ESE 417 Final Project Classification of Wine Quality by Machine Learning

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I. Introduction

Machine learning is a branch of artificial intelligence that enables machines to learn from data and make predictions or decisions without being explicitly programmed. It finds applications in a wide range of domains such as image recognition, natural language processing, and predictive modeling. In this project, we aim to use supervised machine learning algorithms to classify a wine quality data set based on 11 given features. While wine was once viewed as a luxury good, it is now enjoyed by a wider range of consumers. Quality evaluation is a crucial part of the certification process and can help to identify influential factors during the wine production process [citation 1]. In our project, these factors will be used as features for our machine learning algorithm.

The primary objective of this project is to build a machine learning model that can accurately predict the quality of wine into 10 different levels with the given data. Furthermore, we aim to compare the performance of different machine learning algorithms such as Support Vector Machines (SVM), K-Nearest Neighbors (KNN), and Random Forest to determine the most effective algorithm for this task. To improve the accuracy of our model, we have implemented various methods of data cleaning, chosen optimal weight factors, and tuned other hyperparameters.

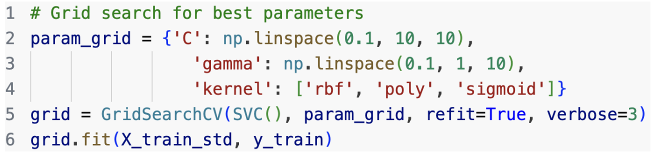
After multiple testing and trial and error iterations, the model was able to achieve an accuracy rate of over 60 percent. Overall, this project demonstrates the effectiveness of supervised machine learning algorithms in predicting the quality of wine based on various influential factors during the production process.

II. Methods

A. Exploratory Data Analysis and Cleaning

B. Grid Search and Weighted Features

Grid search is a widely used hyperparameter optimization technique in machine learning that involves systematically evaluating a range of hyperparameters for a given model. This technique entails creating a grid of all possible combinations of hyperparameters and training a model for each combination. The optimal combination of hyperparameters is then determined by selecting the one that yields the highest accuracy or lowest error rate, depending on the specific problem being addressed.
In the present project, grid search was employed to fine-tune the hyperparameters of the Support Vector Machine (SVM) model. Specifically, the hyperparameters C and gamma were tuned using grid search to optimize the model's performance. These two hyperparameters are of particular importance in determining the efficacy of the SVM model in handling the data at hand.
To accomplish this, a two-stage approach was used, where a broad range of C and gamma values was initially explored, followed by a more focused search of a smaller region to identify the optimal values for these hyperparameters. The implementation of the grid search algorithm used in this project is presented below:



```python
# Grid search for best parameters
param_grid = {'C': np.linspace(0.1, 10, 10),
                'gamma': np.linspace(0.1, 1, 10),
                'kernel': ['rbf', 'poly', 'sigmoid']}
grid = GridSearchCV(SVC(), param_grid, refit=True, verbose=3)
grid.fit(X_train_std, y_train)
```

Fig. 1. Grid Search Code

C. SVM

The Support Vector Machine (SVM) is a supervised machine learning algorithm that has gained popularity for its success in various classification tasks, including wine quality classification. SVM works by identifying a decision boundary that effectively separates the different categories of wine quality in the feature space.

To classify the wine quality, the SVM requires input features such as alcohol content, acidity, sugar content, and other sensory attributes. The objective of the SVM is to find a hyperplane or a linear decision boundary that can best separate the various quality categories of wine samples in the feature space. The dimensionality of this hyperplane is higher than the dimensionality of the data, and it is determined by selecting a marginal maximization hyperplane. This approach ensures that the SVM classifier is robust by calculating the distance between the hyperplane and the nearest data point for each quality category.

However, in cases where the data is not linearly separable, SVMs utilize kernel functions to transform the data to a higher dimensional space, which makes it linearly separable. Among the commonly used kernel functions for wine quality classification are linear, polynomial, radial basis function (RBF), and sigmoid kernels. These kernels map the data into a new feature space, where the SVM can find a hyperplane that separates the different quality categories with a good margin.

