# **Assignment 2 - Wine Quality Prediction**

# 1. Data Exploration

# 1.1 Loading Data

```
In [1]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from scipy import stats

wine = pd.read_csv("winequality-white.csv", delimiter=';')
```

# 1.2 Exploratory Data Analysis (EDA)

In [2]:	wi	wine.head()										
Out[2]:		fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur		density	рН	sulphates	alcohol
	0	7.0	0.27	0.36	20.7	0.045	dioxide 45.0	dioxide 170.0	1.0010	2.00	0.45	8.8
	1	6.3	0.27	0.36	1.6	0.045	14.0	170.0	0.9940		0.45	o.o 9.5
	2	8.1	0.30	0.34	6.9	0.049	30.0	97.0		3.26	0.49	10.1
	3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956		0.40	9.9
	4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9
	4		_	_			_	_	_	_		

This dataset contains 11 features and 1 target:

- Features: fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol
- · Target: quality

#### In [3]: wine.info() <class 'pandas.core.frame.DataFrame'> RangeIndex: 4898 entries, 0 to 4897 Data columns (total 12 columns): Column Non-Null Count Dtype ----- - -----fixed acidity volatile acidity 0 4898 non-null float64 1 4898 non-null float64 2 citric acid 4898 non-null float64 3 residual sugar 4898 non-null float64 4 chlorides 4898 non-null float64 5 free sulfur dioxide float64 4898 non-null 6 total sulfur dioxide 4898 non-null float64 7 float64 density 4898 non-null 8 4898 non-null float64 рΗ 9 sulphates float64 4898 non-null 10 alcohol float64 4898 non-null 11 quality 4898 non-null int64 dtypes: float64(11), int64(1) memory usage: 459.3 KB

There are 4898 entries and all are numerical (long float and long integer). Plus there is no null value in all of the columns.

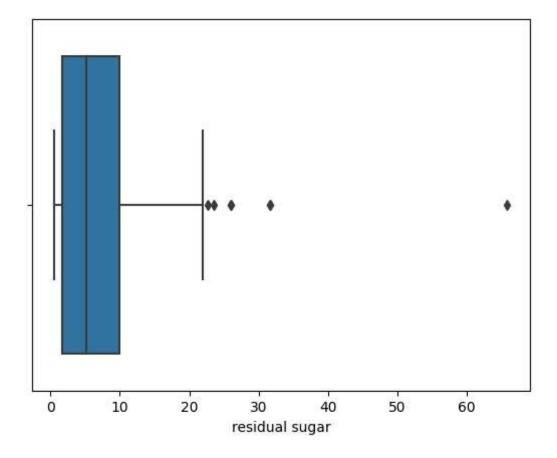
[4]:	wine.c	lescribe()						
4]:		fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfu dioxid
	count	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.00000
	mean	6.854788	0.278241	0.334192	6.391415	0.045772	35.308085	138.36065
	std	0.843868	0.100795	0.121020	5.072058	0.021848	17.007137	42.49806
	min	3.800000	0.080000	0.000000	0.600000	0.009000	2.000000	9.00000
	25%	6.300000	0.210000	0.270000	1.700000	0.036000	23.000000	108.00000
	50%	6.800000	0.260000	0.320000	5.200000	0.043000	34.000000	134.00000
	75%	7.300000	0.320000	0.390000	9.900000	0.050000	46.000000	167.00000
	max	14.200000	1.100000	1.660000	65.800000	0.346000	289.000000	440.00000
	4							

It seems like there are outliers in the residual sugar feature. We can see that 25% of the values are under 1.70 and 75% of them are under 9.90. Taking into account the mean at 6.39, the minimum value of 0.60 and maximum value of 65.80 seems like an outlier.

Using boxplot to visualize the outlier in residual sugar.

```
In [5]: sns.boxplot(x=wine['residual sugar'])
```

Out[5]: <AxesSubplot: xlabel='residual sugar'>



It seems like residual sugar > 20 is considered outlier.

```
In [6]:
            plt.rc('font', size=14)
             plt.rc('axes', labelsize=14, titlesize=14)
             plt.rc('legend', fontsize=14)
             plt.rc('xtick', labelsize=10)
             plt.rc('ytick', labelsize=10)
             wine.hist(bins=50, figsize=(20,15))
             plt.show()
                            fixed acidity
                                                                     volatile acidity
                                                                                                                 citric acid
              600
                                                        400
              500
                                                        300
              300
                                                        200
              100
                                                                                                             0.50
                                                                                                                 0.75 1.00 1.25 1.50
                            residual sugar
                                                                                                              free sulfur dioxide
                                                                       chlorides
                                                       1200
              1400
                                                       1000
              1000
                                                                                                 500
                                                        800
              800
                                                                                                 400
                                                        600
              600
                                                                                                 300
                                                        400
              400
                                                                                                 200
                                                              0.05 0.10 0.15 0.20 0.25 0.30 0.35
                          total sulfur dioxide
                                                        600
                                                                                                 400
              300
                                                        400
                                                        300
                                                                                                 200
              200
                                                        100
                                                                             1.02
                             sulphates
                                                                        alcohol
                                                                                                                  quality
                                                                                                 2000
                                                        250
                                                                                                 1500
                                                        200
                                                        150
                                                        100
```

#### Observations:

- most features are normally distributed except for residual sugar and alcohol
- a lot of features are skewed to the right (fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density)
- from quality, we can see that we have data imbalance problem where we might not have enough samples of high quality wine.

