Machine Learning

Topic: Wine Quality Predictor (Classification)

NOTE: This notebook is where the data was analyzed and the predictive models were built for the app. For App source code, click blue text below:

Source Code

Introduction

Vinho Verde refers to Portuguese wine that originated in the historic Minho province in the far north of the country. The name means "green wine," but translates as "young wine", with wine being released three to six months after the grapes are harvested. They may be red, white, or rosé, and they are usually consumed soon after bottling.

In this project we look at two datasets related to red and white Vinho Verde wine samples, from the north of Portugal. Both datasets will be combined into one for easier analysis and the goal will be to create a predictive model for wine quality adn type based on physicochemical tests.

This data is publicly available for research purposes at the UC Irvine Machine Learning Repository and can be found here:

DATASETS.

Required Libraries ...

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
import shap
from sklearn import preprocessing
from sklearn.metrics import confusion_matrix
from sklearn.model_selection import train_test_split
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import accuracy_score
```

```
from sklearn.linear_model import LogisticRegression

from sklearn.svm import SVC

from sklearn.tree import DecisionTreeClassifier

from sklearn.neighbors import KNeighborsClassifier

import warnings
%load_ext watermark
```

In [2]: warnings.filterwarnings("ignore")

Datasets

Red Wine Data ...

Out[3]:		type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides		total sulfur dioxide	density	рН	sulphates	alcoho
	0	Red	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.
	1	Red	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.
	2	Red	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.

White Wine Data ...

Out[4]:		type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide		density	рН	sulphates	alcoł
	0	White	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	{
	1	White	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9
	2	White	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	1(

Combining the Datasets ...

```
types = [red, white]
In [5]:
        wine = pd.concat(types)
        wine.reset_index(drop = True, inplace = True)
```

Descriptive Analytics

```
In [6]: wine.isnull().sum()
                                0
Out[6]: type
                                0
        fixed acidity
                                0
        volatile acidity
        citric acid
                                0
        residual sugar
        chlorides
        free sulfur dioxide
        total sulfur dioxide
        density
                                0
                                0
        рΗ
        sulphates
                                0
        alcohol
                                0
                                0
        quality
        dtype: int64
```

In [7]: wine.describe().transpose()

Out[7]:

		count	mean	std	min	25%	50%	75%	max
-	fixed acidity	6497.0	7.215307	1.296434	3.80000	6.40000	7.00000	7.70000	15.90000
	volatile acidity	6497.0	0.339666	0.164636	0.08000	0.23000	0.29000	0.40000	1.58000
	citric acid	6497.0	0.318633	0.145318	0.00000	0.25000	0.31000	0.39000	1.66000
	residual sugar	6497.0	5.443235	4.757804	0.60000	1.80000	3.00000	8.10000	65.80000
	chlorides	6497.0	0.056034	0.035034	0.00900	0.03800	0.04700	0.06500	0.61100
	free sulfur dioxide	6497.0	30.525319	17.749400	1.00000	17.00000	29.00000	41.00000	289.00000
	total sulfur dioxide	6497.0	115.744574	56.521855	6.00000	77.00000	118.00000	156.00000	440.00000
	density	6497.0	0.994697	0.002999	0.98711	0.99234	0.99489	0.99699	1.03898
	рН	6497.0	3.218501	0.160787	2.72000	3.11000	3.21000	3.32000	4.01000
	sulphates	6497.0	0.531268	0.148806	0.22000	0.43000	0.51000	0.60000	2.00000
	alcohol	6497.0	10.491801	1.192712	8.00000	9.50000	10.30000	11.30000	14.90000
	quality	6497.0	5.818378	0.873255	3.00000	5.00000	6.00000	6.00000	9.00000

Exploratory Analytics

Correlation Plots

