ASSIGNMENT 3: CMTH 642 DATA ANALYTICS: ADVANCED METHODS

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In [36]:
```
#pip install pingouin --upgrade
```

Preparation:

The dataset is related to white Portuguese "Vinho Verde" wine. For more info: https://archive.ics.uci.edu/ml/datasets/Wine+Quality

Import the following files:

http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white.csv

http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv

In [1]:
```
#imports needed for the this Assignment

import seaborn as sns
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
import pingouin as pg

from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import plot_confusion_matrix
from sklearn.metrics import confusion_matrix
from sklearn.metrics import roc_auc_score, roc_curve, auc, accuracy_score
from sklearn.metrics import classification_report
from sklearn.metrics import accuracy_score
from sklearn.metrics import precision_score
from sklearn.metrics import recall_score
from sklearn.metrics import f1_score
%matplotlib inline
```

In [2]:
```
dataset_1 = pd.read_csv("http://archive.ics.uci.edu/ml/machine-learning-databases/wine-
dataset_2 = pd.read_csv("http://archive.ics.uci.edu/ml/machine-learning-databases/wine-
df_1 = pd.DataFrame(dataset_1)
df_2 = pd.DataFrame(dataset_2)
```

Questions:

1. Combine Red and White wine datasets. (4 points)

In [3]:
```
##### Combine DataFrames with Append() #####
############################################
wine_data_all = df_1.append(df_2, ignore_index=True)
wine_data_all.tail()
```

Out[3]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	q
6492	6.2	0.600	0.08	2.0	0.090	32.0	44.0	0.99490	3.45	0.58	10.5	
6493	5.9	0.550	0.10	2.2	0.062	39.0	51.0	0.99512	3.52	0.76	11.2	
6494	6.3	0.510	0.13	2.3	0.076	29.0	40.0	0.99574	3.42	0.75	11.0	
6495	5.9	0.645	0.12	2.0	0.075	32.0	44.0	0.99547	3.57	0.71	10.2	
6496	6.0	0.310	0.47	3.6	0.067	18.0	42.0	0.99549	3.39	0.66	11.0	

2. Check the datatypes of the attributes. (3 points)

In [4]:
```
wine_data_all.info()
# As you could see the data types of all the attributes below.
# 11 Float and 1 integer
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 6497 entries, 0 to 6496
Data columns (total 12 columns):
 #   Column                Non-Null Count  Dtype  
---  ------                --------------  -----  
 0   fixed acidity         6497 non-null   float64
 1   volatile acidity      6497 non-null   float64
 2   citric acid           6497 non-null   float64
 3   residual sugar        6497 non-null   float64
 4   chlorides             6497 non-null   float64
 5   free sulfur dioxide   6497 non-null   float64
 6   total sulfur dioxide  6497 non-null   float64
 7   density               6497 non-null   float64
 8   pH                    6497 non-null   float64
 9   sulphates             6497 non-null   float64
 10  alcohol               6497 non-null   float64
 11  quality               6497 non-null   int64  
dtypes: float64(11), int64(1)
memory usage: 609.2 KB
```

3. Are there any missing values in the dataset? (4 points)

In [5]:
```
wine_data_all.isnull().sum()
#As can be seen below there is no missing values in the combined dataset.
```

Out[5]:
```
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
```

4.What is the correlation between the attributes other than Quality? (10 points)

Method 1

In [6]:

```
import pingouin as pg
# First we can drope the quality
df_no_quality= wine_data_all.drop(['quality'], axis='columns')

df_no_quality.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 6497 entries, 0 to 6496
Data columns (total 11 columns):
 #   Column                Non-Null Count  Dtype  
---  ------                --------------  -----  
 0   fixed acidity         6497 non-null   float64
 1   volatile acidity      6497 non-null   float64
 2   citric acid           6497 non-null   float64
 3   residual sugar        6497 non-null   float64
 4   chlorides             6497 non-null   float64
 5   free sulfur dioxide   6497 non-null   float64
 6   total sulfur dioxide  6497 non-null   float64
 7   density               6497 non-null   float64
 8   pH                    6497 non-null   float64
 9   sulphates             6497 non-null   float64
 10  alcohol               6497 non-null   float64
dtypes: float64(11)
memory usage: 558.5 KB
```

In [7]:

```
# Now we can calculate the pairwise pearson correlation
corr = pg.pairwise_corr(df_no_quality, method='pearson')
# Sort the correlation by p-values and display the first rows
corr.sort_values(by=['p-unc'])[['X', 'Y', 'n', 'r', 'p-unc']].head()
```

Out[7]:

	X	Y	n	r	p-unc
40	free sulfur dioxide	total sulfur dioxide	6497	0.720934	0.0
29	residual sugar	total sulfur dioxide	6497	0.495482	0.0
6	fixed acidity	density	6497	0.458910	0.0
51	density	alcohol	6497	-0.686745	0.0
30	residual sugar	density	6497	0.552517	0.0

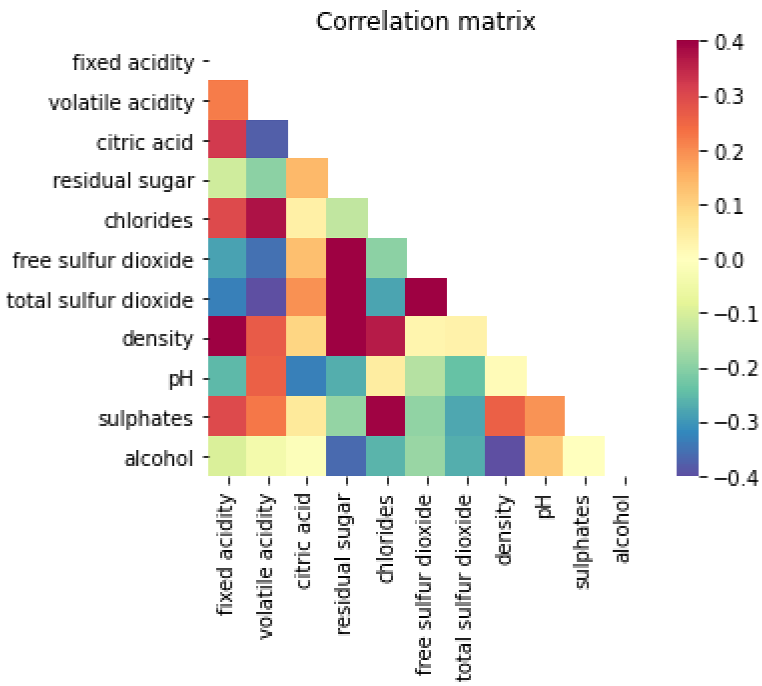
In [8]:
```
df_no_quality.corr().round(2)
```

Out[8]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcoh
fixed acidity	1.00	0.22	0.32	-0.11	0.30	-0.28	-0.33	0.46	-0.25	0.30	-0.1
volatile acidity	0.22	1.00	-0.38	-0.20	0.38	-0.35	-0.41	0.27	0.26	0.23	-0.0
citric acid	0.32	-0.38	1.00	0.14	0.04	0.13	0.20	0.10	-0.33	0.06	-0.0
residual sugar	-0.11	-0.20	0.14	1.00	-0.13	0.40	0.50	0.55	-0.27	-0.19	-0.3
chlorides	0.30	0.38	0.04	-0.13	1.00	-0.20	-0.28	0.36	0.04	0.40	-0.2
free sulfur dioxide	-0.28	-0.35	0.13	0.40	-0.20	1.00	0.72	0.03	-0.15	-0.19	-0.1
total sulfur dioxide	-0.33	-0.41	0.20	0.50	-0.28	0.72	1.00	0.03	-0.24	-0.28	-0.2
density	0.46	0.27	0.10	0.55	0.36	0.03	0.03	1.00	0.01	0.26	-0.6
pH	-0.25	0.26	-0.33	-0.27	0.04	-0.15	-0.24	0.01	1.00	0.19	0.1
sulphates	0.30	0.23	0.06	-0.19	0.40	-0.19	-0.28	0.26	0.19	1.00	-0.0
alcohol	-0.10	-0.04	-0.01	-0.36	-0.26	-0.18	-0.27	-0.69	0.12	-0.00	1.0

In [9]:
```
corrs = df_no_quality.corr()
mask = np.zeros_like(corrs)
mask[np.triu_indices_from(mask)] = True
sns.heatmap(corrs, cmap='Spectral_r', mask=mask, square=True, vmin=-.4, vmax=.4)
plt.title('Correlation matrix')
```

Out[9]: Text(0.5, 1.0, 'Correlation matrix')