Checking class imbalance.

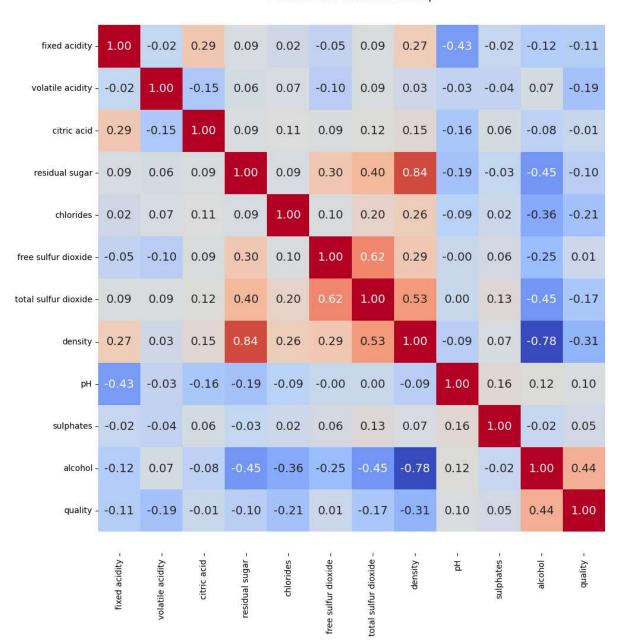
```
In [7]: | wine['quality'].value_counts()
Out[7]: quality
             2198
        6
        5
             1457
        7
              880
        8
              175
        4
              163
        3
              20
        9
                5
        Name: count, dtype: int64
```

## 1.3 Visualize Correlation between Features and Target

```
In [8]: corr = wine.corr()

plt.figure(figsize=(12, 12))
sns.heatmap(corr, annot=True, fmt='.2f', cmap='coolwarm', square=True, cbar=Fa
lse)
b, t = plt.ylim()
plt.ylim(b+0.5, t-0.5)
plt.title("Feature Correlation Heatmap")
plt.show()
```

#### Feature Correlation Heatmap



We can see that alcohol has the highest correlation with the wine quality followed by density, chlorides, and volatile acidity.

# 2. Data Preprocessing

# 2.1 Handling Outliers

Using z-score to find and remove outliers with threshold set to 3.

```
In [9]: | z = np.abs(stats.zscore(wine))
        wine = wine[(z < 3).all(axis=1)]
        print(wine.shape)
        wine['quality'].value_counts()
        (4487, 12)
Out[9]: quality
        6
              2038
        5
              1309
        7
               855
        8
               161
               124
        Name: count, dtype: int64
```

After removing outliers, there are 4487 entries left. This means there are about 411 outliers (about 8.4%).

# 2.2 Split Features and Target

```
In [10]: X = wine.drop('quality', axis=1)
    print(X.shape)

y = wine['quality']
    print(y.shape)

(4487, 11)
    (4487,)
```

## 2.3 Perform Feature Scaling

```
In [11]: from sklearn.preprocessing import StandardScaler
    scaler = StandardScaler()
    X = scaler.fit_transform(X)
```

## 2.4 Split Training and Test Data

```
In [12]: from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, rando
    m_state=42, stratify=y)
    print(X_train.shape)
    print(Y_test.shape)

    print(y_test.shape)

(3589, 11)
    (898, 11)
    (3589,)
    (898,)
```

# 3. Binary Classification

# 3.1 Categorizing Wine Quality

For binary classification task:

- high quality >= 7 quality rating
- low quality < 7 quality rating

```
In [13]: y_train_hq = (y_train >= 7)
y_test_hq = (y_test >= 7)
```

