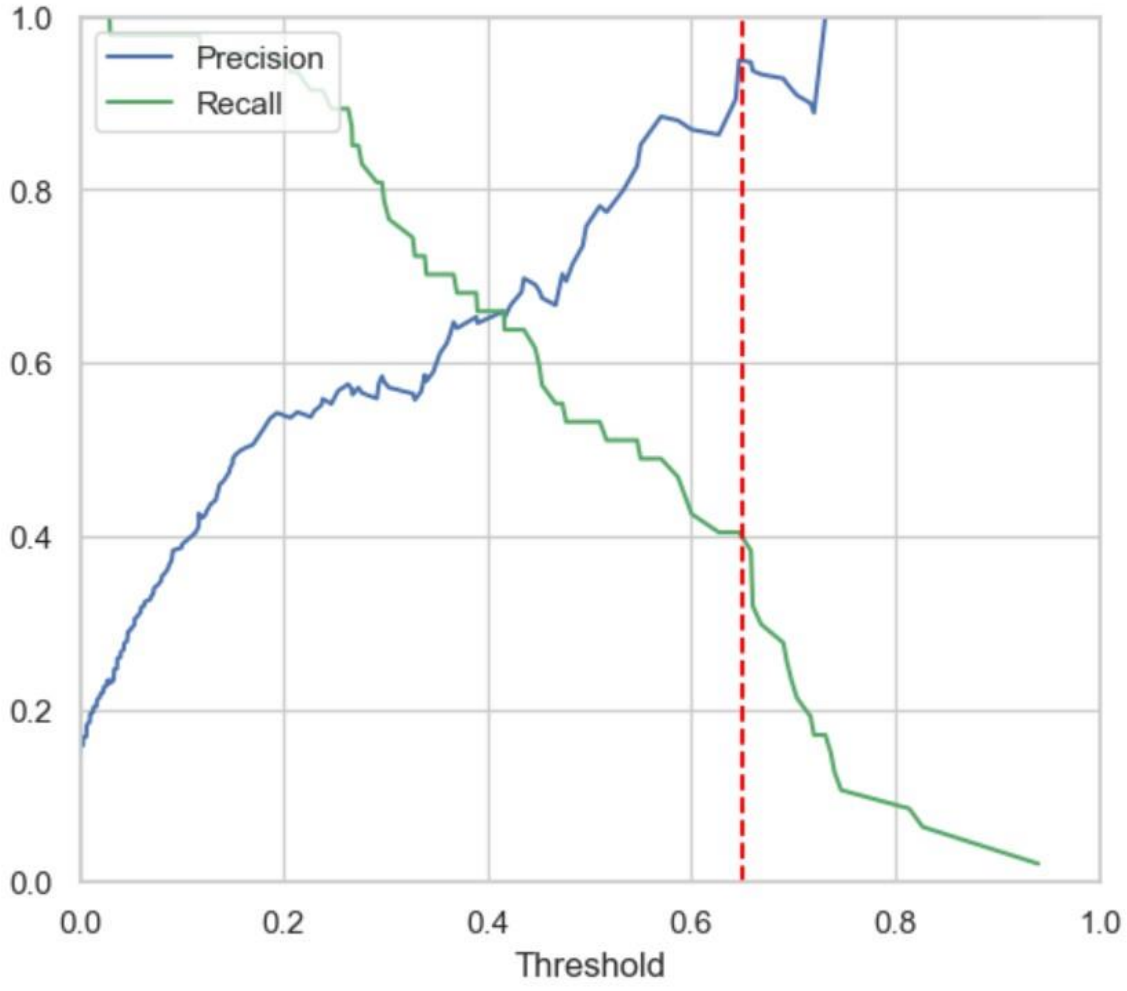


Business Case

In this case, we will assume that our client is a small brewery which needs to make sure that all of its investments are profitable. Therefore, precision is more important than recall. Our solution is to adjust the threshold in our calculation of precision, recall, and F1 score.
Adjusting the threshold is important because it allows us to directly control the balance between precision and recall, finding the "sweet spot" where both metrics are adequately balanced depending on whether we prioritize identifying all positive cases (high recall) or minimizing false positives (high precision). . Key points about threshold adjustment:

- **Impact on Precision and Recall:**
  A higher threshold leads to higher precision (fewer false positives) but lower recall (more false negatives), while a lower threshold increases recall but decreases precision.
- **Importance for Imbalanced Datasets:**
  In datasets where one class is significantly smaller than the other, adjusting the threshold can be crucial to accurately evaluate the model's performance on the minority class.
- **Precision-Recall Curve:**
  Visualizing the precision-recall curve helps identify the optimal threshold by showing how precision and recall change as the threshold varies.

From the precision recall curve of our best model Random Forest (after tuning), we adjust the threshold to increase precision and we find at threshold 0.65 the precision is much higher at 0.95 albeit at slightly lower recall



```
Best Parameters (Random Forest): {'max_depth': 15, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 300}
Accuracy (Tuned Random Forest): 0.90625
Confusion Matrix (Tuned Random Forest):
 [[272   1]
 [ 29  18]]
Classification Report (Tuned Random Forest):
              precision    recall  f1-score   support

           0       0.90      1.00      0.95       273
           1       0.95      0.38      0.55        47

    accuracy                           0.91       320
   macro avg       0.93      0.69      0.75       320
weighted avg       0.91      0.91      0.89       320
```

CONCLUSION:

Our Random Forest model performs much better than the Logistic Regression model, suggesting there is a complex, non-linear relationship between the features and hi quality target variable.