```
fig = plt.figure(figsize=(15,5))
In [8]:
            grid = fig.add gridspec(1,3)
            ax0 = fig.add_subplot(grid[0,0])
            sns.heatmap(red.corr(), cmap='coolwarm', annot=False, ax=ax0)
            ax0.set title('Red Wine Correlation')
            ax1 = fig.add_subplot(grid[0,1])
            sns.heatmap(white.corr(), cmap='coolwarm', annot=False, ax=ax1)
            ax1.set_title('White Wine Correlation')
            ax2 = fig.add subplot(grid[0,2])
            sns.heatmap(wine.corr(), cmap='coolwarm', annot=False, ax=ax2)
            ax2.set_title('Overall Correlation')
            plt.tight_layout()
                           Red Wine Correlation
                                                                     White Wine Correlation
                                                                                                                Overall Correlation
                                                 1.0
               fixed acidity
                                                         fixed acidity
                                                                                                   fixed acidity -
                                                                                           - 0.8
                                                 - 0.8
                                                                                                                                     - 0.8
              volatile acidity
                                                        volatile acidity
                                                                                                  volatile acidity
                 citric acid
                                                           citric acid
                                                                                                     citric acid
                                                                                           0.6
                                                        residual sugar
               residual sugar
                                                                                                  residual sugai
                                                                                           0.4
                                                 0.4
                                                                                                                                     0.4
                 chlorides
                                                           chlorides
                                                                                                     chlorides
            free sulfur dioxide
                                                      free sulfur dioxide
                                                                                           - 0.2
                                                                                                free sulfur dioxide
                                                 - 0.2
                                                                                                                                     0.2
            total sulfur dioxide
                                                      total sulfur dioxide
                                                                                               total sulfur dioxide
                                                 0.0
                                                           sulphates
                                                  -0.4
                                                             alcohol
                                                                                                      alcohol
```

The variable with the highest correlation to the quality score is 'alcohol' across all three dataframes. The weakest correlation overall appears to be density.

By Type

```
In [9]: fig = plt.figure(figsize=(15,5))
grid = fig.add_gridspec(1,3)

ax0 = fig.add_subplot(grid[0,0])
sns.countplot(data=wine, x='type', ax=ax0)
ax0.bar_label(ax0.containers[0])

ax1 = fig.add_subplot(grid[0,1])
sns.boxplot(data=wine, x="quality", y='type', ax=ax1)

ax2 = fig.add_subplot(grid[0,2])
sns.countplot(data=wine, x="quality", hue="type", ax=ax2)
for container in ax2.containers:
    ax2.bar_label(container)
```

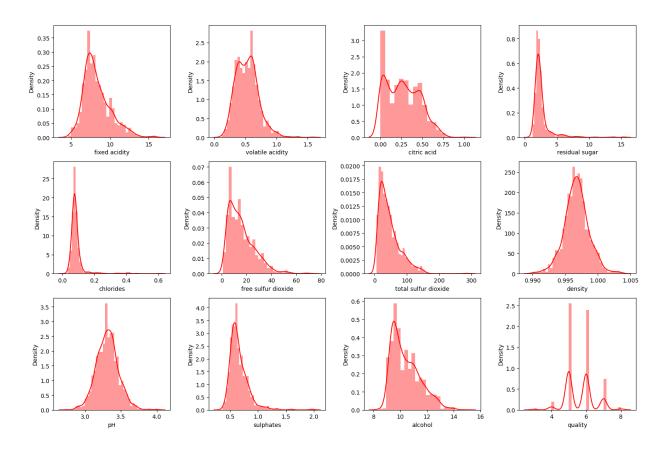
plt.tight_layout() 5000 4898 Red Red White White White White White White White White Ped White Whit

- In the charts above, we learn that the overwhelming majority of the samples in the dataset is white wine, totaling just a little over three times the amount of white wine.
- The median score between the two wine types is between 5 and 6, with the highest scores being 9 and 8 for white and red wine, respectively. The lowest for both is a score of 3.
- The majority of red wines had a quality score of 5, while the majority of white wines had a score of 6.

Red Wine Distributions

```
In [10]: plt.figure(figsize = (15,10))

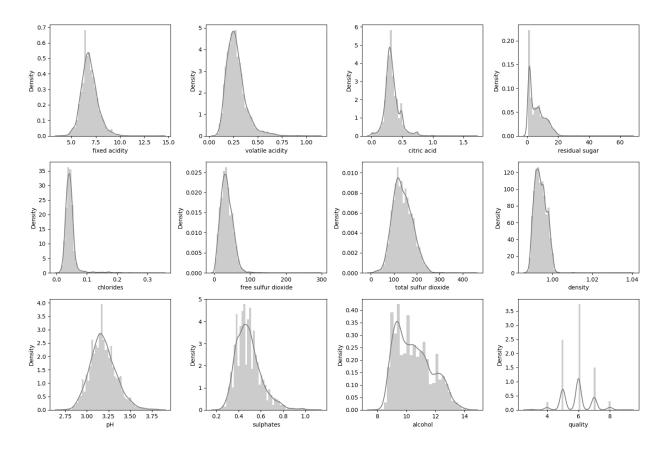
for i in range(1,13):
    plt.subplot(3,4,i)
    sns.distplot(red[red.columns[i]],color='red')
    plt.tight_layout()
```



White Wine Distributions