# 3.2 Model Training

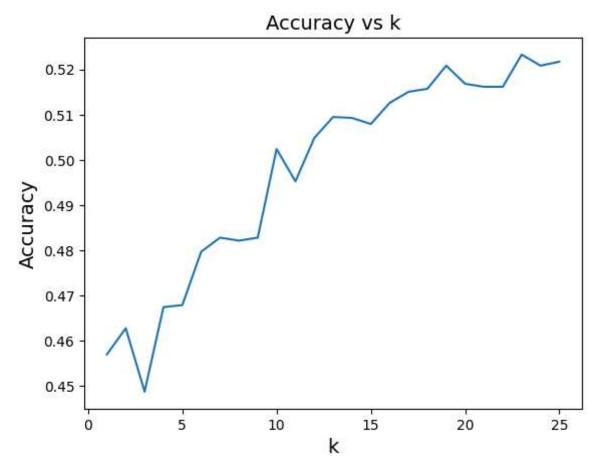
#### 3.2.1 Logistic Regression

### 3.2.2 Support Vector Machine (SVM)

## 3.2.3 K-Nearest Neighbors (KNN)

Before training, lets see how the accuracy changed with number of K.

```
In [16]:
         from sklearn.neighbors import KNeighborsClassifier
         from sklearn.model_selection import cross val score
         # Range of k from 1 to 26
         k_range = range(1, 26)
         # List of cv scores
         cv_scores = []
         # Perform 10-fold cross validation
         for k in k_range:
             knn = KNeighborsClassifier(n_neighbors=k)
             scores = cross_val_score(knn, X, y, cv=10, scoring='accuracy')
             cv_scores.append(scores.mean())
         # Plot accuracy vs k
         plt.plot(k_range, cv_scores)
         plt.xlabel('k')
         plt.ylabel('Accuracy')
         plt.title('Accuracy vs k')
         plt.show()
```



We can see that highest accuracy is achieved when k equals to 19 or 23. Train the model with k = 23.

#### 3.2.4 Decision Tree

#### 3.2.5 Random Forest

# 3.3 Model Evaluation

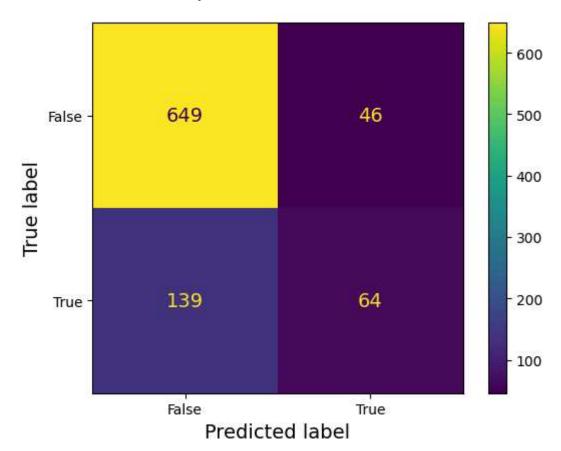
In model evaluation, the trained model will be cross-validated using 10-fold and tested using the test set.

```
In [20]: # Cross-validation using 10-fold with accuracy scoring
    y_cv_logreg = cross_val_score(logreg, X_train, y_train_hq, cv=10, scoring='accuracy')
    y_cv_svm = cross_val_score(svm, X_train, y_train_hq, cv=10, scoring='accuracy')
    y_cv_knn = cross_val_score(knn, X_train, y_train_hq, cv=10, scoring='accuracy')
    y_cv_dt = cross_val_score(dt, X_train, y_train_hq, cv=10, scoring='accuracy')
    y_cv_rf = cross_val_score(rf, X_train, y_train_hq, cv=10, scoring='accuracy')

# Predict using the test set
    y_pred_logreg = logreg.predict(X_test)
    y_pred_svm = svm.predict(X_test)
    y_pred_dt = dt.predict(X_test)
    y_pred_df = dt.predict(X_test)
    y_pred_rf = rf.predict(X_test)
```

### 3.3.1 Evaluation of Logistic Regression

	precision	recall	f1-score	support
False True	0.824 0.582	0.934 0.315	0.875 0.409	695 203
accuracy macro avg weighted avg	0.703 0.769	0.625 0.794	0.794 0.642 0.770	898 898 898

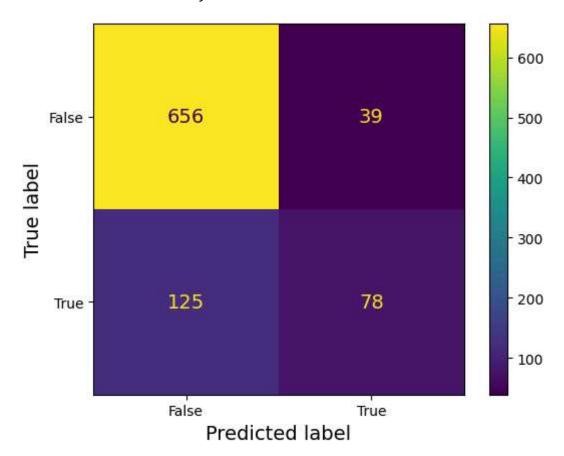


3.3.2 Evaluation of SVM

```
In [22]: print(classification_report(y_test_hq, y_pred_svm, digits=3, zero_division=1))
    print('Cross-validation accuracy score:', y_cv_svm.mean())

    plt.rc('font', size=14)
    ConfusionMatrixDisplay.from_predictions(y_test_hq, y_pred_svm)
    plt.show()
```

	precision	recall	f1-score	support
False	0.840	0.944	0.889	695
True	0.667	0.384	0.487	203
accuracy			0.817	898
macro avg	0.753	0.664	0.688	898
weighted avg	0.801	0.817	0.798	898