Method 2

In [10]:

```
wine_data_all.iloc[0:,0:11].corr().abs()
```

Out[10]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sul
fixed acidity	1.000000	0.219008	0.324436	0.111981	0.298195	0.282735	0.329054	0.458910	0.252700	0.2
volatile acidity	0.219008	1.000000	0.377981	0.196011	0.377124	0.352557	0.414476	0.271296	0.261454	0.2
citric acid	0.324436	0.377981	1.000000	0.142451	0.038998	0.133126	0.195242	0.096154	0.329808	0.0
residual sugar	0.111981	0.196011	0.142451	1.000000	0.128940	0.402871	0.495482	0.552517	0.267320	0.1
chlorides	0.298195	0.377124	0.038998	0.128940	1.000000	0.195045	0.279630	0.362615	0.044708	0.3
free sulfur dioxide	0.282735	0.352557	0.133126	0.402871	0.195045	1.000000	0.720934	0.025717	0.145854	0.1
total sulfur dioxide	0.329054	0.414476	0.195242	0.495482	0.279630	0.720934	1.000000	0.032395	0.238413	0.2
density	0.458910	0.271296	0.096154	0.552517	0.362615	0.025717	0.032395	1.000000	0.011686	0.2
pH	0.252700	0.261454	0.329808	0.267320	0.044708	0.145854	0.238413	0.011686	1.000000	0.1
sulphates	0.299568	0.225984	0.056197	0.185927	0.395593	0.188457	0.275727	0.259478	0.192123	1.0
alcohol	0.095452	0.037640	0.010493	0.359415	0.256916	0.179838	0.265740	0.686745	0.121248	0.0

Q4 Note:

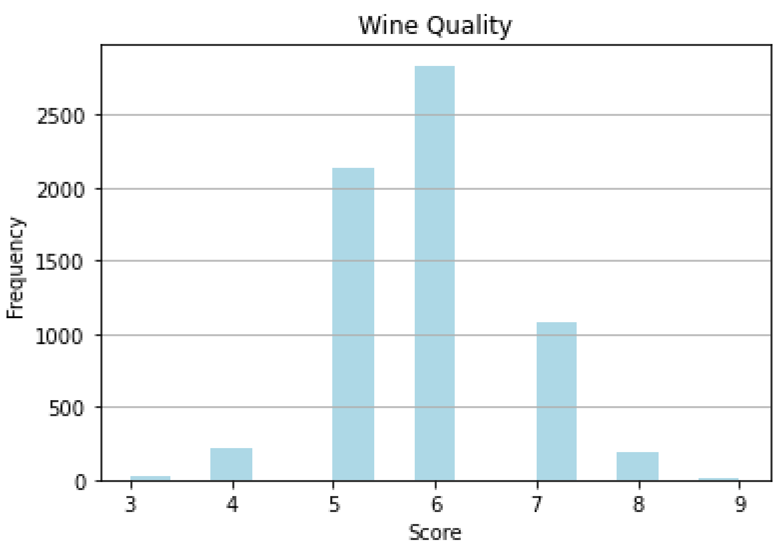
A correlation is a number between -1 and +1 that measures the degree of association between two Attributes (call them X and Y). A positive value for the correlation implies a positive association. In this case large values of X tend to be associated with large values of Y and small values of X tend to be associated with small values of Y. A negative value for the correlation implies a negative or inverse association. In this case large values of X tend to be associated with small values of Y and vice versa.

As you can see above the values of both methods are the correlation values...of all attributes except quality.

5. Graph the frequency distribution of wine quality by using Quality. (10 points)

In [11]:

```
wine_data_all['quality'].plot.hist(grid=True, bins=15,
                       color='LightBlue')
plt.title('Wine Quality')
plt.xlabel('Score')
plt.ylabel('Frequency')
plt.grid(axis='x', alpha=0.75)
# AS you can easily get the frequency distribution of wine quality below.
```



6. Reduce the levels of rating for quality to three levels as high, medium andlow. Assign the levels of 3 and 4 to level 0; 5 and 6 to level 1; and 7,8 and 9to level 2. (10 points)

In [13]:

```
# first we get with quality column in the dataset for all
wine_data_all['quality_label'] = wine_data_all.quality.apply(lambda q: 'Low' if q <= 4
wine_data_all.head()
```

Out[13]:

fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quali

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quali
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	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	

In [14]:

```
# Now We do not need the quality anymore as we new column ...so we can remove it .
wine_data_all= wine_data_all.drop(['quality'], axis='columns')

wine_data_all.head()
```

Out[14]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quali
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	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	

In [15]:

```
wine_data_all.quality_label.value_counts()
# Below you could see the dataset values as per three categories.
# You can tell dataset is balanced and could do further experiments.
```

Out[15]:

```
Medium    4974
High      1277
Low        246
Name: quality_label, dtype: int64
```

7. Normalize the numeric attributes. (10 points)

In [16]:

```
#To Normalizing numeric data with help of the function below
def normalize(x):
  return ((x - min(x)) / (max(x) - min(x)))
```

