Predicting Wine Quality Using Machine Learning: An Exploratory Study and Model Comparison

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- Module: Probability and Statistics for Artificial Intelligence
- Date: 20/06/2025

Local Development Env. Setup

1. Install python: 3.11.3
2. Installed VSCode
3. Add Python and jupyter extension
4. Set kernel
5. conda install -n base ipykernel jupyter
6. conda -V >> conda 23.5.2
7. pip install jupyter notebook pandas numpy matplotlib scipy scikit-learn pandoc nbconvert[webpdf] nbconvert notebook-as-pdf seaborn xgboost shap openpyxl
8. run >> jupyter notebook
9. Github url for code repo: https://github.com/usd-ms-aai/aai-500-project-g4

In [1]:
```
# Import necessary libraries for data analysis, visualization, and machine learning
import pandas as pd  # For data manipulation and analysis
import numpy as np  # For numerical operations
import matplotlib.pyplot as plt  # For plotting graphs
import seaborn as sns  # For advanced data visualization
from sklearn.model_selection import train_test_split, GridSearchCV  # For splitting
from sklearn.preprocessing import StandardScaler  # For feature scaling
from sklearn.linear_model import LinearRegression, LogisticRegression  # For regres
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier  # For e
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score  # Fo
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score
from xgboost import XGBRegressor, XGBClassifier  # For XGBoost models
import shap  # For model interpretability
```

In [2]:
```
# Load the wine quality dataset from an Excel file
# The dataset contains physicochemical properties and quality ratings for white win
data = pd.read_excel('winequality-white123.xlsx')
```

In [3]:
```
# Display the first few rows of the dataset to understand its structure
print(data.head())

# 1. Data Cleaning/Preparation
# Check for missing values in the dataset to ensure data quality
print("\nChecking for missing values:")
print(data.isnull().sum())  # Confirm no missing data

# Separate features (X) and target variable (y)
```

```python
X = data.drop('quality', axis=1)  # Features: all columns except 'quality'
y = data['quality']  # Target: wine quality rating
```

```
   fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0            7.0              0.27         0.36            20.7      0.045   
1            6.3              0.30         0.34             1.6      0.049   
2            8.1              0.28         0.40             6.9      0.050   
3            7.2              0.23         0.32             8.5      0.058   
4            7.2              0.23         0.32             8.5      0.058   

   free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0                 45.0                 170.0   1.0010  3.00       0.45   
1                 14.0                 132.0   0.9940  3.30       0.49   
2                 30.0                  97.0   0.9951  3.26       0.44   
3                 47.0                 186.0   0.9956  3.19       0.40   
4                 47.0                 186.0   0.9956  3.19       0.40   

   alcohol  quality  
0      8.8        6  
1      9.5        6  
2     10.1        6  
3      9.9        6  
4      9.9        6  

Checking for missing values:
fixed acidity           0
volatile acidity        0
citric acid             0
residual sugar          0
chlorides               0
free sulfur dioxide     0
total sulfur dioxide    0
density                 0
pH                      0
sulphates               0
alcohol                 0
quality                 0
dtype: int64
```