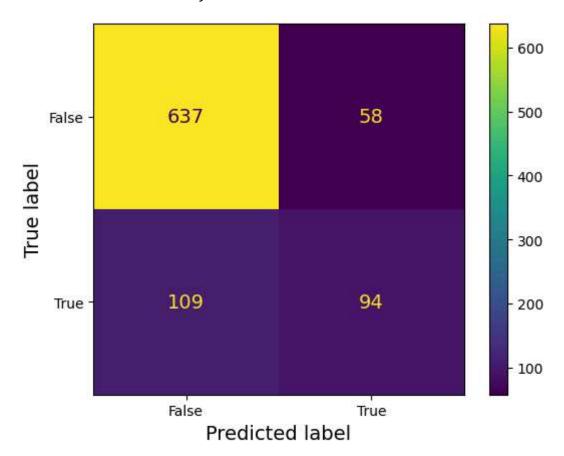


## 3.3.3 Evaluation of KNN

```
In [23]: print(classification_report(y_test_hq, y_pred_knn, digits=3, zero_division=1))
    print('Cross-validation accuracy score:', y_cv_knn.mean())

    plt.rc('font', size=14)
    ConfusionMatrixDisplay.from_predictions(y_test_hq, y_pred_knn)
    plt.show()
```

	precision	recall	f1-score	support
False True	0.854 0.618	0.917 0.463	0.884 0.530	695 203
True	0.018	0.403	0.550	203
accuracy			0.814	898
macro avg	0.736	0.690	0.707	898
weighted avg	0.801	0.814	0.804	898

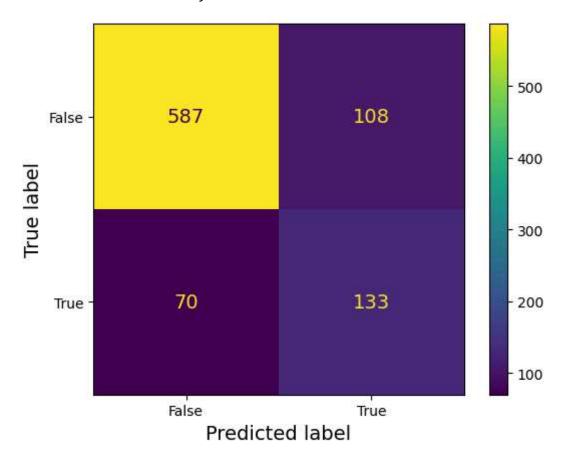


### 3.3.4 Evaluation of Decision Tree

In [24]: print(classification\_report(y\_test\_hq, y\_pred\_dt, digits=3, zero\_division=1))
 print('Cross-validation accuracy score:', y\_cv\_dt.mean())

 plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test\_hq, y\_pred\_dt)
 plt.show()

	precision	recall	f1-score	support
False	0.893	0.845	0.868	695
True	0.552	0.655	0.599	203
accuracy			0.802	898
macro avg	0.723	0.750	0.734	898
weighted avg	0.816	0.802	0.807	898

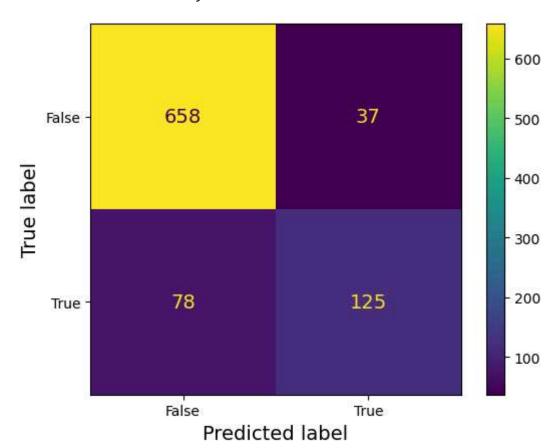


### 3.3.5 Evaluation of Random Forest

In [25]: print(classification\_report(y\_test\_hq, y\_pred\_rf, digits=3, zero\_division=1))
 print('Cross-validation accuracy score:', y\_cv\_rf.mean())

 plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test\_hq, y\_pred\_rf)
 plt.show()

	precision	recall	f1-score	support
False	0.894	0.947	0.920	695
True	0.772	0.616	0.685	203
accuracy			0.872	898
macro avg	0.833	0.781	0.802	898
weighted avg	0.866	0.872	0.867	898



