Midterm Project

Carlos Olivas ID# 861045506

Below we will attempt to create a predictive model for wine. The data to be used contains 11 features that describe each wine and a quality score for the wine. The scores were given by wine experts. This data was previously used by a research group that found that the best model was a support vector machine (SVM). I think it would be safe to trust them. So we too will create an SVM model.

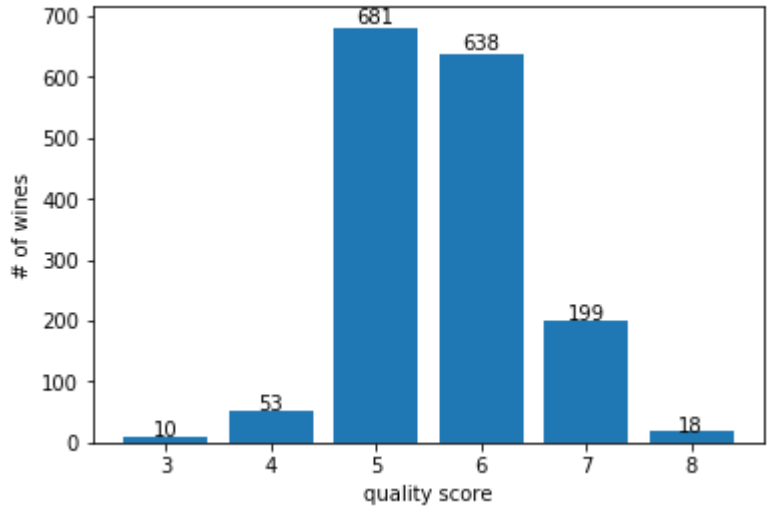
We'll start by importing all the necessary libraries.

In [47]:
```
import pandas as pd
import numpy as np
from sklearn.svm import SVC
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.metrics import confusion_matrix, accuracy_score, classification_report
from sklearn.model_selection import GridSearchCV
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
from imblearn.under_sampling import RandomUnderSampler
from imblearn.over_sampling import RandomOverSampler, ADASYN
```

In [7]:
```
# read in the data from the csv file into a pandas DataFrame
wine_data = pd.read_csv('winequality-red.csv', sep=';')

# format the column names
wine_data.columns = wine_data.columns.str.strip().str.lower().str.replace(' ', '_')
```

We know that the data does not have any missing values, so that step will be skipped. To begin, we'll create a graph to show the distribution of the wines amongst the different quality scores to get a better understanding of our data.

In [8]:
```
# get the count for each quality score to be used to show how imbalanced the data is
quality_counts = wine_data['quality'].value_counts()

# create and show bar graph to show distribution of wines' in quality scores
bars = plt.bar(quality_counts.keys(), quality_counts)
plt.xlabel('quality score')
plt.ylabel('# of wines')

# add annotations to the bars
for bar in bars:
    bar_height = bar.get_height()
    plt.text(bar.get_x() + bar.get_width()/2., 1.01*bar_height, str(bar_height), ha='center')
plt.show()
```



As we can see, although the possible quality score can range from 1-10, the data contains wines with scores between 3-8. Next we will begin to create a basic SVM model. The data will be split into a 70-30, with 70% training data, 15% validation data, and 15% test data.

In [15]:
```
# split the data into sets for training, validation, and test
y = wine_data['quality']
x = wine_data.drop('quality', axis=1)

# split data as 70% train and 30% test
x_train, x_test, y_train, y_test = train_test_split(x, y, test_size=0.3)

# split test data into validation data and test data
x_val, x_test, y_val, y_test = train_test_split(x_test, y_test, test_size=0.5)

# scale the data
sc = StandardScaler()
x_train_s = sc.fit_transform(x_train)
x_val_s = sc.transform(x_val)
x_test_s = sc.transform(x_test)

# create the model using SVM
svc = SVC()
# svc = SVC(gamma='scale', decision_function_shape='ovo')
svc.fit(x_train_s, y_train)
svc_predict = svc.predict(x_val_s)

svc_acc_score = accuracy_score(y_val, svc_predict)

print('SVM basic accuracy: %f' % svc_acc_score)
```

```
SVM basic accuracy: 0.683333
```

In [16]:
```
svc.fit(x_train_s, y_train)
y_pred = svc.predict(x_test_s)

svc_acc_score = accuracy_score(y_test, y_pred)

print('SVM basic accuracy: %f' % (svc_acc_score))
```

```
SVM basic accuracy: 0.600000
```

The default values of the SVC render a 68.33% accuracy with the validation data, and 60% with the testing data. We'll see if we can find better parameters to increase that percentage using Grid Search.

