Grid Search and Pipelining

November 1, 2018

1 Pipelining in machine learning

```
In [2]: import numpy as np
        import pandas as pd
        import seaborn as sns

        from sklearn import tree
        from sklearn.externals import joblib
        from sklearn.decomposition import PCA
        from sklearn.pipeline import Pipeline
        from sklearn.datasets import load_iris
        from sklearn.metrics import accuracy_score
        from sklearn.ensemble import RandomForestClassifier
        from sklearn.svm import SVC
        from sklearn.linear_model import SGDClassifier
        from sklearn.metrics import confusion_matrix, classification_report
        from sklearn.preprocessing import StandardScaler, LabelEncoder
        from sklearn.model_selection import train_test_split, GridSearchCV, cross_val_score

        import matplotlib.pyplot as plt
        %matplotlib inline
```

1.1 Loading the dataset into memory

```
In [17]: iris = load_iris()
         X_train, X_test, y_train, y_test = train_test_split(iris.data,
                                                             iris.target,
                                                             test_size=0.2,
                                                             random_state=42)
```

1.2 Constructing pipelines for data processing

`sklearn.pipeline.Pipeline(steps, memory=None)`

```
In [18]: pipe_lr = Pipeline([('scl', StandardScaler()),
                             ('pca', PCA(n_components=2)),
                             ('clf', LogisticRegression(random_state=42))])
```

```
        pipe_svm = Pipeline([('scl', StandardScaler()),
                             ('pca', PCA(n_components=2)),
                             ('clf', svm.SVC(random_state=42))])

        pipe_dt = Pipeline([('scl', StandardScaler()),
                            ('pca', PCA(n_components=2)),
                            ('clf', tree.DecisionTreeClassifier(random_state=42))])

        # List of pipelines for ease of iteration
        pipelines = [pipe_lr, pipe_svm, pipe_dt]

        # Dictionary of pipelines and classifier types for ease of reference
        pipe_dict = {0: 'Logistic Regression', 1: 'Support Vector Machine', 2: 'Decision Tree
```

1.3 Fitting the data to the pipelines

```
In [19]: # Fit the pipelines
         for pipe in pipelines:
             pipe.fit(X_train, y_train)

         # Compare accuracies
         for idx, val in enumerate(pipelines):
             print('%s pipeline test accuracy: %.3f' % (pipe_dict[idx], val.score(X_test, y_te

         # Identify the most accurate model on test data
         best_acc = 0.0
         best_clf = 0
         best_pipe = ''
         for idx, val in enumerate(pipelines):
             if val.score(X_test, y_test) > best_acc:
                 best_acc = val.score(X_test, y_test)
                 best_pipe = val
                 best_clf = idx
         print('Classifier with best accuracy: %s' % pipe_dict[best_clf])

         # Save pipeline to file
         joblib.dump(best_pipe, 'best_pipeline.pkl', compress=1)
         print('Saved %s pipeline to file' % pipe_dict[best_clf])
```

```
Logistic Regression pipeline test accuracy: 0.933
Support Vector Machine pipeline test accuracy: 0.900
Decision Tree pipeline test accuracy: 0.867
Classifier with best accuracy: Logistic Regression
Saved Logistic Regression pipeline to file
```

2 Integrating pipeline with grid search

```
In [20]: from sklearn.grid_search import GridSearchCV
```

2.0.1 List of parameters for the decision tree classifier

```
In [21]: print('Decision tree model hyperparameters:\n', pipe_dt.steps[2][1].get_params())
```

```
Decision tree model hyperparameters:
 {'class_weight': None, 'criterion': 'gini', 'max_depth': None, 'max_features': None, 'max_lea
```