### Ranking:

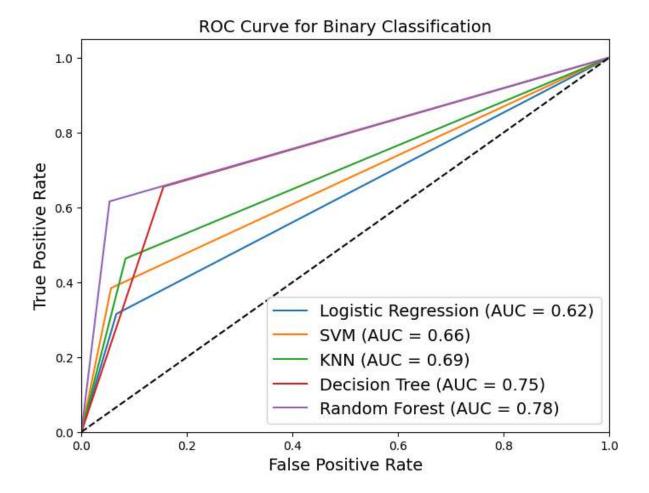
CV Accuracy: RF, DT, SVM, KNN, LOGREG
Precision: RF, DT, KNN, SVM, LOGREG
Recall: RF, KNN, DT, SVM, LOGREG
F1-Score: RF, DT, KNN, SVM, LOGREG

#### Observations:

- Random Forest is the best at binary classification for this white wine quality prediction.
- However, Decision Tree is better at recall high quality wine.

# 3.4 ROC Curve Analysis

```
In [26]: | from sklearn.metrics import roc_curve, auc
         models = [logreg, svm, knn, dt, rf]
         model_names = ['Logistic Regression', 'SVM', 'KNN', 'Decision Tree', 'Random F
         orest']
         plt.figure(figsize=(8, 6))
         # Plot ROC curve for each model
         for model, name in zip(models, model_names):
             y_pred = model.predict(X_test)
             fpr, tpr, thresholds = roc_curve(y_test_hq, y_pred)
             roc_auc = auc(fpr, tpr)
             plt.plot(fpr, tpr, label='%s (AUC = %0.2f)' % (name, roc_auc))
         # Plot the random guess line
         plt.plot([0, 1], [0, 1], 'k--')
         plt.xlim([0.0, 1.0])
         plt.ylim([0.0, 1.05])
         plt.xlabel('False Positive Rate')
         plt.ylabel('True Positive Rate')
         plt.title('ROC Curve for Binary Classification')
         plt.legend(loc="lower right")
         plt.show()
```

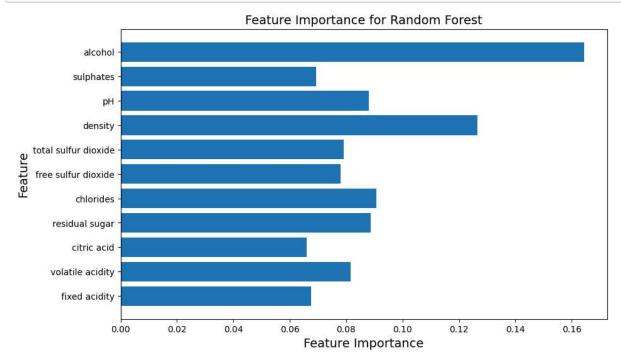


From the ROC curve, we can observe that Random Forest have the highest ROC AUC which is 0.78. Although this value is quite low (ROC AUC = 1 being the perfect), it is the best we can achieved among the 5 chosen algorithms with imbalanced dataset.

## 3.5 Feature Importance for Binary Classification

```
In [27]: feature_importances = rf.feature_importances_

# Plot the feature importance for Random Forest
plt.figure(figsize=(10, 6))
plt.barh(wine.columns[:-1], feature_importances)
plt.xlabel('Feature Importance')
plt.ylabel('Feature')
plt.title('Feature Importance for Random Forest')
plt.show()
```



For binary classification, alcohol and density are the most important features to distinguish low quality wine and high quality wine (binary). This might not be the case for multiclass classification.

# 4. Multiclass Classification

# 4.1 Model Training

Logistic Regression and Support Vector Machine, by default, is limited to binary classification problems. However, we can utilize extensions like One-vs-One (OvO) and One-vs-Rest (OvR) to be used for multiclass classification problems. Other algorithms such as K-Nearest Neighbors, Decision Tree, and Random Forest inherently support multiclass classification.

### 4.1.1 Logistic Regression

One-vs-One approach.

One-vs-Rest approach.

### 4.1.2 Support Vector Machines (SVM)

One-vs-One approach.