In [17]:
```
parameters = [{'C': [1, 10, 100, 1000], 'kernel': ['linear']},
              {'C': [1, 10, 100, 1000], 'kernel': ['rbf'],
               'gamma': [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]}]
grid_search = GridSearchCV(estimator=svc, param_grid=parameters, scoring='accuracy', cv=3)
grid_search.fit(x_train_s, y_train)
best_accuracy = grid_search.best_score_
best_parameters = grid_search.best_params_
print(best_parameters)
print('Automated projected accuracy: %f' % best_accuracy)
```

```
{'C': 1, 'gamma': 0.6, 'kernel': 'rbf'}
Automated projected accuracy: 0.645219
```

The greatest accuracy the grid search was able to achieve with the indicated parameters came out less than the accuracy we were able to achieve with the default setting for SVC. Granted, it was only cross-validating with the training data itself. The penalty and the kernel are the same as the default values for SVC. We will see how the gamma selected by the grid search performs against the validation data.

In [21]:
```
svc.gamma = 0.6
svc.fit(x_train_s, y_train)
y_pred = svc.predict(x_val_s)
svc_acc_score = accuracy_score(y_val, y_pred)
print('SVM accuracy w/gamma = 0.6: %f' % (svc_acc_score))
```

```
SVM accuracy w/gamma = 0.6: 0.687500
```

The accuracy against the valdation data was better than the grid search projection and the default settings. So I wanted to see what other values for gamma could produce:

In [22]:
```
for g in [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]:
    svc.gamma = g
    svc.fit(x_train_s, y_train)
    y_pred = svc.predict(x_val_s)

    svc_acc_score = accuracy_score(y_val, y_pred)

    print('SVM accuracy w/gamma = %0.1f: %f' % (g, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.1: 0.691667
SVM accuracy w/gamma = 0.2: 0.691667
SVM accuracy w/gamma = 0.3: 0.691667
SVM accuracy w/gamma = 0.4: 0.695833
SVM accuracy w/gamma = 0.5: 0.691667
SVM accuracy w/gamma = 0.6: 0.687500
SVM accuracy w/gamma = 0.7: 0.695833
SVM accuracy w/gamma = 0.8: 0.712500
SVM accuracy w/gamma = 0.9: 0.695833
```