2.1 Selected hyperparameters for grid search

- **criterion** - This is the function used to evaluate the quality of the split; we will use both options available in Scikit-learn: Gini impurity and information gain (entropy)
- **min_samples_leaf** - This is the minimum number of samples required for a valid leaf node; we will use the integer range 1 to 5
- **max_depth** - The is the maximum depth of the tree; we will use the integer range 1 to 5
- **min_samples_split** - This is the minimum number of samples required in order to split a non-leaf node; we will use the integer range 1 to 5
- **presort** - This indicates whether or not to presort the data in order to speed up the location of best splits during fitting; this does not have any effect on the resulting model accuracy (only on training times).

```
In [22]: param_range = [1, 2, 3, 4, 5]

         # Set grid search params
         grid_params = [{'clf__criterion': ['gini', 'entropy'],
                         'clf__min_samples_leaf': param_range,
                         'clf__max_depth': param_range,
                         'clf__min_samples_split': param_range[1:],
                         'clf__presort': [True, False]}]
```

```
In [23]: # Construct grid search
         gs = GridSearchCV(estimator=pipe_dt,
                           param_grid=grid_params,
                           scoring='accuracy',
                           cv=10)
```

```
In [24]: # Fit using grid search
         gs.fit(X_train, y_train)

         # Best accuracy
         print('Best accuracy: %.3f' % gs.best_score_)

         # Best params
         print('\nBest params:\n', gs.best_params_)
```

```
Best accuracy: 0.925

Best params:
 {'clf__criterion': 'gini', 'clf__max_depth': 2, 'clf__min_samples_leaf': 1, 'clf__min_samples_
```

3 Managing multiple models, pipelines and grid searches

```
In [13]: # Construct some pipelines
         pipe_lr = Pipeline([('scl', StandardScaler()),
                             ('clf', LogisticRegression(random_state=42))])

         pipe_lr_pca = Pipeline([('scl', StandardScaler()),
                             ('pca', PCA(n_components=2)),
                             ('clf', LogisticRegression(random_state=42))])

         pipe_rf = Pipeline([('scl', StandardScaler()),
                             ('clf', RandomForestClassifier(random_state=42))])

         pipe_rf_pca = Pipeline([('scl', StandardScaler()),
                             ('pca', PCA(n_components=2)),
                             ('clf', RandomForestClassifier(random_state=42))])

         pipe_svm = Pipeline([('scl', StandardScaler()),
                             ('clf', svm.SVC(random_state=42))])

         pipe_svm_pca = Pipeline([('scl', StandardScaler()),
                             ('pca', PCA(n_components=2)),
                             ('clf', svm.SVC(random_state=42))])
```

3.1 Setting up the grid search parameters for each classifier

```
In [13]: param_range = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
         param_range_fl = [1.0, 0.5, 0.1]

         grid_params_lr = [{'clf__penalty': ['l1', 'l2'],
                            'clf__C': param_range_fl,
                            'clf__solver': ['liblinear']}]

         grid_params_rf = [{'clf__criterion': ['gini', 'entropy'],
                            'clf__min_samples_leaf': param_range,
                            'clf__max_depth': param_range,
                            'clf__min_samples_split': param_range[1:]}]

         grid_params_svm = [{'clf__kernel': ['linear', 'rbf'],
                             'clf__C': param_range}]
```

3.2 Execution

```
In [15]: jobs = -1

         gs_lr = GridSearchCV(estimator=pipe_lr,
                              param_grid=grid_params_lr,
                              scoring='accuracy',
                              cv=10)

         gs_lr_pca = GridSearchCV(estimator=pipe_lr_pca,
                                  param_grid=grid_params_lr,
                                  scoring='accuracy',
                                  cv=10)

         gs_rf = GridSearchCV(estimator=pipe_rf,
                              param_grid=grid_params_rf,
                              scoring='accuracy',
                              cv=10,
                              n_jobs=jobs)

         gs_rf_pca = GridSearchCV(estimator=pipe_rf_pca,
                                  param_grid=grid_params_rf,
                                  scoring='accuracy',
                                  cv=10,
                                  n_jobs=jobs)

         gs_svm = GridSearchCV(estimator=pipe_svm,
                               param_grid=grid_params_svm,
                               scoring='accuracy',
                               cv=10,
                               n_jobs=jobs)

         gs_svm_pca = GridSearchCV(estimator=pipe_svm_pca,
                                   param_grid=grid_params_svm,
                                   scoring='accuracy',
                                   cv=10,
                                   n_jobs=jobs)
```

```
In [16]: grids = [gs_lr, gs_lr_pca, gs_rf, gs_rf_pca, gs_svm, gs_svm_pca]


         grid_dict = {0: 'Logistic Regression', 1: 'Logistic Regression w/PCA',
                      2: 'Random Forest', 3: 'Random Forest w/PCA',
                      4: 'Support Vector Machine', 5: 'Support Vector Machine w/PCA'}
```