```
In [11]: plt.figure(figsize = (15,10))

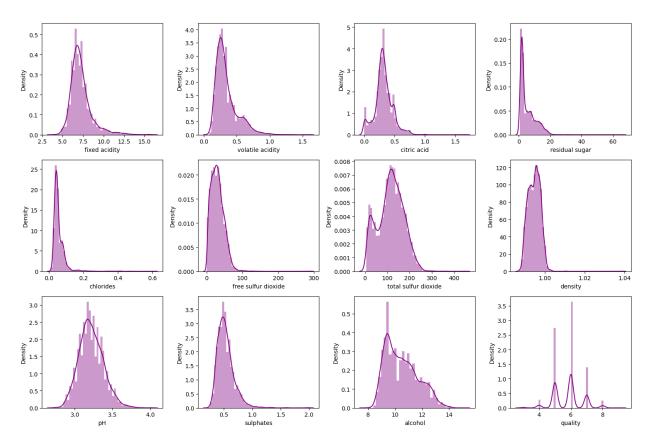
for i in range(1,13):
    plt.subplot(3,4,i)
    sns.distplot(white[white.columns[i]], color='gray')
    plt.tight_layout()
```



Overall Distributions

```
In [12]: plt.figure(figsize = (15,10))

for i in range(1,13):
    plt.subplot(3,4,i)
    sns.distplot(wine[wine.columns[i]],color='purple')
    plt.tight_layout()
```



The above distribution plots point to outliers being present in our dataset. We will keep this in mind for later when we are ready to build our models.

Ranking Quality Scores

In this section we will split the 'quality' column into 3 bins labeled 'Low', 'Medium', and 'High' and each value of 'quality' will receive a corresponding label.

```
In [13]: group_names=['Low','Medium','High']
bin = pd.cut(wine['quality'], 3, labels=group_names)
wine['quality'] = bin
wine
```

		_		_
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\cup	ич	1 4	. –	

•		type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	рН	sulphates	а
	0	Red	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.99780	3.51	0.56	
	1	Red	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.99680	3.20	0.68	
	2	Red	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.99700	3.26	0.65	
	3	Red	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.99800	3.16	0.58	
	4	Red	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.99780	3.51	0.56	
	•••												
	6492	White	6.2	0.21	0.29	1.6	0.039	24.0	92.0	0.99114	3.27	0.50	
	6493	White	6.6	0.32	0.36	8.0	0.047	57.0	168.0	0.99490	3.15	0.46	
	6494	White	6.5	0.24	0.19	1.2	0.041	30.0	111.0	0.99254	2.99	0.46	
	6495	White	5.5	0.29	0.30	1.1	0.022	20.0	110.0	0.98869	3.34	0.38	
	6496	White	6.0	0.21	0.38	0.8	0.020	22.0	98.0	0.98941	3.26	0.32	

6497 rows × 13 columns

Low 2384 High 198

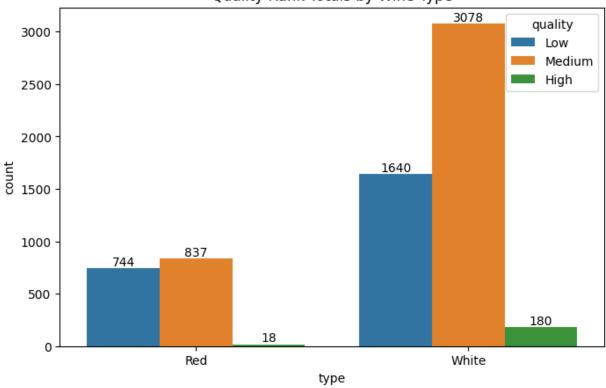
Name: quality, dtype: int64

This split for the quality scores makes sense as it makes high ranking wines few and far between while the large majority of the dataset is Medium to Low rank.

```
In [15]: plt.figure(figsize=(8,5))

counts = sns.countplot(x = 'type', hue = 'quality', data = wine)
for container in counts.containers:
        counts.bar_label(container)
plt.title('Quality Rank Totals by Wine Type')
plt.show()
```





Transforming Categorical Features

Now that we have ranked our quality scores we can create dummy variables for this column and the 'type' column in order to have a completely numeric dataset for our classification models.

Reassignment for quality ranks ...