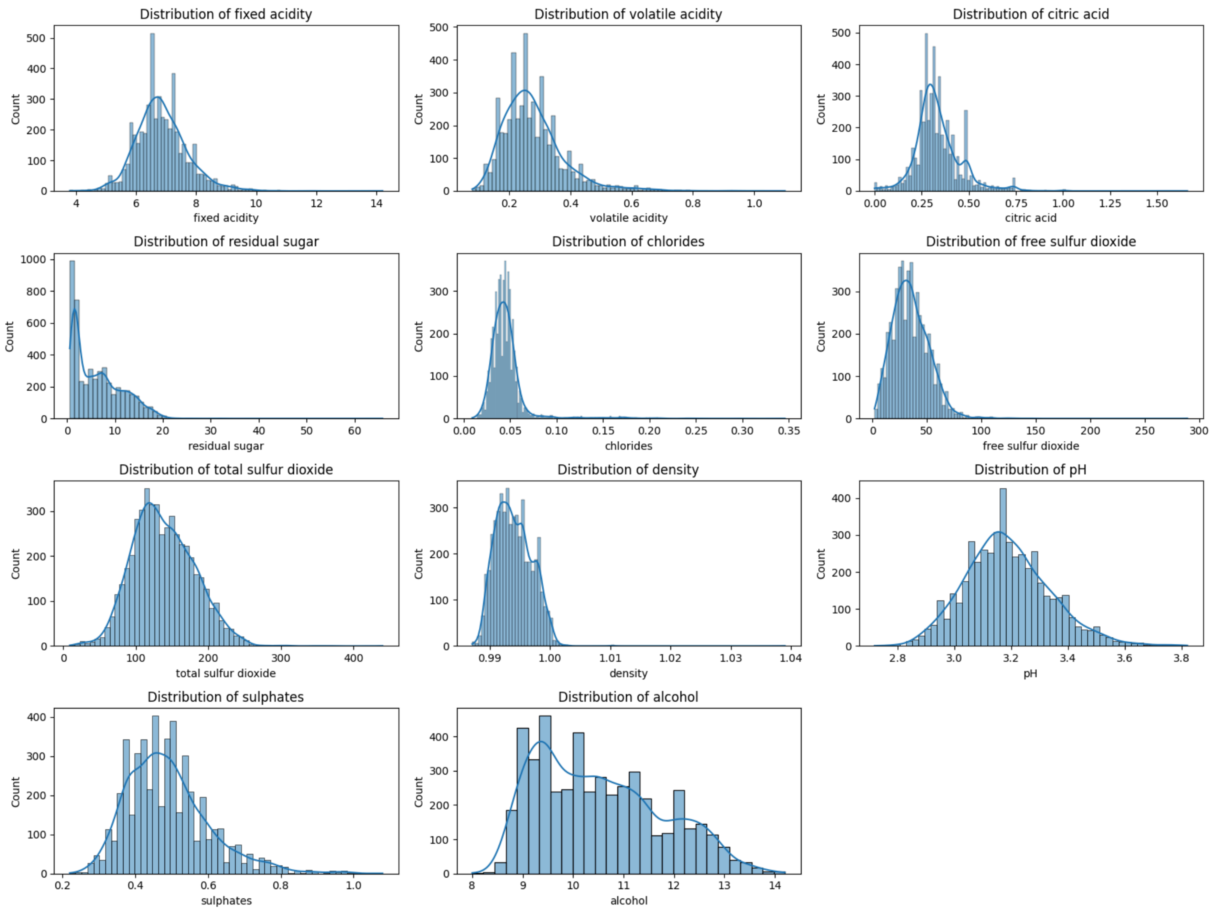
In [4]:

```python
# Option 1: Regression (predict actual quality)
# Option 2: Classification (Good vs Bad wine based on threshold quality >= 7)

# Define a binary classification target: Good (quality >= 7) vs Bad (quality < 7)
quality_threshold = 7
y_class = (y >= quality_threshold).astype(int)  # 1 = Good, 0 = Bad

# Feature Scaling: Standardize features to have mean=0 and variance=1
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)

# Split data into training and test sets for regression
X_train_reg, X_test_reg, y_train_reg, y_test_reg = train_test_split(X_scaled, y, te

# Split data into training and test sets for classification
X_train_clf, X_test_clf, y_train_clf, y_test_clf = train_test_split(X_scaled, y_cla
```

In [5]:
```python
# 2. Exploratory Data Analysis (EDA)
# Display summary statistics for each feature to understand data distribution and c
print("\nSummary statistics:")
print(data.describe())
```