3.3 Fitting the grid search objects

```
In [19]: print('Performing model optimizations...')
         best_acc = 0.0
```

```
    best_clf = 0
    best_gs = ''
    for idx, gs in enumerate(grids):
        print('\nEstimator: %s' % grid_dict[idx])
        # Fit grid search
        gs.fit(X_train, y_train)
        # Best params
        print('Best params: %s' % gs.best_params_)
        # Best training data accuracy
        print('Best training accuracy: %.3f' % gs.best_score_)
        # Predict on test data with best params
        y_pred = gs.predict(X_test)
        # Test data accuracy of model with best params
        print('Test set accuracy score for best params: %.3f ' % accuracy_score(y_test, y
        # Track best (highest test accuracy) model
        if accuracy_score(y_test, y_pred) > best_acc:
            best_acc = accuracy_score(y_test, y_pred)
            best_gs = gs
            best_clf = idx
    print('\nClassifier with best test set accuracy: %s' % grid_dict[best_clf])

    # Save best grid search pipeline to file
    dump_file = 'best_gs_pipeline.pkl'
    joblib.dump(best_gs, dump_file, compress=1)
    print('\nSaved %s grid search pipeline to file: %s' % (grid_dict[best_clf], dump_file
```

```
Performing model optimizations...

Estimator: Logistic Regression
Best params: {'clf__C': 1.0, 'clf__penalty': 'l1', 'clf__solver': 'liblinear'}
Best training accuracy: 0.917
Test set accuracy score for best params: 0.967

Estimator: Logistic Regression w/PCA
Best params: {'clf__C': 0.5, 'clf__penalty': 'l1', 'clf__solver': 'liblinear'}
Best training accuracy: 0.858
Test set accuracy score for best params: 0.933

Estimator: Random Forest
Best params: {'clf__criterion': 'gini', 'clf__max_depth': 3, 'clf__min_samples_leaf': 2, 'clf_
Best training accuracy: 0.942
Test set accuracy score for best params: 1.000

Estimator: Random Forest w/PCA
Best params: {'clf__criterion': 'entropy', 'clf__max_depth': 5, 'clf__min_samples_leaf': 1, 'c
Best training accuracy: 0.917
Test set accuracy score for best params: 0.900
```

```
Estimator: Support Vector Machine
Best params: {'clf__C': 3, 'clf__kernel': 'linear'}
Best training accuracy: 0.967
Test set accuracy score for best params: 0.967

Estimator: Support Vector Machine w/PCA
Best params: {'clf__C': 4, 'clf__kernel': 'rbf'}
Best training accuracy: 0.925
Test set accuracy score for best params: 0.900

Classifier with best test set accuracy: Random Forest

Saved Random Forest grid search pipeline to file: best_gs_pipeline.pkl
```

4 On my own dataset

In this notebook, First I have done some exploration on the data using matplotlib and seaborn. Then, I use different classifier models to predict the quality of the wine.

1. **Random Forest Classifier**
2. **Stochastic Gradient Descent Classifier**
3. **Support Vector Classifier(SVC)**

Then I use cross validation evaluation technique to optimize the model performance.