```
In [16]: quality = {"Low" : 0,"Medium": 1,"High" : 2}
wine["quality"] = wine["quality"].map(quality)
wine.head()
```

Out[16]:

	type	fixed acidity	volatile acidity		residual sugar	chlorides	free sulfur dioxide		density	рН	sulphates	alcoho
0	Red	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.
1	Red	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.
2	Red	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.
3	Red	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.
4	Red	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.

Reassignment for wine type ...

```
In [17]: type_ = {"Red" : 0, "White": 1}
wine["type"] = wine["type"].map(type_)
```

wine.head()

Out[17]:		type	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide		density	рН	sulphates	alcoho
	0	0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.
	1	0	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.
	2	0	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.
	3	0	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.
	4	0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.
													•

Split and Scale

This split will be used to predict quality ...

```
In [18]: X = wine.drop(['quality'],axis=1)
Y = wine['quality']
```

And this split will be used to predict type ...

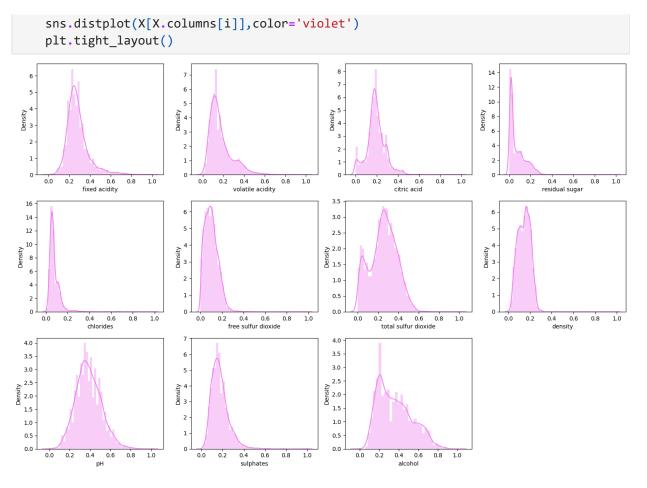
We began here by splitting our dataset into independent (X) and dependent (Y) variables to fit onto our models.

After having done this we scaled the independent variables, this means that the data was transformed so that it all fits within a specific scale like, in this case, 0-1. This will be useful for our data since our features exhibit a wide range of values. For example, the highest value for Total Sulfur Dioxide was 440 but for Chlorides the highest value was a mere 0.6.

By scaling our variables, it will help compare different variables on equal footing while also improve the performance of our machine learning algorithms, as they often perform better with data that is in a common range.

```
In [22]: plt.figure(figsize = (15,10))

for i in range(1,12):
    plt.subplot(3,4,i)
```



^ here we can see that all values for each feature falls between 0 and 1.

Now we will split the independent and dependent variables into training and test sets for our models.

```
In [23]:
         X_train, X_test, Y_train, Y_test = train_test_split(X,Y, test_size = 0.2, random_state
         X2_train, X2_test, Y2_train, Y2_test = train_test_split(X2,Y2, test_size = 0.2, random
In [24]:
         80% of our data will be used to train our models and the remaining 20% will be used for testing.
In [25]:
         print("The shape of X_train is:", X_train.shape)
         print("The shape of X_test is:", X_test.shape)
         print("The shape of Y_train is:", Y_train.shape)
         print("The shape of Y_test is:", Y_test.shape)
         The shape of X_train is: (5197, 12)
         The shape of X test is: (1300, 12)
         The shape of Y train is: (5197,)
         The shape of Y_test is: (1300,)
         print("The shape of X_train is:", X2_train.shape)
         print("The shape of X_test is:", X2_test.shape)
         print("The shape of Y_train is:", Y2_train.shape)
         print("The shape of Y_test is:", Y2_test.shape)
```

```
The shape of X_train is: (5197, 12)
The shape of X_test is: (1300, 12)
The shape of Y_train is: (5197,)
The shape of Y test is: (1300,)
```

Predictive Models for Wine Quality

Finally, we have arrived at the best part. We will begin to build and tune our predictive models here.

For this project I will focus on four classification algorithms from the sklearn library :

- Logistic Regression
- Support Vector Classifier
- Decision Tree Classifier and
- K-Neighbours Classifier

Before that lets build a function to plot the confusion matrix for each model as we go along for better visualization.