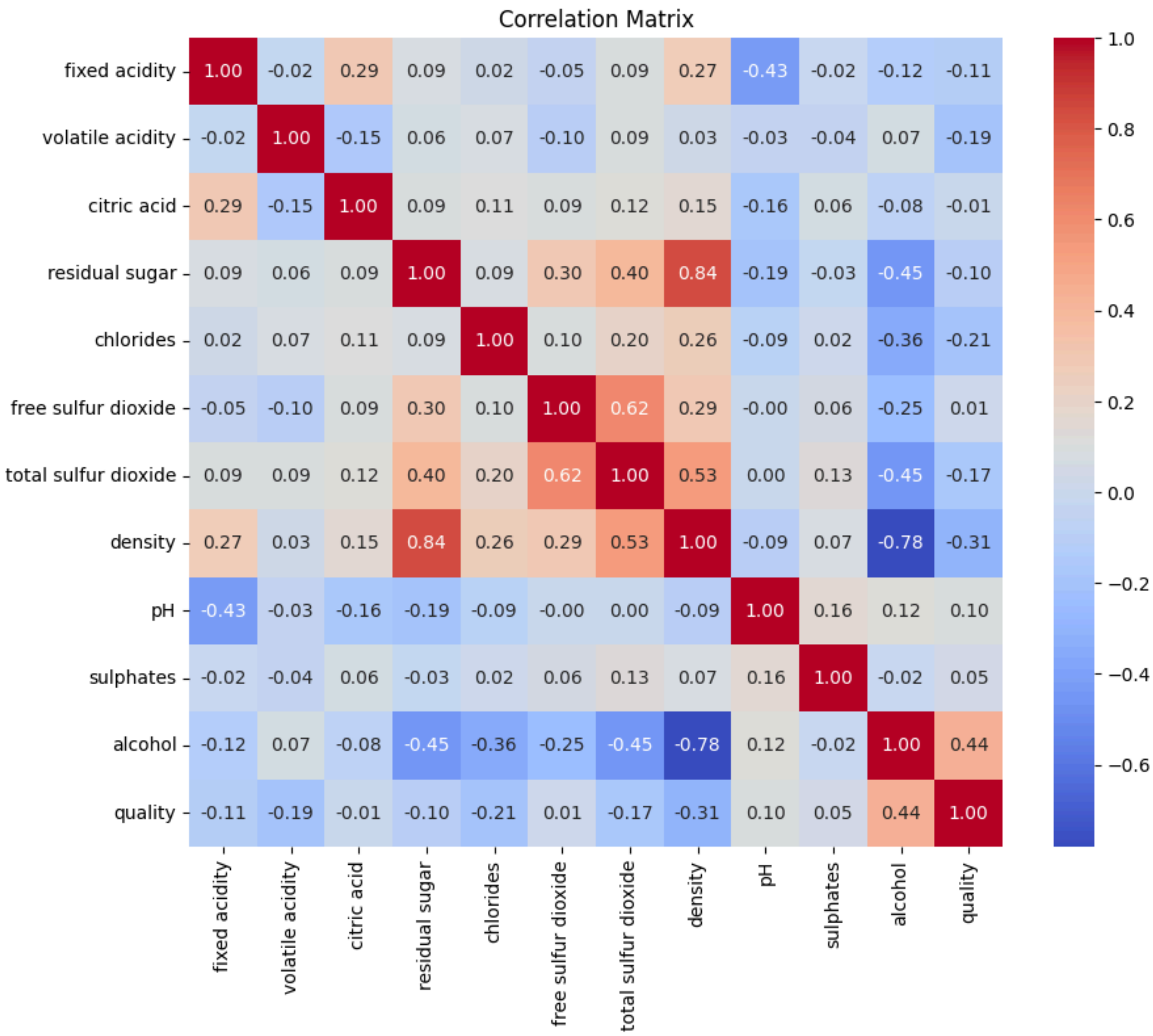
```
Summary statistics:
       fixed acidity  volatile acidity  citric acid  residual sugar  \
count    4898.000000       4898.000000  4898.000000     4898.000000
mean        6.854788          0.278241     0.334192        6.391415
std         0.843868          0.100795     0.121020        5.072058
min         3.800000          0.080000     0.000000        0.600000
25%         6.300000          0.210000     0.270000        1.700000
50%         6.800000          0.260000     0.320000        5.200000
75%         7.300000          0.320000     0.390000        9.900000
max        14.200000          1.100000     1.660000       65.800000

         chlorides  free sulfur dioxide  total sulfur dioxide      density  \
count  4898.000000          4898.000000           4898.000000  4898.000000
mean      0.045772            35.308085            138.360657     0.994027
std       0.021848            17.007137             42.498065     0.002991
min       0.009000             2.000000              9.000000     0.987110
25%       0.036000            23.000000            108.000000     0.991723
50%       0.043000            34.000000            134.000000     0.993740
75%       0.050000            46.000000            167.000000     0.996100
max       0.346000           289.000000            440.000000     1.038980

                pH    sulphates      alcohol      quality
count  4898.000000  4898.000000  4898.000000  4898.000000
mean      3.188267     0.489847    10.514267     5.877909
std       0.151001     0.114126     1.230621     0.885639
min       2.720000     0.220000     8.000000     3.000000
25%       3.090000     0.410000     9.500000     5.000000
50%       3.180000     0.470000    10.400000     6.000000
75%       3.280000     0.550000    11.400000     6.000000
max       3.820000     1.080000    14.200000     9.000000
```