One-vs-Rest approach.

## 4.1.3 K-Nearest Neighbors (KNN)

#### 4.1.4 Decision Tree

#### 4.1.5 Random Forest

### 4.2 Model Evaluation

For multiclass classification, it is recommended to find AUC score using cross validation method by passing roc\_auc\_ovr parameter. Evaluating the model with this method is advantageous when there is a high class imbalance. Also it does not require to set a classification threshold.

```
In [35]: # Cross-validation using 10-fold with accuracy scoring
         y_cv_ovo_logreg = cross_val_score(ovo_logreg, X_train, y_train, cv=10, scoring
         ='accuracy')
         y_cv_ovr_logreg = cross_val_score(ovr_logreg, X_train, y_train, cv=10, scoring
         ='accuracy')
         y cv ovo svm = cross val score(ovo svm, X train, y train, cv=10, scoring='accu
         racy')
         y_cv_ovr_svm = cross_val_score(ovr_svm, X_train, y_train, cv=10, scoring='accu
         racy')
         y_cv_knn = cross_val_score(knn, X_train, y_train, cv=10, scoring='accuracy')
         y cv dt = cross val score(dt, X train, y train, cv=10, scoring='accuracy')
         y cv rf = cross_val_score(rf, X_train, y_train, cv=10, scoring='accuracy')
         # Predict using the test set
         y_pred_ovo_logreg = ovo_logreg.predict(X_test)
         y pred ovr logreg = ovr logreg.predict(X test)
         y pred ovo svm = ovo svm.predict(X test)
         v pred ovr svm = ovr svm.predict(X test)
         y pred knn = knn.predict(X test)
         y pred dt = dt.predict(X test)
         y pred rf = rf.predict(X test)
```

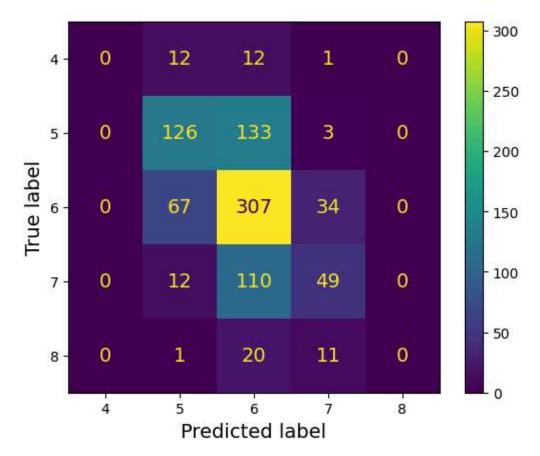
#### 4.2.1 Evaluation of Logistic Regression

One-vs-One.

In [36]: print(classification\_report(y\_test, y\_pred\_ovo\_logreg, digits=3, zero\_division
=1))
 print('Cross-validation accuracy score:', y\_cv\_ovo\_logreg.mean())

plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test, y\_pred\_ovo\_logreg)
 plt.show()

	precision	recall	f1-score	support
4	1.000	0.000	0.000	25
5	0.578	0.481	0.525	262
6	0.527	0.752	0.620	408
7	0.500	0.287	0.364	171
8	1.000	0.000	0.000	32
accuracy			0.537	898
macro avg	0.721	0.304	0.302	898
weighted avg	0.567	0.537	0.504	898

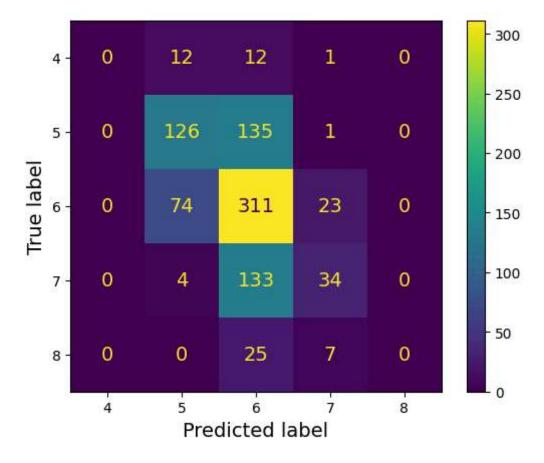


One-vs-Rest.

```
In [37]: print(classification_report(y_test, y_pred_ovr_logreg, digits=3, zero_division
=1))
    print('Cross-validation accuracy score:', y_cv_ovr_logreg.mean())

plt.rc('font', size=14)
    ConfusionMatrixDisplay.from_predictions(y_test, y_pred_ovr_logreg)
    plt.show()
```

	precision	recall	f1-score	support
4	1.000	0.000	0.000	25
5	0.583	0.481	0.527	262
6	0.505	0.762	0.607	408
7	0.515	0.199	0.287	171
8	1.000	0.000	0.000	32
accuracy			0.524	898
macro avg	0.721	0.288	0.284	898
weighted avg	0.561	0.524	0.484	898

