**Project Name:** Classifying Wine Using Logistic Regression and SVM Models

**Course:** PROG39051 Machine Learning Techniques

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## Introduction

“An alcoholic beverage derived from fermented grapes is called wine.” (Mani, Krishnankutty, Swaminathan, & Theerthagiri, 2023) In the world of winemaking, each bottle of wine is a piece of art. Hence, it is essential to understand the quality and the making of this wine, which is a challenge and considered to be a multi – faceted problem. However, to solve this problem, which is usually very expensive, we decided to work on a project that intricately focuses on using a machine learning model to classify wine, based on its quality and its chemical formulations. This view would help to perform a more efficient assessment of wine quality.

## Literature Review

As we’ve heard, the older the wine the better it tastes. When it comes to wine quality there are several elements that need to be taken into consideration. “To judge the quality of wine we need to understand the correlation among the wine elements.” (Trivedi & Sehrawat, 2018) The main goal of this research project is to understand and predict the quality of wine as good or bad. We selected Logistic Regression and Support Vector Machines (SVM) for our project based on the effectiveness in classification tasks and multi – class classification.

**Support Vector Machines (SVM)**

Support Vector Machines constitute a well-known family of algorithms utilized for classification and regression tasks. One major advantage of SVM is its ability to maintain learning capacity even with a high number of features. This classifier transforms examples into points within an n-dimensional space through non-linear transformations. Subsequently, SVM seeks to find the hyperplane that maximizes the distance between points from positive and negative classes (Gómez-Meire et al., 2014.) In other words, the core concept of SVM relies on the kernel function to discover the hyperplane capable of separating instances into categories. There are two pivotal hyperparameters in SVM, namely the penalty factor C and the choice of kernel function.

**C**: This parameter serves as a regularization parameter that balances maximizing the margin and minimizing training error.

**Kernel**: the kernel parameter, with options including linear, polynomial (poly), and radial basis function (rbf), plays a critical role in finding the optimal separation for various datasets (Del Bimbo et al., 2021).

**Logistic Regression**

Logistic Regression is a statistical technique used to analyze datasets where one or more independent variables lead to a result. Often employed for binary classification, Logistic Regression predicts the likelihood of an event occurring by fitting data to a logistic or sigmoid function (Mani et al., 2023). In Logistic Regression, three primary hyperparameters are vital:

**Solver:** This specifies the algorithm used in the optimization problem. Options include {‘newton-cg’, ‘lbfgs’, ‘liblinear’, ‘sag’, ‘saga’}, with the default being 'lbfgs'.

**Penalty** (Regularization): Intended to reduce model generalization error, the penalty discourages and regulates overfitting. Options for the penalty are {‘l1’, ‘l2’, ‘elasticnet’, ‘none’}, with the default being 'l2'.

**C** (Regularization Strength): Collaborating with the penalty term, C helps control overfitting. Lower values indicate stronger regularization, while higher values instruct the model to give greater weight to the training data (Gusarov, 2022).

The features included in our dataset are:

1. Alcohol
2. Malic Acid
3. Ash
4. Magnesium
5. Total phenols
6. Flavonoids
7. Non – Flavonoid phenols
8. Proanthocyanins
9. Color intensity
10. Hue
11. Total phenols
12. . OD280/OD315 of diluted wines
13. Proline

Quality is a highly essential ingredient for the success of any company, selling any kind of products to the public. Therefore, it is essential that optimal care is taken to measure the quality of the product, in our – wine. The features we listed above are essential to offer a comprehensive view of the dataset, and through the project we will analyze the various relationships between these features and how they affect the type of wine. “As the demand for wine is drastically increasing these days, the urge to better estimate its quality has become the need of the hour.” (Tingwei, 2021)

## Implementation

### Data Loading and Understanding

The first step in the implementation is to load the dataset and gain a comprehensive understanding of its structure and contents.

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### Data Preprocessing

Data preprocessing is a vital step that ensures the accuracy, completeness, and relevance of data for analysis or machine learning models. These tasks involve several key processes:

#### Data Cleaning:

Data cleaning involves addressing issues like missing data, duplicates, and outliers, which can impact analysis or model training.

##### Handling missing data

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The dataset does not have any missing data.

##### Handling duplicated data

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The dataset does not have any duplicated data.

##### Handling outliers

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A group of yellow rectangular objects

Description automatically generated with medium confidence

The boxplot displays some unusual data points, marked by the small circles, in 'Ash', 'Alcalinity\_of\_ash', 'Magnesium', 'Proanthocyanins', and 'Color\_intensity'. These points are positioned more than 1.5 times the interquartile range (IQR) away from the quartiles, indicating they might be outliers.