The SVM model trained without performing any cleaning on the data obtained an accuracy of 57%. However, after cleaning the data, the accuracy improved to 63%. The SVM model's default parameters were $kernel =' rbf', C = 1.0, randomstate = 0, degree = 3, gamma =' auto'$. After normalizing the data, the researchers retrained the model, which improved the accuracy from 57% to 61%. To further improve the model's accuracy, grid search was used for tuning the hyperparameters, where they varied C from 0.1 to 10 and gamma from 0.1 to 1 using three kernel functions, namely rbf, poly, and sigmoid. The best parameters for the grid search were found to be 'C': 2.3, 'gamma': 0.7, 'kernel': 'rbf', which increased the accuracy from 61% to 63%. The researchers then refined the grid search by narrowing down C from 1.8 to 2.8 and gamma from 0.6 to 0.8, leading to the final optimal hyperparameters of 'C': 2.326, 'gamma': 0.705, 'kernel': 'rbf'.

D. Random Forest

Random Forest is an ensemble learning algorithm that is used for classification tasks. It works by constructing multiple decision trees and then combining their predictions to make a final prediction. The algorithm randomly selects a subset of features and a subset of training samples for each decision tree, which helps to reduce overfitting and improve the performance of the model.Also, to simplify the process, the sklearn method of RandomForestClassifier() is used to classify the wine quality. (sklearn). There are eleven features imputed to the ML algorithm. Because the correlation of the wine quality is more related to some features than others, the features need to be considered differently while imputed into the machine learning algorithm. Here are the weights for each feature used in the program :1: 10, 2: 10, 3: 69, 4: 1, 5: 1, 6: 1, 7: 1, 8: 34, 9: 10, 10: 10, 11: 80. Those weights are estimated from the input importance of the people originally conducting the experiments.
Due to their great variety of hyperparameters, to optimize the accuracy of the method four are used which are $nestimators, maxdepth, randomstate, classweight$.
The grid search is implemented to come up with the best combination of the hyperparameters, $'maxdepth' : 15,' nestimators' : 700$. With given depth and number of estimators the Machine learning algorithm would output the best performances.

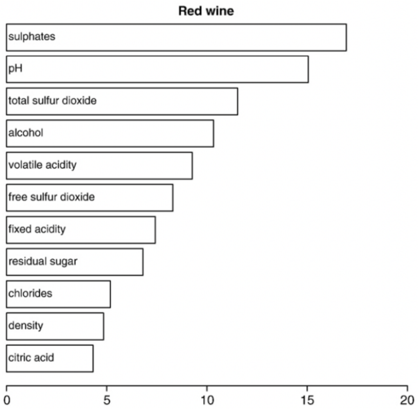


Fig. 2. Red Wine Weight

III. Result and Analysis

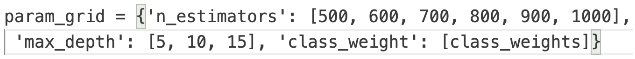
Implementing the three method mentioned above shows Random Forest does the best in all the methods.

A. KNN

B. SVM

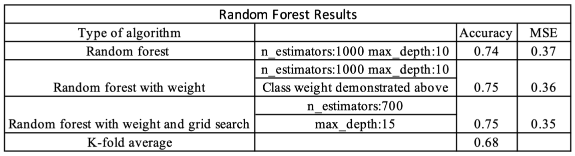
C. Random Forest

The grid search parameters demonstrated as following: After trials and errors, the features with the most importance are citric acid and alcohol. The density of the wine still has some weight impact to the wine but not as much. The other variables are not as important. Even the consideration chlorides, free sulfur dioxide and total sulfur dioxide would disrupt the judgment of the algorithm and lower the accuracy of the classification.
(1: 10, 2: 10, 3: 69, 4: 1, 5: 1, 6: 1, 7: 1, 8: 34, 9: 10, 10: 10, 11: 80)
All method used the random state of 3



```
param_grid = {'n_estimators': [500, 600, 700, 800, 900, 1000],
 'max_depth': [5, 10, 15], 'class_weight': [class_weights]}
```

Fig. 3. Random Forest Grid Search Code



Random Forest Results			
Type of algorithm		Accuracy	MSE
Random forest	n_estimators:1000 max_depth:10	0.74	0.37
Random forest with weight	n_estimators:1000 max_depth:10 Class weight demonstrated above	0.75	0.36
Random forest with weight and grid search	n_estimators:700 max_depth:15	0.75	0.35
K-fold average		0.68	

Fig. 4. Random Forest Result