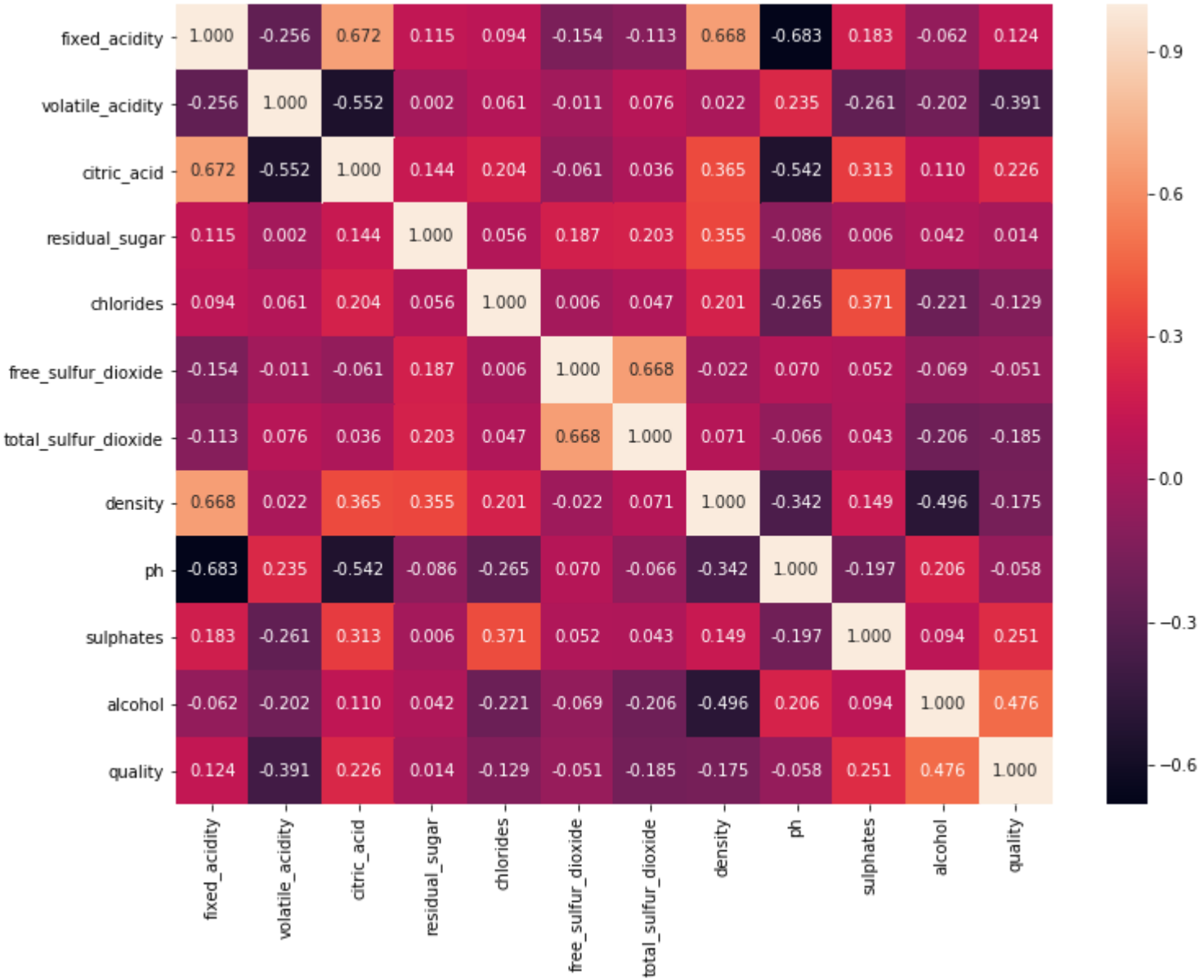
We can see that a gamma value of 0.8 actually produces the best accuracy of about 71.25%. Now, let's see how this performs on the test data.

In [20]:
```
svc.gamma = 0.8
svc.fit(x_train_s, y_train)
y_pred = svc.predict(x_test_s)

svc_acc_score = accuracy_score(y_test, y_pred)

print('SVM accuracy w/gamma = %0.1f: %f' % (svc.gamma, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.8: 0.579167
```

The acuruacy of predicting the test data quality scores actually went down. So, there is room for improvement. So the following will be attempts to increase the accuracy with the validation data before using the model on the test data. One method we can follow is feature selection. The first method of feature selection we will attempt will be to remove the features that seem to have the lowest correlation to the wine's quality score. Below, we will see a heatmap of the correlation of each feature to the quality score of each wine.

In [23]:
```
plt.figure(figsize=(12, 9))
sns.heatmap(wine_data.corr(), annot=True, annot_kws={"size": 10}, fmt='.3f', linewidths=0)
plt.show()
```



If we look at the last row of the heatmap, we can see that the least correlated feature is the residual sugar, followed by free sulfur dioxide and pH. So we'll remove those features from the data and see if that will help improve the model.

In [24]:
```
x_train_fs = x_train.drop(['residual_sugar', 'free_sulfur_dioxide', 'ph'], axis=1)
x_val_fs = x_val.drop(['residual_sugar', 'free_sulfur_dioxide', 'ph'], axis=1)
x_test_fs = x_test.drop(['residual_sugar', 'free_sulfur_dioxide', 'ph'], axis=1)
```

Now we have to rescale everything and run the model again using different values for gamma to find the best predictive accuracy.