```
def plot_confusion_matrix(y,y_predict):
    cm = confusion_matrix(y, y_predict)
    ax= plt.subplot()
    sns.heatmap(cm, cmap='coolwarm',annot=True,fmt = " ", ax = ax);
    ax.set_xlabel('Predicted labels')
    ax.set_ylabel('True labels')
    ax.set_title('Confusion Matrix');
    ax.xaxis.set_ticklabels(['Low','Medium','High']); ax.yaxis.set_ticklabels(['Low','Medium','High']);
```

Logistic Regression

```
In [28]: lr = LogisticRegression()
    lr.fit(X_train,Y_train)
    accuracy = lr.score(X_test, Y_test)
    print('Log Regression Accuracy:',(accuracy*100).round(2),'%')
```

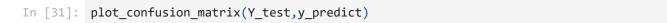
Log Regression Accuracy: 70.69 %

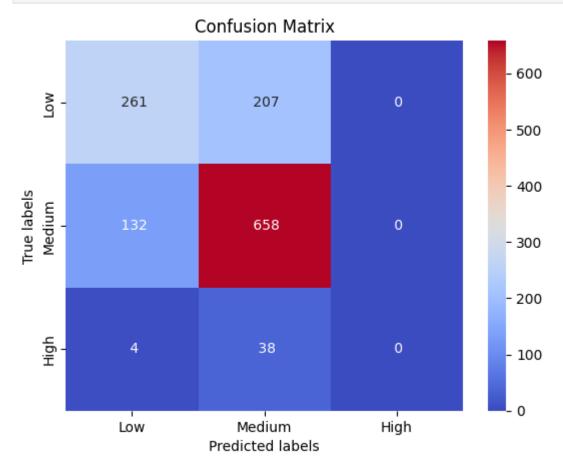
Our Logisitic Regression model gave us a preliminary accuracy score of 70.69%, which is quite low. Let's tune our model to see if we can improve on that number.

```
Best Parameters : {'C': 1, 'penalty': 'l2', 'solver': 'lbfgs'}
GridSearch Score : 71.48 %
```

Tuned Logistic Regression Model Accuracy: 70.69 %

Our tuned model returned the same preliminary score and below is the confusion matrix for the 1300 samples in the test set.





Support Vector Machine

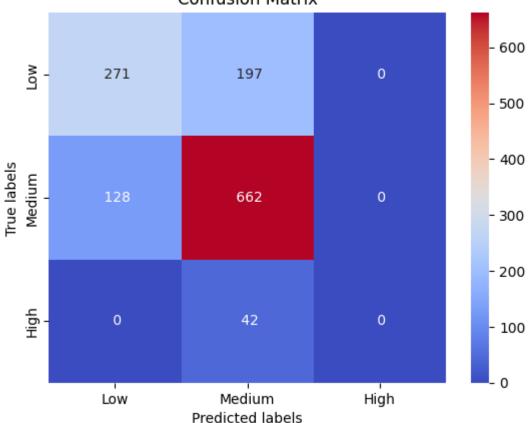
```
In [32]: svm = SVC()
    svm.fit(X_train,Y_train)
    accuracy = svm.score(X_test, Y_test)
    print('Support Vector Accuracy:',(accuracy*100).round(2),'%')
```

Support Vector Accuracy: 72.0 %

Our Support Vector model gave us a preliminary accuracy score of 72%, which is slightly better than the Log Regression model but still low. Let's tune our model to see if we can improve on that number.