In [6]:
```python
# Plot the distribution of each feature to visualize their spread and detect outlie
features = X.columns
plt.figure(figsize=(16,12))
for i, feature in enumerate(features):
    plt.subplot(4,3,i+1)
    sns.histplot(data[feature], kde=True)
    plt.title(f'Distribution of {feature}')
plt.tight_layout()
plt.show()
```

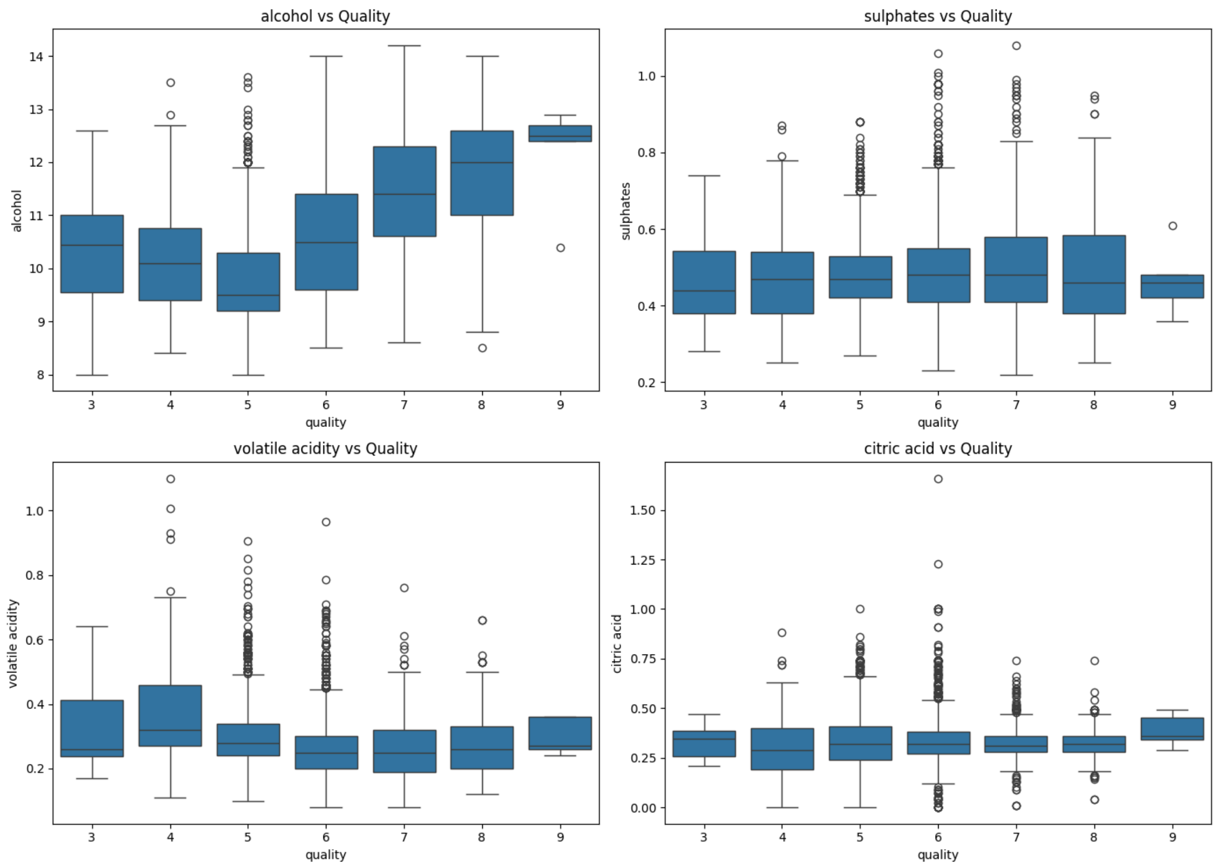


In [7]:

```
# Plot the correlation matrix to examine relationships between features and with th
plt.figure(figsize=(10,8))
corr = data.corr()
sns.heatmap(corr, annot=True, fmt=".2f", cmap='coolwarm')
plt.title('Correlation Matrix')
plt.show()
```



In [8]:
```python
# Create boxplots to visualize the relationship between wine quality and key featur
key_features = ['alcohol', 'sulphates', 'volatile acidity', 'citric acid']
plt.figure(figsize=(14,10))
for i, feature in enumerate(key_features):
    plt.subplot(2,2,i+1)
    sns.boxplot(x='quality', y=feature, data=data)
    plt.title(f'{feature} vs Quality')
plt.tight_layout()
plt.show()
```



In [9]:
```
# 3. Model Selection and Training
# Define Regression models to predict wine quality as a continuous variable
models_reg = {
    "Linear Regression": LinearRegression(),
    "Random Forest": RandomForestRegressor(random_state=42),
    "XGBoost": XGBRegressor(random_state=42, eval_metric='rmse')
}
```

In [10]:
```
# Train and evaluate each regression model, reporting key performance metrics
print("\nRegression Model Performance:")
for name, model in models_reg.items():
    model.fit(X_train_reg, y_train_reg)  # Train the model
    y_pred = model.predict(X_test_reg)  # Predict on test set
    rmse = np.sqrt(mean_squared_error(y_test_reg, y_pred))  # Root Mean Squared Err