In [25]:
```
# re-scale the data
sc = StandardScaler()
x_train_fs_s = sc.fit_transform(x_train_fs)
x_val_fs_s = sc.transform(x_val_fs)
x_test_fs_s = sc.transform(x_test_fs)

for g in [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]:
    svc.gamma = g
    svc.fit(x_train_fs_s, y_train)
    y_pred = svc.predict(x_val_fs_s)

    svc_acc_score = accuracy_score(y_val, y_pred)

    print('SVM accuracy w/gamma = %0.1f: %f' % (g, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.1: 0.650000
SVM accuracy w/gamma = 0.2: 0.675000
SVM accuracy w/gamma = 0.3: 0.679167
SVM accuracy w/gamma = 0.4: 0.666667
SVM accuracy w/gamma = 0.5: 0.675000
SVM accuracy w/gamma = 0.6: 0.675000
SVM accuracy w/gamma = 0.7: 0.670833
SVM accuracy w/gamma = 0.8: 0.687500
SVM accuracy w/gamma = 0.9: 0.679167
```

As we can see, a gamma value of 0.8, inclusively, would render the predictive accuracy of 68.75% of the validation data. An improvement from the highest predictive accuracy from above. Let's see if the improvement is also seen in with the test data.

In [27]:
```
svc.gamma = 0.8
svc.fit(x_train_fs_s, y_train)
y_pred = svc.predict(x_test_fs_s)

svc_acc_score = accuracy_score(y_test, y_pred)

print('SVM accuracy w/gamma = %0.1f: %f' % (svc.gamma, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.8: 0.591667
```

The predictive accuracy of the test data dropped to 59.17%. But, perhaps we can tru a different method of feature selection. Another method we can try is univariate selection. This uses scikit-learn's SelectKBest class to run different statistical tests to show the best features.

In [28]:
```
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import chi2

bestfeatures = SelectKBest(score_func=chi2, k=11)
fit = bestfeatures.fit(x_train,y_train)
dfscores = pd.DataFrame(fit.scores_)
dfcolumns = pd.DataFrame(x_train.columns)

#concat two dataframes for better visualization
featureScores = pd.concat([dfcolumns,dfscores],axis=1)
featureScores.columns = ['Specs','Score']  #naming the dataframe columns
print(featureScores.nlargest(10,'Score'))  #print 10 best features
```

```
                  Specs        Score
6   total_sulfur_dioxide  1850.537651
5    free_sulfur_dioxide   135.582551
10               alcohol    34.633674
1       volatile_acidity     9.485278
0          fixed_acidity     8.658984
2            citric_acid     8.625872
3         residual_sugar     5.666101
9               sulphates     2.762647
4               chlorides     0.775297
8                      ph     0.117185
```

For this instance we chose to use the chi-squared test. The test allows us to see which features are most likely to be independent and be irrelevant to the classification. Based on the scores above, it would seem that ph and chlorides would be good feature to exclude from the model.

In [36]:
```
x_train_fs = x_train.drop(['ph'], axis=1)
x_val_fs = x_val.drop(['ph'], axis=1)
x_test_fs = x_test.drop(['ph'], axis=1)

# re-scale the data
sc = StandardScaler()
x_train_fs_s = sc.fit_transform(x_train_fs)
x_val_fs_s = sc.transform(x_val_fs)
x_test_fs_s = sc.transform(x_test_fs)

for g in [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]:
    svc.gamma = g
    svc.fit(x_train_fs_s, y_train)
    y_pred = svc.predict(x_val_fs_s)

    svc_acc_score = accuracy_score(y_val, y_pred)

    print('SVM accuracy w/gamma = %0.1f: %f' % (g, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.1: 0.675000
SVM accuracy w/gamma = 0.2: 0.695833
SVM accuracy w/gamma = 0.3: 0.700000
SVM accuracy w/gamma = 0.4: 0.691667
SVM accuracy w/gamma = 0.5: 0.691667
SVM accuracy w/gamma = 0.6: 0.687500
SVM accuracy w/gamma = 0.7: 0.700000
SVM accuracy w/gamma = 0.8: 0.687500
SVM accuracy w/gamma = 0.9: 0.700000
```

We can see that removing the feature ph has given us a marginally better predictive accuracy of about 70% with gamma values of 0.1. This will be the accepted feature selection. Now we will see how this model predicts the test data.