```
In [33]: svm_params = {'C':[0.01,0.1,1],
                        'kernel':['linear', 'rbf','poly','sigmoid'],
                        'degree':[2,3,4,5],
                        'decision_function_shape':['ovo', 'ovr'],
                        'gamma':[0.01,0.1,1.0]}
         svm_cv = GridSearchCV(svm,svm_params,cv=5)
         svm_cv.fit(X_train, Y_train)
         print("Best Parameters :",svm_cv.best_params_)
         print("GridSearch Score:",(svm_cv.best_score_*100).round(2),'%')
         Best Parameters : {'C': 1, 'decision_function_shape': 'ovo', 'degree': 5, 'gamma': 1.
         0, 'kernel': 'poly'}
         GridSearch Score: 72.46 %
In [34]: y_predict=svm_cv.best_estimator_.predict(X_test)
         print("Tuned Logistic Regression Model Accuracy:",
               (accuracy_score(Y_test, y_predict)*100).round(2),'%')
         Tuned Logistic Regression Model Accuracy: 71.77 %
In [35]:
         plot_confusion_matrix(Y_test,y_predict)
```

Confusion Matrix



Decision Tree

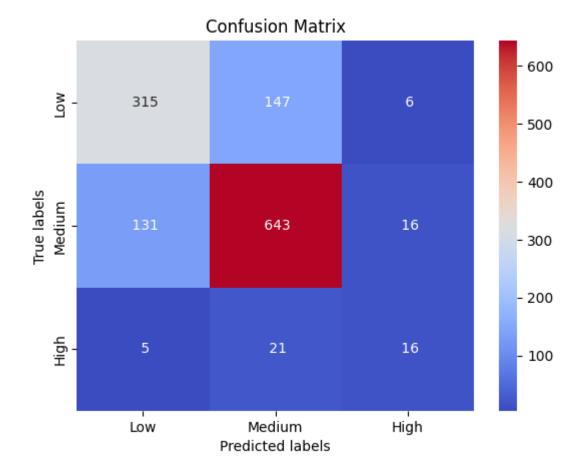
```
In [36]: tree = DecisionTreeClassifier()
    tree.fit(X_train,Y_train)
```

```
accuracy = tree.score(X_test, Y_test)
print('Decision Tree Accuracy:',(accuracy*100).round(2),'%')
```

Decision Tree Accuracy: 73.31 %

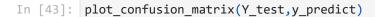
Our decision tree model gave us a slightly higher preliminary accuracy score than the previous two models but we are still stuck in the low 70's.

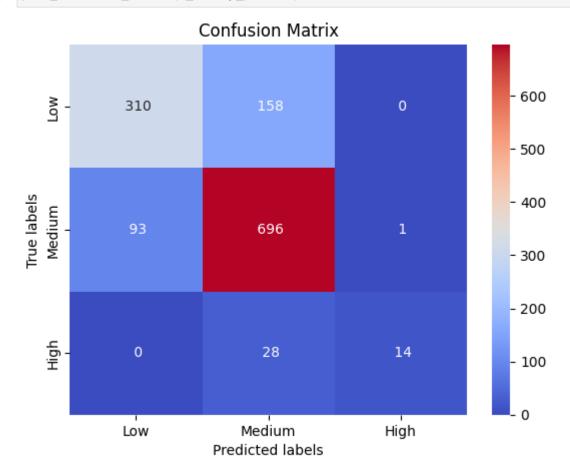
```
In [37]: tree_params = {'criterion':['gini','entropy','log_loss'],
                         'splitter': ['best', 'random'],
                         'max_depth': ['None',2, 4, 6, 8, 10, 12, 14, 16, 18, 20],
                         'min_samples_split': [2, 4, 6, 8, 10, 12, 14, 16, 18, 20],
                         'min_samples_leaf': [1, 2, 3, 4, 5, 6, 7, 8 , 9, 10, 11, 12, 13, 14, 15
                         'max_features': ['auto', 'sqrt','log2']}
         tree_cv = GridSearchCV(tree,tree_params,cv=5)
         tree_cv.fit(X_train, Y_train)
         print("Best Parameters :",tree_cv.best_params_)
         print("GridSearch Score :",(tree_cv.best_score_*100).round(2),'%')
         Best Parameters : {'criterion': 'log_loss', 'max_depth': 18, 'max_features': 'log2',
         'min_samples_leaf': 1, 'min_samples_split': 2, 'splitter': 'best'}
         GridSearch Score : 72.62 %
In [38]: y_predict = tree_cv.best_estimator_.predict(X_test)
         print("Tuned Decision Tree Model Accuracy:",
              (accuracy_score(Y_test, y_predict)*100).round(2),'%')
         Tuned Decision Tree Model Accuracy: 74.92 %
         plot_confusion_matrix(Y_test,y_predict)
In [39]:
```



K-Nearest-Neighbors