    mae = mean_absolute_error(y_test_reg, y_pred)  # Mean Absolute Error
    r2 = r2_score(y_test_reg, y_pred)  # R-squared score
    print(f"{name} - RMSE: {rmse:.3f}, MAE: {mae:.3f}, R²: {r2:.3f}")
```

```
Regression Model Performance:
Linear Regression - RMSE: 0.754, MAE: 0.586, R²: 0.265
Random Forest - RMSE: 0.590, MAE: 0.419, R²: 0.551
XGBoost - RMSE: 0.617, MAE: 0.439, R²: 0.509
```

In [11]:
```
# Define classification models to predict if a wine is 'Good' or 'Bad'
models_clf = {
    "Logistic Regression": LogisticRegression(max_iter=500, random_state=42),
    "Random Forest": RandomForestClassifier(random_state=42),
    #"XGBoost": XGBClassifier(use_label_encoder=False, eval_metric='logloss', rando
```

```
    "XGBoost": XGBClassifier(eval_metric='logloss', random_state=42)
}
```

In [12]:

```
# Train and evaluate each classification model, reporting accuracy, precision, reca
print("\nClassification Model Performance:")
for name, model in models_clf.items():
    model.fit(X_train_clf, y_train_clf)  # Train the model
    y_pred = model.predict(X_test_clf)  # Predict on test set
    acc = accuracy_score(y_test_clf, y_pred)  # Accuracy
    prec = precision_score(y_test_clf, y_pred)  # Precision
    rec = recall_score(y_test_clf, y_pred)  # Recall
    f1 = f1_score(y_test_clf, y_pred)  # F1-score
    print(f"{name} - Accuracy: {acc:.3f}, Precision: {prec:.3f}, Recall: {rec:.3f},
```

```
Classification Model Performance:
Logistic Regression - Accuracy: 0.787, Precision: 0.582, Recall: 0.282, F1-score: 0.
380
Random Forest - Accuracy: 0.893, Precision: 0.859, Recall: 0.643, F1-score: 0.736
XGBoost - Accuracy: 0.883, Precision: 0.792, Recall: 0.670, F1-score: 0.726
```