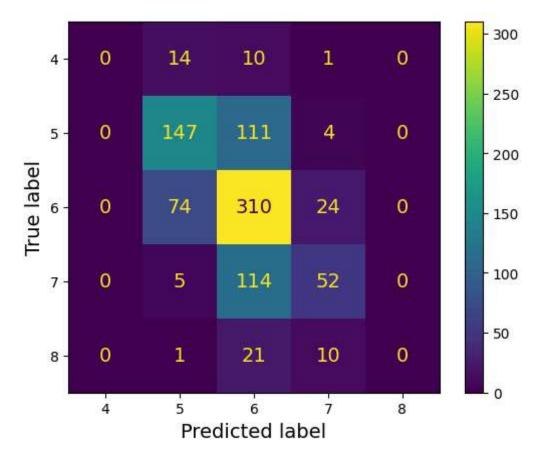


Although the OvR method achieved higher cross-validation accuracy, the OvO achieved better performance in all aspects (accuracy, precision, recall, f1-score) during testing.

In [38]: print(classification\_report(y\_test, y\_pred\_ovo\_svm, digits=3, zero\_division=
1))
 print('Cross-validation accuracy score:', y\_cv\_ovo\_svm.mean())

plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test, y\_pred\_ovo\_svm)
 plt.show()

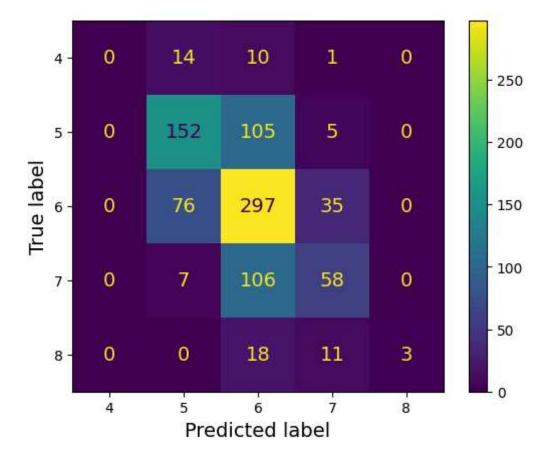
	precision	recall	f1-score	support
4	1.000	0.000	0.000	25
5	0.610	0.561	0.584	262
6	0.548	0.760	0.637	408
7	0.571	0.304	0.397	171
8	1.000	0.000	0.000	32
accuracy			0.567	898
macro avg	0.746	0.325	0.324	898
weighted avg	0.599	0.567	0.535	898



```
In [39]: print(classification_report(y_test, y_pred_ovr_svm, digits=3, zero_division=
1))
    print('Cross-validation accuracy score:', y_cv_ovr_svm.mean())

plt.rc('font', size=14)
    ConfusionMatrixDisplay.from_predictions(y_test, y_pred_ovr_svm)
    plt.show()
```

	precision	recall	f1-score	support
4	1.000	0.000	0.000	25
5	0.610	0.580	0.595	262
6	0.554	0.728	0.629	408
7	0.527	0.339	0.413	171
8	1.000	0.094	0.171	32
accuracy			0.568	898
macro avg	0.738	0.348	0.362	898
weighted avg	0.594	0.568	0.544	898



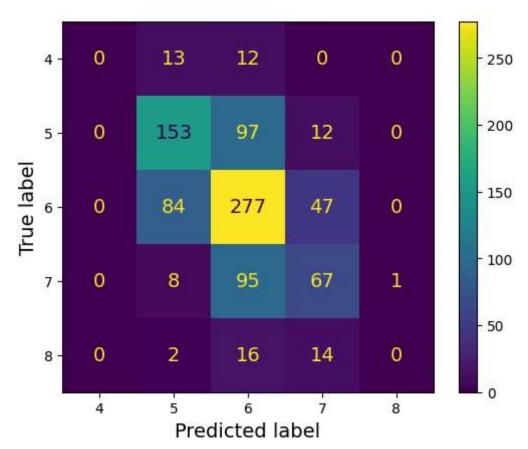
SVM however achieved better performance using the OvR method. Plus, it is the first time a model is able to predict samples with quality class 8.