In [39]:
```
svc.gamma = 0.3
svc.fit(x_train_fs_s, y_train)
y_pred = svc.predict(x_test_fs_s)

svc_acc_score = accuracy_score(y_test, y_pred)

print('SVM accuracy w/gamma = %0.1f: %f' % (svc.gamma, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.3: 0.604167
```

While this is the best accuracy we've seen at 60.41%, it could hopefully get better. As we saw above, there is a ridiculously greater number of wines with quality scores 5 and 6 than any of the other scores. This imbalance in the data could cause the model to bias towards the over-represented classes. One method to correct this would be to undersample the over-represented classes. This would entail randomly removing wines of the majority class from the training data.

In [32]:
```
x_train_fs = x_train.drop(['ph'], axis=1)
x_val_fs = x_val.drop(['ph'], axis=1)
x_test_fs = x_test.drop(['ph'], axis=1)

# resample the training data using under-sampling
rus = RandomUnderSampler(random_state=0, sampling_strategy='majority')
x_train_fsu, y_train_u = rus.fit_resample(x_train_fs, y_train)

# re-scale the data
sc = StandardScaler()
x_train_fsu_s = sc.fit_transform(x_train_fsu)
x_val_fs_s = sc.transform(x_val_fs)
x_test_fs_s = sc.transform(x_test_fs)

for g in [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]:
    svc.gamma = g
    svc.fit(x_train_fsu_s, y_train_u)
    y_pred = svc.predict(x_val_fs_s)

    svc_acc_score = accuracy_score(y_val, y_pred)

    print('SVM accuracy w/gamma = %0.1f: %f' % (g, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.1: 0.383333
SVM accuracy w/gamma = 0.2: 0.395833
SVM accuracy w/gamma = 0.3: 0.408333
SVM accuracy w/gamma = 0.4: 0.395833
SVM accuracy w/gamma = 0.5: 0.387500
SVM accuracy w/gamma = 0.6: 0.387500
SVM accuracy w/gamma = 0.7: 0.387500
SVM accuracy w/gamma = 0.8: 0.391667
SVM accuracy w/gamma = 0.9: 0.391667
```

As we can see, the projected prediction accuracies went down. This could be due to the smaller size of the training data. Another method we can attempt is over-sampling, wherein the minority class is oversampled with replacement.

In [33]:
```
ros = RandomOverSampler(sampling_strategy='minority')

x_train_fs = x_train.drop(['ph'], axis=1)
x_val_fs = x_val.drop(['ph'], axis=1)
x_test_fs = x_test.drop(['ph'], axis=1)

x_train_fso, y_train_o = ros.fit_sample(x_train_fs, y_train)

# re-scale the data
sc = StandardScaler()
x_train_fso_s = sc.fit_transform(x_train_fso)
x_val_fs_s = sc.transform(x_val_fs)
x_test_fs_s = sc.transform(x_test_fs)

for g in [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]:
    svc.gamma = g
    svc.fit(x_train_fso_s, y_train_o)
    y_pred = svc.predict(x_val_fs_s)

    svc_acc_score = accuracy_score(y_val, y_pred)

    print('SVM accuracy w/gamma = %0.1f: %f' % (g, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.1: 0.637500
SVM accuracy w/gamma = 0.2: 0.683333
SVM accuracy w/gamma = 0.3: 0.695833
SVM accuracy w/gamma = 0.4: 0.679167
SVM accuracy w/gamma = 0.5: 0.683333
SVM accuracy w/gamma = 0.6: 0.687500
SVM accuracy w/gamma = 0.7: 0.704167
SVM accuracy w/gamma = 0.8: 0.695833
SVM accuracy w/gamma = 0.9: 0.700000
```

In [34]:
```
svc.gamma = 0.1
svc.fit(x_train_fso_s, y_train_o)
y_pred = svc.predict(x_test_fs_s)
svc_acc_score = accuracy_score(y_test, y_pred)

print('SVM accuracy w/gamma = %0.1f: %f' % (svc.gamma, svc_acc_score))
```

```
SVM accuracy w/gamma = 0.1: 0.587500
```

Unfortunately, oversampling the minority data did not produce a a great prediction accuracy. Let's see a few evaluation metrics of our most effective iteration of our model.