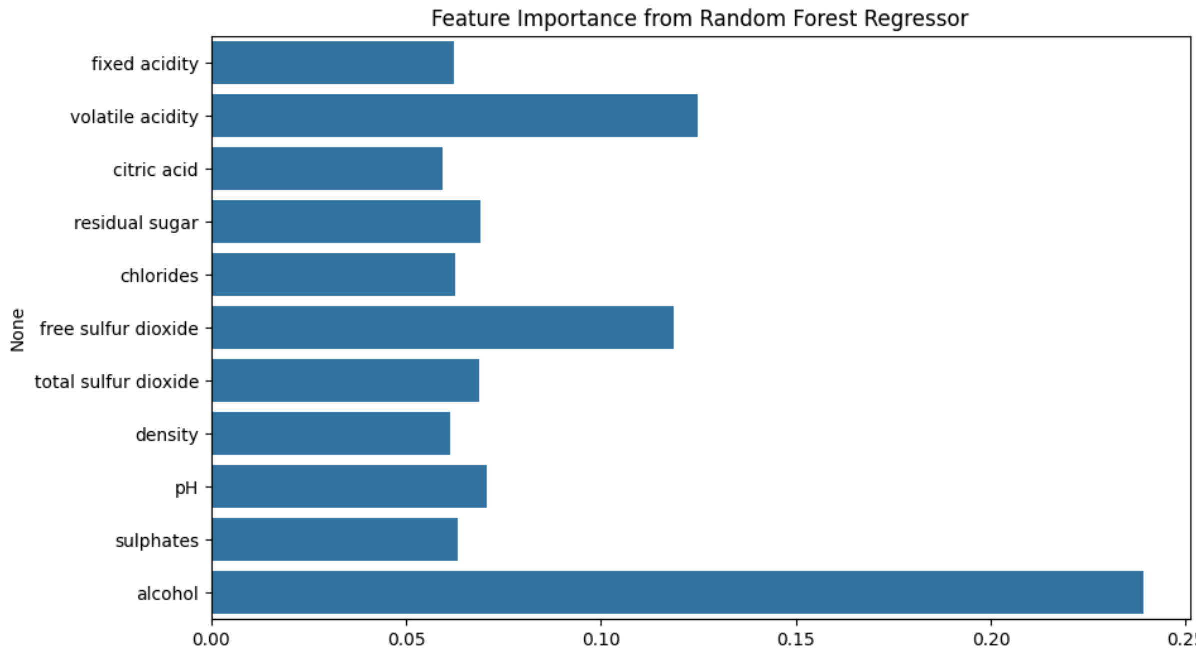
In [13]:

```
# Generate and display the confusion matrix for the best classifier (Random Forest)
best_clf = RandomForestClassifier(random_state=42)
best_clf.fit(X_train_clf, y_train_clf)
y_pred_best = best_clf.predict(X_test_clf)
cm = confusion_matrix(y_test_clf, y_pred_best)
print("\nConfusion Matrix for Random Forest Classifier:")
print(cm)
```

```
Confusion Matrix for Random Forest Classifier:
[[729  24]
 [ 81 146]]
```