In [17]:

```
X = list(set(list(wine_data_all)) - set(['quality_label']))
X
```

Out[17]:

```
['fixed acidity',
 'residual sugar',
 'pH',
```

```
 'citric acid',
 'alcohol',
 'chlorides',
 'density',
 'total sulfur dioxide',
 'volatile acidity',
 'free sulfur dioxide',
 'sulphates']
```

In [18]:

```
df_new_wine_data_all = wine_data_all.iloc[:,].copy()
df_new_wine_data_all[X] = df_new_wine_data_all[X].apply(normalize)
df_new_wine_data_all.head()
```

Out[18]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates
0	0.264463	0.126667	0.216867	0.308282	0.059801	0.152778	0.377880	0.267785	0.217054	0.129213
1	0.206612	0.146667	0.204819	0.015337	0.066445	0.045139	0.290323	0.132832	0.449612	0.151685
2	0.355372	0.133333	0.240964	0.096626	0.068106	0.100694	0.209677	0.154039	0.418605	0.123596
3	0.280992	0.100000	0.192771	0.121166	0.081395	0.159722	0.414747	0.163678	0.364341	0.101124
4	0.280992	0.100000	0.192771	0.121166	0.081395	0.159722	0.414747	0.163678	0.364341	0.101124

In [19]:

```
df_new_wine_data_all.describe()
# Observe the values below
```

Out[19]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	
count	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497
mean	0.282257	0.173111	0.191948	0.074283	0.078129	0.102518	0.252868	(
std	0.107143	0.109758	0.087541	0.072972	0.058195	0.061630	0.130235	(
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	(
25%	0.214876	0.100000	0.150602	0.018405	0.048173	0.055556	0.163594	(
50%	0.264463	0.140000	0.186747	0.036810	0.063123	0.097222	0.258065	(
75%	0.322314	0.213333	0.234940	0.115031	0.093023	0.138889	0.345622	(
max	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1

8. Divide the dataset to training and test sets. (10 points)

In [20]:

```
# We use the dataset from above as moving forward to split the dataset into train and t
df_train, df_test, y_train, y_test = train_test_split(df_new_wine_data_all[X], df_new_w
```

In [21]:

```
df_train.head()
```

```
# you could see the dataset records are randomly taken for train/test sets.
```

Out[21]:

	fixed acidity	residual sugar	pH	citric acid	alcohol	chlorides	density	total sulfur dioxide	volatile acidity	free sulfu dioxid
6249	0.280992	0.026074	0.465116	0.006024	0.550725	0.093023	0.119722	0.092166	0.360000	0.02430
3975	0.190083	0.016871	0.364341	0.156627	0.565217	0.039867	0.061500	0.294931	0.106667	0.20833
3007	0.099174	0.059816	0.565891	0.192771	0.666667	0.038206	0.047233	0.396313	0.126667	0.19791
5089	0.214876	0.019939	0.658915	0.150602	0.260870	0.107973	0.198381	0.099078	0.193333	0.06944
5321	0.553719	0.023006	0.333333	0.283133	0.434783	0.094684	0.206092	0.041475	0.106667	0.01736

In [22]:

```
df_new_wine_data_all['quality_label'].head()
```

Out[22]:

```
0    Medium
1    Medium
2    Medium
3    Medium
4    Medium
Name: quality_label, dtype: object
```

In [23]:

```
# same here for test set
df_test.head()
```

Out[23]:

	fixed acidity	residual sugar	pH	citric acid	alcohol	chlorides	density	total sulfur dioxide	volatile acidity	free sulfu dioxid
5316	0.669421	0.021472	0.403101	0.307229	0.347826	0.186047	0.240794	0.032258	0.200000	0.02083
5210	0.429752	0.033742	0.465116	0.186747	0.217391	0.139535	0.212840	0.211982	0.253333	0.06250
3518	0.305785	0.009202	0.364341	0.246988	0.449275	0.068106	0.081357	0.288018	0.080000	0.08680
1622	0.223140	0.108896	0.302326	0.295181	0.101449	0.059801	0.165606	0.375576	0.240000	0.05208
2443	0.231405	0.029141	0.333333	0.198795	0.289855	0.071429	0.116638	0.491935	0.160000	0.13541

In [24]:

```
y_test.head()
```

Out[24]:

```
5316    Medium
5210    Medium
3518    Medium
1622    Medium
2443    Medium
Name: quality_label, dtype: object
```

9.Use the KNN algorithm to predict the quality of wine using its attributes.(12 points)