```
In [40]: KNN = KNeighborsClassifier()
         KNN.fit(X_train,Y_train)
         accuracy = KNN.score(X_test, Y_test)
         print('KNN Model Accuracy:',(accuracy*100).round(2),'%')
         KNN Model Accuracy: 71.0 %
In [41]:
         knn_params = {'n_neighbors': list(range(1,50)),
                        'weights':['uniform','distance'],
                        'algorithm': ['auto', 'ball_tree', 'kd_tree', 'brute'],
                        'p': [1,2]}
         knn_cv = GridSearchCV(KNN,knn_params,cv=10)
         knn_cv.fit(X_train, Y_train)
         print("Best Parameters :",knn_cv.best_params_)
         print("GridSearch Score :",(knn_cv.best_score_*100).round(2),'%')
         Best Parameters : {'algorithm': 'auto', 'n_neighbors': 18, 'p': 1, 'weights': 'distan
         ce'}
         GridSearch Score: 79.85 %
In [42]: y_predict=knn_cv.best_estimator_.predict(X_test)
         print("Tuned K-Neighbors model accuracy:",
              ( accuracy_score(Y_test, y_predict)*100).round(2),'%')
         Tuned K-Neighbors model accuracy: 78.46 %
```





Comparisons

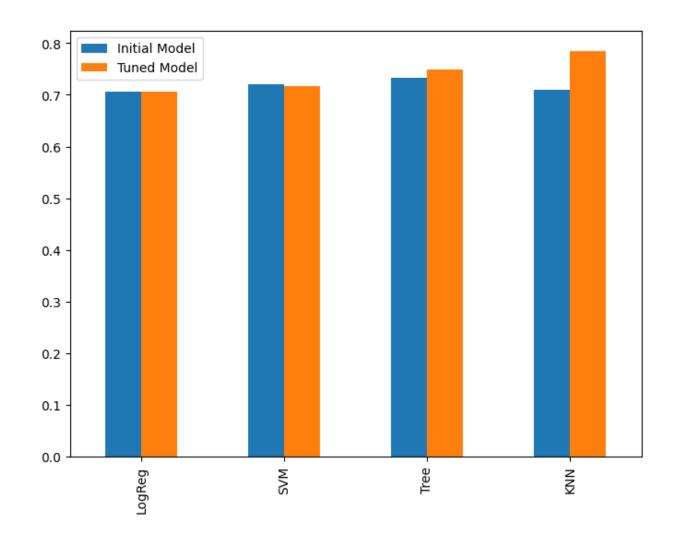
Between the four models, the best one to predict wine quality was the K-Nearest-Neigbors classifier after tuning.

Out[44]:	Initial Model	Tuned Model
Out[44]:	Initial Model	Tuned Model

LogReg	0.706923	0.706923
SVM	0.720000	0.717692
Tree	0.733077	0.749231
KNN	0.710000	0.784615

```
In [45]: scores.plot.bar(figsize=(8,6))
```

Out[45]: <AxesSubplot: >



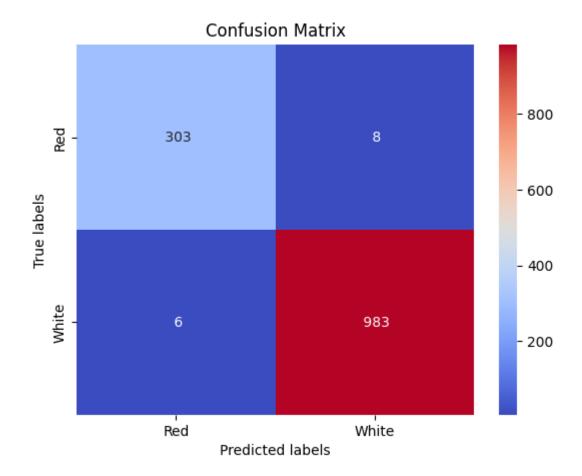
Predictive Models for Wine Type

```
In [46]:

def plot_confusion_matrix2(y,y_predict):
    cm = confusion_matrix(y, y_predict)
    ax= plt.subplot()
    sns.heatmap(cm, cmap='coolwarm',annot=True,fmt = " ", ax = ax);
    ax.set_xlabel('Predicted labels')
    ax.set_ylabel('True labels')
    ax.set_title('Confusion Matrix');
    ax.xaxis.set_ticklabels(['Red','White']); ax.yaxis.set_ticklabels(['Red','White'])
```

Logistic Regression

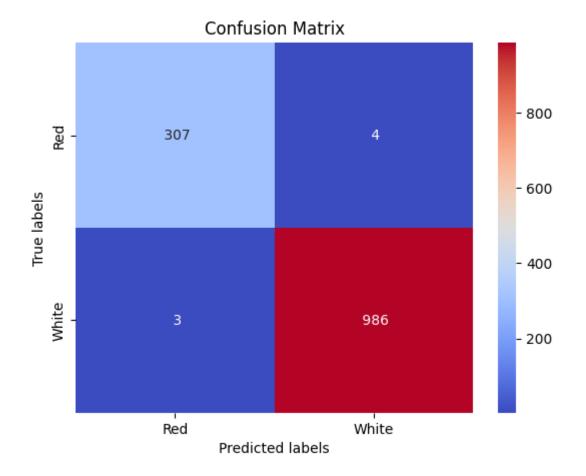
```
In [47]: lr = LogisticRegression()
    lr.fit(X2_train,Y2_train)
    lr_accuracy = lr.score(X2_test, Y2_test)
    print('Log Regression Accuracy:',(lr_accuracy*100).round(2),'%')
    Log Regression Accuracy: 98.92 %
In [48]: y_predict = lr.predict(X2_test)
    plot_confusion_matrix2(Y2_test,y_predict)
```



Here we can see that our Log Regression model gave us a fantastic score of 98.92%, accurately predicting 1,286 samples out of 1,300. With a score like this, there is no need to tune our model or to even train any other ones. However, we will continue on with other models to see what scores we get and also, just for fun.

Support Vector Machine

```
In [49]: svm = SVC()
svm.fit(X2_train,Y2_train)
svm_accuracy = svm.score(X2_test, Y2_test)
print('Support Vector Accuracy:',(svm_accuracy*100).round(2),'%')
Support Vector Accuracy: 99.46 %
In [50]: y_predict = svm.predict(X2_test)
plot_confusion_matrix2(Y2_test,y_predict)
```

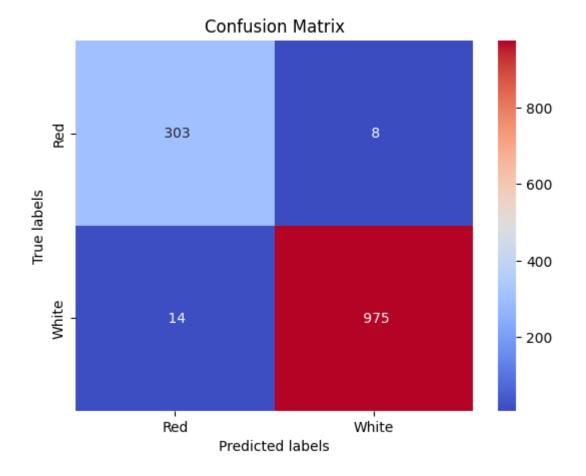


Decision Tree

```
In [51]: tree = DecisionTreeClassifier()
    tree.fit(X2_train,Y2_train)
    tree_accuracy = tree.score(X2_test, Y2_test)
    print('Decision Tree Accuracy:',(tree_accuracy*100).round(2),'%')

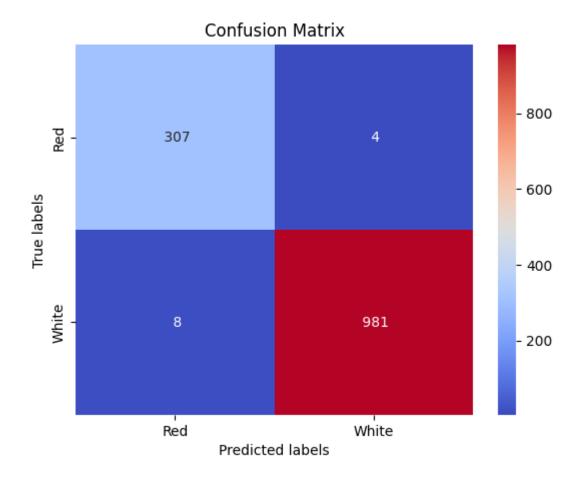
Decision Tree Accuracy: 98.31 %

In [52]: y_predict = tree.predict(X2_test)
    plot_confusion_matrix2(Y2_test,y_predict)
```



K-Nearest-Neighbors

```
In [53]: KNN = KNeighborsClassifier()
   KNN.fit(X2_train,Y2_train)
   KNN_accuracy = KNN.score(X2_test, Y2_test)
   print('KNN Model Accuracy:',(KNN_accuracy*100).round(2),'%')
   KNN Model Accuracy: 99.08 %
In [54]: y_predict = KNN.predict(X2_test)
   plot_confusion_matrix2(Y2_test,y_predict)
```



Comparisons

The best model for predicting wine types is our Support Vector Classifier with a score of 99.46 %