#### 4.2.3 Evaluation of KNN

In [40]: print(classification\_report(y\_test, y\_pred\_knn, digits=3, zero\_division=1))
 print('Cross-validation accuracy score:', y\_cv\_knn.mean())

 plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test, y\_pred\_knn)
 plt.show()

	precision	recall	f1-score	support
4	1.000	0.000	0.000	25
5 6	0.588 0.557	0.584 0.679	0.586 0.612	262 408
7	0.479	0.392	0.431	171
8	0.000	0.000	0.000	32
accuracy			0.553	898
macro avg	0.525	0.331	0.326	898
weighted avg	0.544	0.553	0.531	898

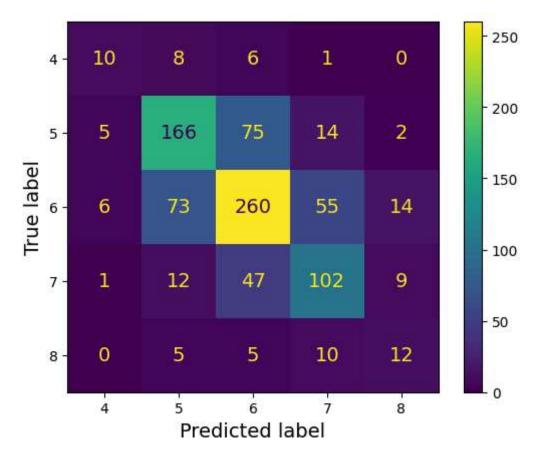


### 4.2.4 Evaluation of Decision Tree

In [41]: print(classification\_report(y\_test, y\_pred\_dt, digits=3, zero\_division=1))
 print('Cross-validation accuracy score:', y\_cv\_dt.mean())

 plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test, y\_pred\_dt)
 plt.show()

	precision	recall	f1-score	support
4	0.455	0.400	0.426	25
5	0.629	0.634	0.631	262
6	0.662	0.637	0.649	408
7	0.560	0.596	0.578	171
8	0.324	0.375	0.348	32
accuracy			0.612	898
macro avg	0.526	0.528	0.526	898
weighted avg	0.615	0.612	0.613	898

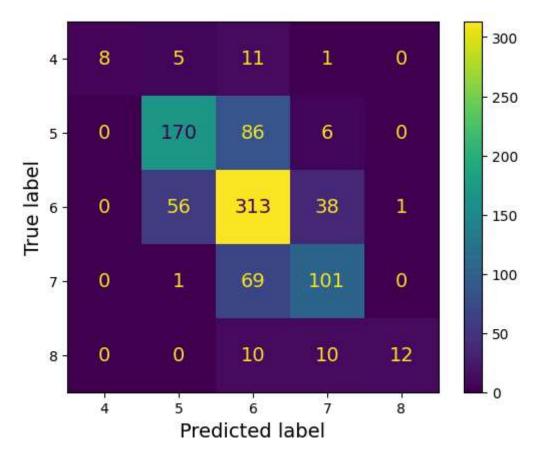


### **4.2.5** Evaluation of Random Forest

In [42]: print(classification\_report(y\_test, y\_pred\_rf, digits=3, zero\_division=1))
 print('Cross-validation accuracy score:', y\_cv\_rf.mean())

 plt.rc('font', size=14)
 ConfusionMatrixDisplay.from\_predictions(y\_test, y\_pred\_rf)
 plt.show()

	precision	recall	f1-score	support
4	1.000	0.320	0.485	25
5	0.733	0.649	0.688	262
6	0.640	0.767	0.698	408
7	0.647	0.591	0.618	171
8	0.923	0.375	0.533	32
266118261			0.673	898
accuracy				
macro avg	0.789	0.540	0.604	898
weighted avg	0.689	0.673	0.668	898

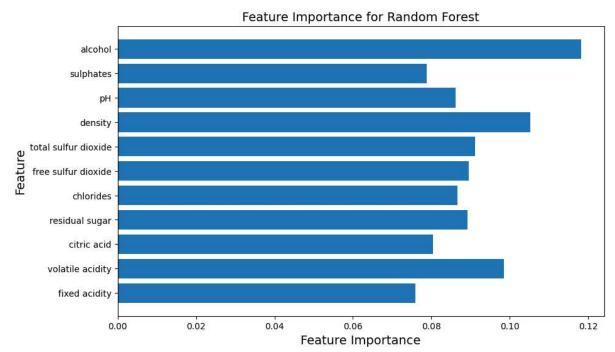


Random forest is the best algorithm for the multiclass classification of wine quality. It achieved the highest cross-validation accuracy, testing accuracy, precision, recall, and f1-score. However, decision tree is better at recall for minority classes. This is the exact case as in binary classification.

# 4.3 Feature Importance for Multiclass Classification

```
In [43]: feature_importances = rf.feature_importances_

# PLot the feature importance for Random Forest
plt.figure(figsize=(10, 6))
plt.barh(wine.columns[:-1], feature_importances)
plt.xlabel('Feature Importance')
plt.ylabel('Feature')
plt.title('Feature Importance for Random Forest')
plt.show()
```



For multiclass classification, alcohol and density are still the most important features as in binary classification. However, we can also see that volatile acidity has high importance during training.