In [25]:

```
# Predictions using KNN classifier
```

```
knn_pred = KNeighborsClassifier(algorithm = 'ball_tree', leaf_size = 12, n_neighbors =
knn_pred.fit(df_train[X], y_train)
```

Out[25]:
```
KNeighborsClassifier(algorithm='ball_tree', leaf_size=12, n_neighbors=12, p=1,
                     weights='distance')
```

In [26]:
```
# train the model first train set
print('KNeighbors Classifier Training Accuracy: {:2.2%}'.format(accuracy_score(y_train,
# see the Accuracy is 100% for training
```

```
KNeighbors Classifier Training Accuracy: 100.00%
```

In [28]:
```
# Now start prediction with test set
y_pred = knn_pred.predict(df_test)
y_pred
```

Out[28]:
```
array(['Medium', 'Medium', 'Medium', ..., 'Medium', 'High', 'Medium'],
      dtype=object)
```

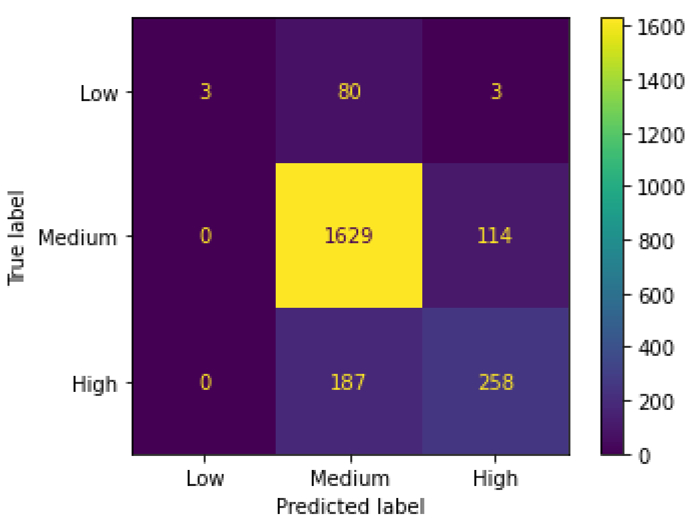
In [29]:
```
# train the model first train set
print('KNeighbors Classifier Test Accuracy: {:2.2%}'.format(accuracy_score(y_test, y_pr
# As you see the accuracy below its not exceptional but okay.
```

```
KNeighbors Classifier Test Accuracy: 83.11%
```

10.Display the confusion matrix to evaluate the model performance. (12 points)

In [30]:
```
plot_confusion_matrix(knn_pred, df_test, y_test, labels=['Low','Medium','High'])
```

Out[30]:
```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1e8f1b18ee0>
```



In [31]:
```
matrix = confusion_matrix(y_test,y_pred, labels=['Low','Medium','High'])
print('Classification report : \n',matrix)
```

```
Classification report :
 [[   3   80    3]
 [   0 1629  114]
 [   0  187  258]]
```

11. Evaluate the model performance by computing Accuracy, Precision and Recall(Sensitivity). (15 points)

In [32]:
```
# You can observe classification report for precision, recall f1-score and accuracy
matrix_report = classification_report(y_test,y_pred, labels=['Low','Medium','High'])
print('Classification report : \n',matrix_report)
```

```
Classification report :
               precision    recall  f1-score   support

         Low       1.00      0.03      0.07        86
      Medium       0.86      0.93      0.90      1743
        High       0.69      0.58      0.63       445

    accuracy                           0.83      2274
   macro avg       0.85      0.52      0.53      2274
weighted avg       0.83      0.83      0.81      2274
```

We you can see one Accuracy(0.83) as a whole, and you could also see the values of each group for Sensitivity(recall), Precision for each group, at the above report.

Now here we can also find the specificity for each group in the following:

In [33]:
```
# For 'Low' group
low_Specificity =(matrix[1,1]+matrix[1,2]+matrix[2,1]+matrix[2,2]) /(matrix[1,1]+matrix
print('Low_Specificity : ', low_Specificity )
```

```
Low_Specificity :  1.0
```

In [34]:
```
# For 'Medium' group
Medium_Specificity =(matrix[0,0]+matrix[0,2]+matrix[2,0]+matrix[2,2]) /(matrix[0,0]+mat
print('Medium_Specificity : ',round(Medium_Specificity,3) )
```

```
Medium_Specificity :  0.497
```

In [35]:
```
# For 'High' group
High_Specificity =(matrix[0,0]+matrix[0,1]+matrix[1,0]+matrix[1,1]) /(matrix[0,0]+matri
print('High_Specificity : ',round(High_Specificity,3) )
```

```
High_Specificity :  0.936
```

In [ ]:
```

```