In [56]:
```
x_train_fs = x_train.drop(['ph'], axis=1)
x_val_fs = x_val.drop(['ph'], axis=1)
x_test_fs = x_test.drop(['ph'], axis=1)

# re-scale the data
sc = StandardScaler()
x_train_fs_s = sc.fit_transform(x_train_fs)
x_val_fs_s = sc.transform(x_val_fs)
x_test_fs_s = sc.transform(x_test_fs)

# predict the quality scores of the test data
svc.gamma = 0.3
svc.fit(x_train_fs_s, y_train)
y_pred = svc.predict(x_test_fs_s)

conf_mtrx = confusion_matrix(y_test, y_pred)
svc_acc_score = accuracy_score(y_test, y_pred)
classif_report = classification_report(y_test, y_pred)

print('SMV model using RBF kernel and gamma value of 0.3:\n')
print('Accuracy Score: %f\n' % (svc_acc_score))
print('Confusion Matrix:')
print(conf_mtrx)
print()
print("Classification report:")
print(classif_report)
```

```
SMV model using RBF kernel and gamma value of 0.3:

Accuracy Score: 0.604167

Confusion Matrix:
[[ 0  0  3  0  0  0]
 [ 0  0  8  1  0  0]
 [ 0  0 65 19  1  0]
 [ 0  0 37 71  3  0]
 [ 0  0  0 19  9  0]
 [ 0  0  0  2  2  0]]

Classification report:
              precision    recall  f1-score   support

           3       0.00      0.00      0.00         3
           4       0.00      0.00      0.00         9
           5       0.58      0.76      0.66        85
           6       0.63      0.64      0.64       111
           7       0.60      0.32      0.42        28
           8       0.00      0.00      0.00         4

    accuracy                           0.60       240
   macro avg       0.30      0.29      0.29       240
weighted avg       0.57      0.60      0.58       240


C:\Users\Carlos Olivas\AppData\Roaming\Python\Python36\site-packages\sklearn\metrics\classification.py:1437:
UndefinedMetricWarning: Precision and F-score are ill-defined and being set to 0.0 in labels with no predicte
d samples.
  'precision', 'predicted', average, warn_for)
C:\Users\Carlos Olivas\AppData\Roaming\Python\Python36\site-packages\sklearn\metrics\classification.py:1437:
UndefinedMetricWarning: Precision and F-score are ill-defined and being set to 0.0 in labels with no predicte
d samples.
  'precision', 'predicted', average, warn_for)
C:\Users\Carlos Olivas\AppData\Roaming\Python\Python36\site-packages\sklearn\metrics\classification.py:1437:
UndefinedMetricWarning: Precision and F-score are ill-defined and being set to 0.0 in labels with no predicte
d samples.
  'precision', 'predicted', average, warn_for)
```

So the greatest accuracy we achieved of the test data was 60.41%, with an SVM model with an RBF kernel (default kernel) and a gamma value of 0.3 where we applied feature selection to remove the 'ph' feature. Removal of additional features only caused our accuracy scores to drop. With the confusion matrix, we are able to see exactly what predictions our model made of the test data. Of the incorrect classifications, the majority of those were incorrect classifications into quality scores of 5 or 6. This is to be expected due to the data imbalance. We can also see that the lowest populated quality scores of 3, 4, and 8 had 0 accuracte classifications. This is more clearly explained in the classification report. Again, this is an effect of the data imbalance, but also a result of having such a small amount of data for those classes in the training set. From the classification report, we can see that the best classifications were made when classifying wines of quality score 5 and 6. The summarative f-1 score shows that the best classifications correlate with the population of each score in the data set. This could also just be some element of luck. If there are more elements of a certain class, it is more likely that items of that class are classified correctly into that class.

Different divisions of the data into training and testing sets would give different prediction accuracies. I believe that it would be difficult to produce an accurate model of this data due to the fact that the quality scores are subjective. There are multiple examples where wine experts were tricked into giving a cheaper wine a higher rating just by placing it in a different bottle. So the consistency of the wine experts' ratings could be doubtful. Here is an article where such a conclusion was made: https://www.theguardian.com/lifeandstyle/2013/jun/23/wine-tasting-junk-science-analysis (https://www.theguardian.com/lifeandstyle/2013/jun/23/wine-tasting-junk-science-analysis)