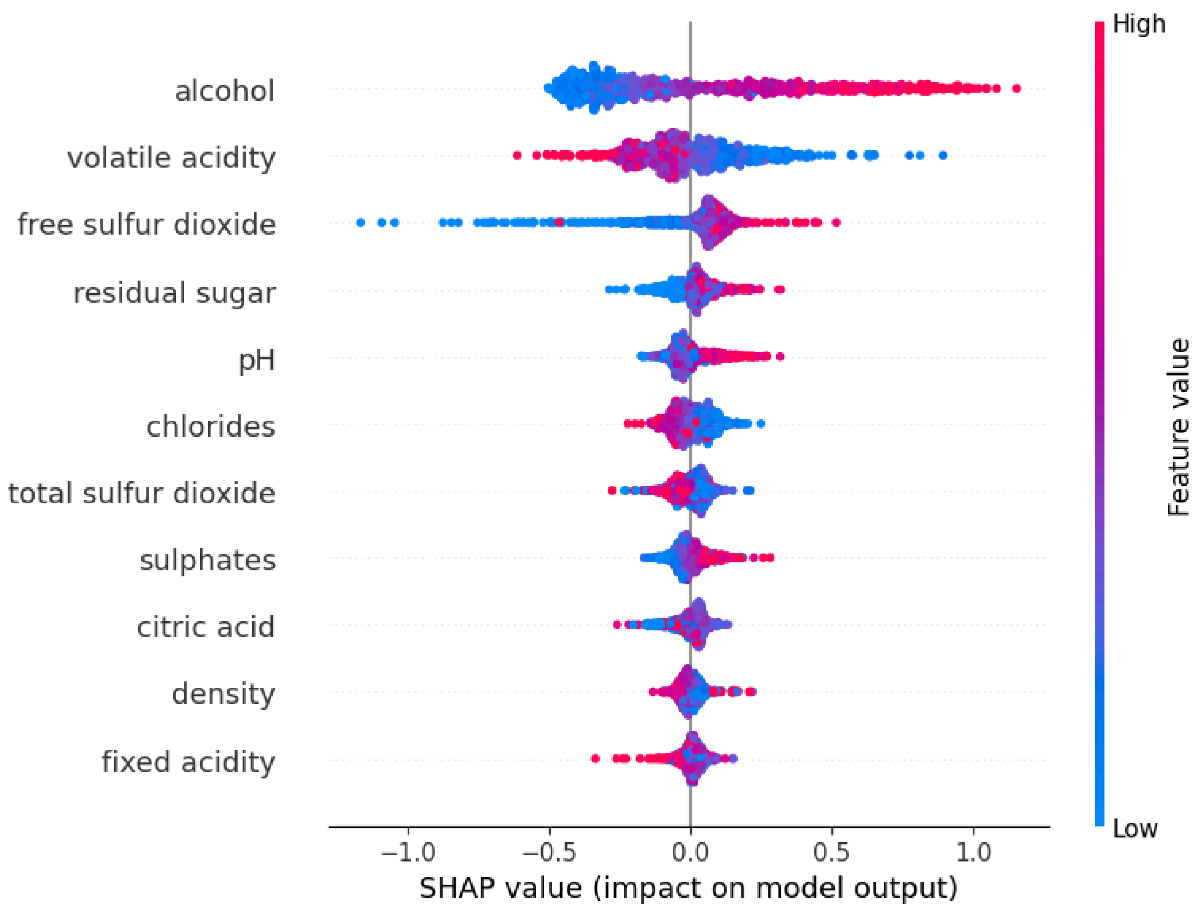
In [14]:

```
# 4. Feature Importance (Random Forest Regressor example)
# Fit a Random Forest Regressor and extract feature importances
best_reg = RandomForestRegressor(random_state=42)
best_reg.fit(X_train_reg, y_train_reg)
importances = best_reg.feature_importances_

# Visualize feature importances using a bar plot
plt.figure(figsize=(10,6))
sns.barplot(x=importances, y=features)
plt.title('Feature Importance from Random Forest Regressor')
plt.show()
```



In [15]:
```
# 5. Use SHAP to explain the predictions of the Random Forest Regressor
explainer = shap.TreeExplainer(best_reg)
shap_values = explainer.shap_values(X_test_reg)
```

In [16]:
```
# Generate a SHAP summary plot to visualize feature impact on model output
shap.summary_plot(shap_values, features=X_test_reg, feature_names=features)
```



Conclusion

1. Feature Impact: The analysis revealed that certain features, such as alcohol content and volatile acidity, have a significant impact on wine quality. Both feature importance and SHAP analysis consistently highlighted these variables as key drivers in predicting wine quality.

2. Model Performance: Ensemble models like Random Forest and XGBoost outperformed simpler models in both regression and classification tasks, demonstrating the value of using advanced machine learning techniques for complex, real-world datasets like wine quality prediction.