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#### Handling class imbalances

Class imbalances occur when the distribution of values for the class is not uniform, potentially leading to biased model performance. Techniques such as oversampling, undersampling, or adjusting class weights are commonly used to address this imbalance. For this project, the 'oversampling' technique will be employed due to the small dataset size (only 161 rows).

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#### Feature Selection

Feature selection is essential for reducing model complexity, overfitting, and training time.

When deciding on a feature selection method, we need to consider various factors, including dataset characteristics, computational cost, and modeling objectives.

**Correlation Matrix with Heatmap:** Inappropriate for our categorical target variable.

**RFE (Recursive Feature Elimination):** Not ideal for our two selected machine learning algorithms.

**SelectKBest:** Efficient and straightforward, suitable for quick feature selection.

**ExtraTreesClassifier:** Offers insights into feature importance and handles non-linear relationships well, aligning with our goal of creating logistic regression and SVC classifiers for wine type classification.

Considering our categorical target variable and the requirements of our logistic regression and SVC models, we've chosen ExtraTreesClassifier for feature selection.

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#### Data Transformation - Normalization:

Before building the model, it's essential to normalize the data since the unit of measurement might differ across features. This process ensures that all features contribute equally to the model. Here are the two steps involved:

- Step1: Visualize the distribution of each numerical column using a histogram to assess its normality. Look for a bell curve shape, which indicates a Gaussian distribution.

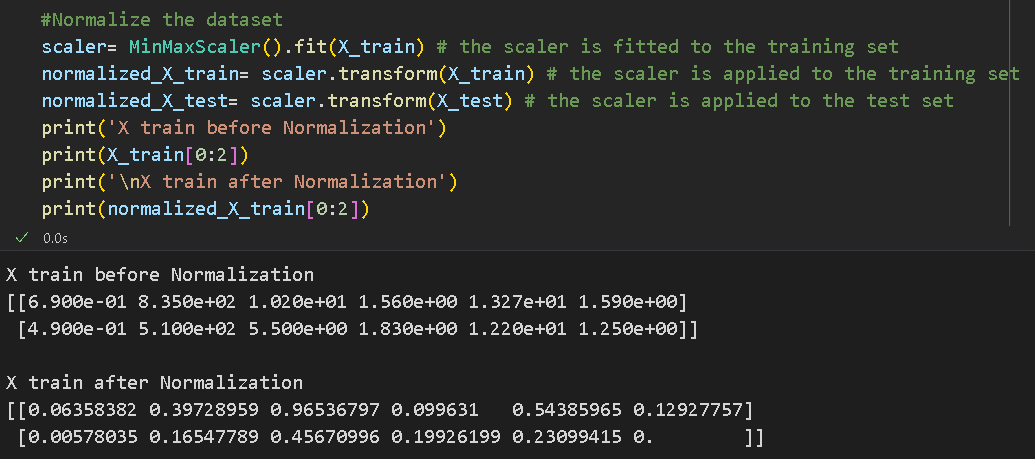
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A graph of different columns

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- Step2 Normalize the features based on the observed distribution. Since all columes exhibit non-Gaussian distributions, Min-Max Normalization will be applied to these columns.



### Model Building

#### Logistic Regression Model Building

For building the Logistic Regression model, I used the LogisticRegression from sklearn library, initializing with the following hyperparameters:

**max\_iter:** This parameter specifies the maximum number of iterations for the solver to converge. In this project, I chose the default value of 200 for simplicity.

**penalty:** 'l2' is a common choice for Logistic Regression and is the default in scikit-learn. It helps with regularization.

**C:** The default value of 1.0 is chosen for C, controlling the regularization strength. Since the dataset is not extremely large or small, the default is suitable.

**solver:** 'lbfgs' is suitable for small datasets like this project.

**random\_state:** I set the random\_state to a fixed seed (42) for reproducibility and to ensure consistent results across runs.

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#### SVM Model Building

For building the SVM model, I used the SVC Classifier from sklearn library, initializing with the following hyperparameters:

**kernel:** 'rbf' is a good default choice for non-linear classification problems. It can handle complex relationships between features.

**C:** The default value of 1.0 is chosen for C, controlling the regularization strength. Since the dataset is not extremely large or small, the default is suitable.

**random\_state:** I set the random\_state to a fixed seed (42) for reproducibility and to ensure consistent results across runs.

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## Evaluation

#### Logistic Regression Model Building

##### Evaluate the model using a confusion matrix.

A confusion matrix is a matrix that breaks down correctly and incorrectly classified into: True positive (TP): Correctly predicting the positive class. True Negative (TN): Correctly predicting the negative class. False Positive (FP): Incorrectly predicting the positive class.

A diagram of positive and negative

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The confusion matrix shows the following:

* Rows correspond to the actual classes.
* Columns correspond to the predicted classes.
* The diagonal elements (top-left to bottom-right) represent the number of correct predictions for each class.
* Off-diagonal elements represent incorrect predictions (Evidently AI, n.d.).

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**Confusion Matrix:** both the train and test confusion matrix show high accuracy in classifying samples as there are only two misclassifications on the training data and test data.

##### Evaluate the model using an accuracy score.

The accuracy score calculates the accuracy by comparing the predicted labels to the true labels and returns a value between 0 and 1, where 1 indicates perfect accuracy. The model has achieved high accuracy on both the training and test data, which suggests that it is performing well and generalizing effectively to unseen data.

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**Accuracy:** The accuracy scores of 98% on the training set and 96% on the test set indicate that the Logistic Regression model performs exceptionally well in both training and unseen data.

##### Evaluate the model using a classification\_report

The classification\_report function provides a detailed report with various metrics such as precision, recall, and F1-score for each class in the classification. These metrics are commonly used to evaluate the model's performance.

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**Classification Report:** The precision, recall, and F1-score metrics provide a detailed view of the model's performance for each class. The weighted average F1-score of 0.96 for the test set demonstrates a strong overall performance.

#### SVM Model Building

##### Evaluate the model using a confusion matrix.

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**Confusion Matrix:** both the train and test confusion matrices show high accuracy in classifying samples as there is only one misclassification on the training data.

##### Evaluate the model using an accuracy score.

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**Accuracy:** The accuracy scores of 0.99 on the training set and 1.0 on the test set indicate that the SVM model performs exceptionally well in both training and unseen data.

##### Evaluate the model using a classification\_report

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**Classification Report:** The precision, recall, and F1-score metrics provide a detailed view of the model's performance for each class. The weighted average F1-score of 1.0 for the test set demonstrates a strong overall performance.

#### Compare Logistic Regression Model and SVM Model

Based on the evaluation metrics for both the Logistic Regression and SVM models:

* Confusion Matrix:
* Logistic Regression: The confusion matrix for both the training and test sets shows high accuracy, with only two misclassifications in the training data and the test data.
* SVM: The confusion matrix for both the training and test sets also shows high accuracy, with only one misclassification in the training data.
* Accuracy Score:
* Logistic Regression: Achieved an accuracy score of 0.99 on the training set and 0.96 on the test set. This indicates that the Logistic Regression model performs exceptionally well on both the training and unseen data.
* SVM: Achieved an accuracy score of 0.99 on the training set and 1.0 on the test set. Similar to the Logistic Regression model, the SVM model performs exceptionally well on both the training and unseen data.
* Classification Report:
* Logistic Regression: The precision, recall, and F1-score metrics from the classification report show a strong overall performance. The weighted average F1-score of 0.96 for the test set indicates high precision and recall.
* SVM: The precision, recall, and F1-score metrics from the classification report also show a strong overall performance. The weighted average F1-score of 1.0 for the test set indicates high precision and recall.

In summary, both the Logistic Regression and SVM models demonstrate excellent performance in classifying wine types based on their chemical attributes. They have high accuracy scores, minimal misclassifications in the confusion matrices, and strong precision, recall, and F1-scores according to the classification reports. However, the SVM model shows slightly better performance compared to the Logistic Regression model.

## Conclusion

In conclusion, our research project has been successfully able to achieve and demonstrate the effectiveness of employing Machine Learning models: Logistic Regression and Support Vector Machines (SVMs) to assess the quality of various wine samples based on their chemical formulations. Both the models have shown high accuracy levels and strong performance metrics, in confusion matrices, accuracy, and classification reports. The Regression model provided us with excellent results of an F1 – score of 0.96 for the test set, while the SVM gave us slightly better results with an F1 – score of 1.0, which is indicative of exceptional precision and recall.

These findings help us to understand the potential of Machine Learning Algorithms and the impact they can have to revolutionize the traditional methods of quality assurance in the wine industry. By automating the evaluation process, these models help enhance the quality and accuracy of wine tasting but also reduce the cost, energy, and time which goes into manual assessments.

Our research can help serve as a pathway for potential learnings for future exploration into the application and usage of machine learning across various domains where quality and compositions can be assessed, and results can be analyzed. Therefore, these models can be considered as a significant way to move forward to ensure the consistent production of high – quality and well – made wines, meeting both the customers’ expectations and the high industry standards.

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