1. **Grid Search CV**
2. **Cross Validation Score**

```
In [6]: #Loading dataset
        wine = pd.read_csv('../Dataset/winequality-red.csv', sep=';')
```

```
In [7]: #Let's check how the data is distributed
        wine.head()
```

```
Out[7]:    fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
        0            7.4              0.70         0.00             1.9      0.076
        1            7.8              0.88         0.00             2.6      0.098
        2            7.8              0.76         0.04             2.3      0.092
        3           11.2              0.28         0.56             1.9      0.075
        4            7.4              0.70         0.00             1.9      0.076

           free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
        0                 11.0                  34.0   0.9978  3.51       0.56
        1                 25.0                  67.0   0.9968  3.20       0.68
        2                 15.0                  54.0   0.9970  3.26       0.65
        3                 17.0                  60.0   0.9980  3.16       0.58
        4                 11.0                  34.0   0.9978  3.51       0.56

           alcohol  quality
        0      9.4        5
        1      9.8        5
        2      9.8        5
        3      9.8        6
        4      9.4        5
```

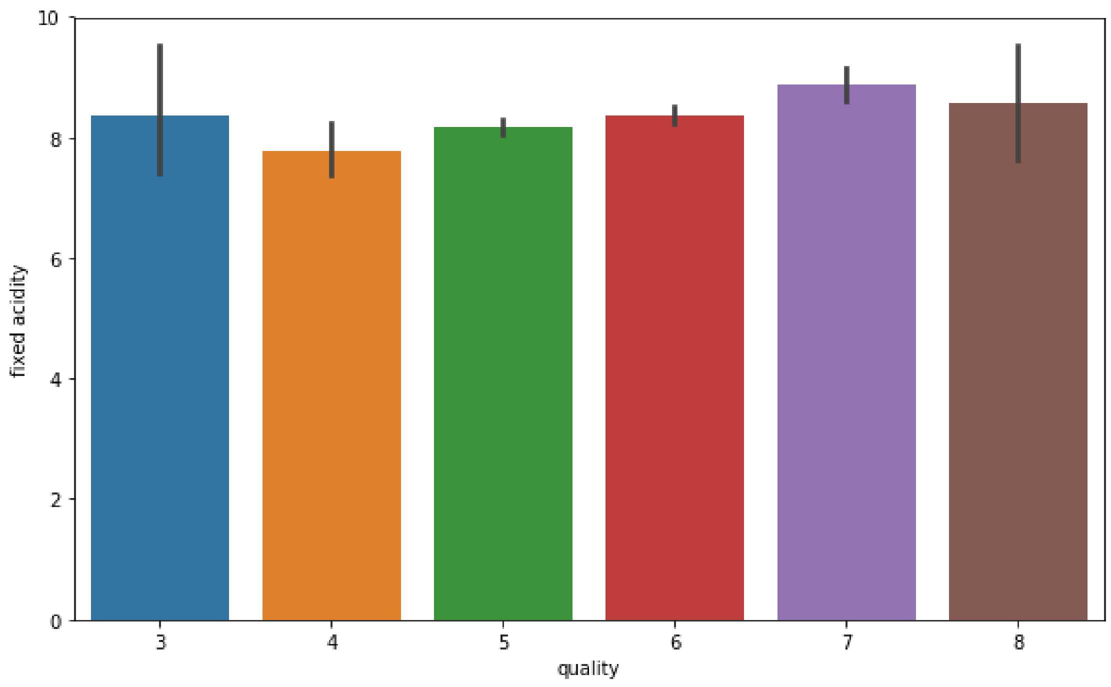
```
In [8]: #Information about the data columns
        wine.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1599 entries, 0 to 1598
Data columns (total 12 columns):
fixed acidity           1599 non-null float64
volatile acidity        1599 non-null float64
citric acid             1599 non-null float64
residual sugar          1599 non-null float64
chlorides               1599 non-null float64
free sulfur dioxide     1599 non-null float64
total sulfur dioxide    1599 non-null float64
density                 1599 non-null float64
pH                      1599 non-null float64
sulphates               1599 non-null float64
alcohol                 1599 non-null float64
quality                 1599 non-null int64
dtypes: float64(11), int64(1)
memory usage: 150.0 KB
```

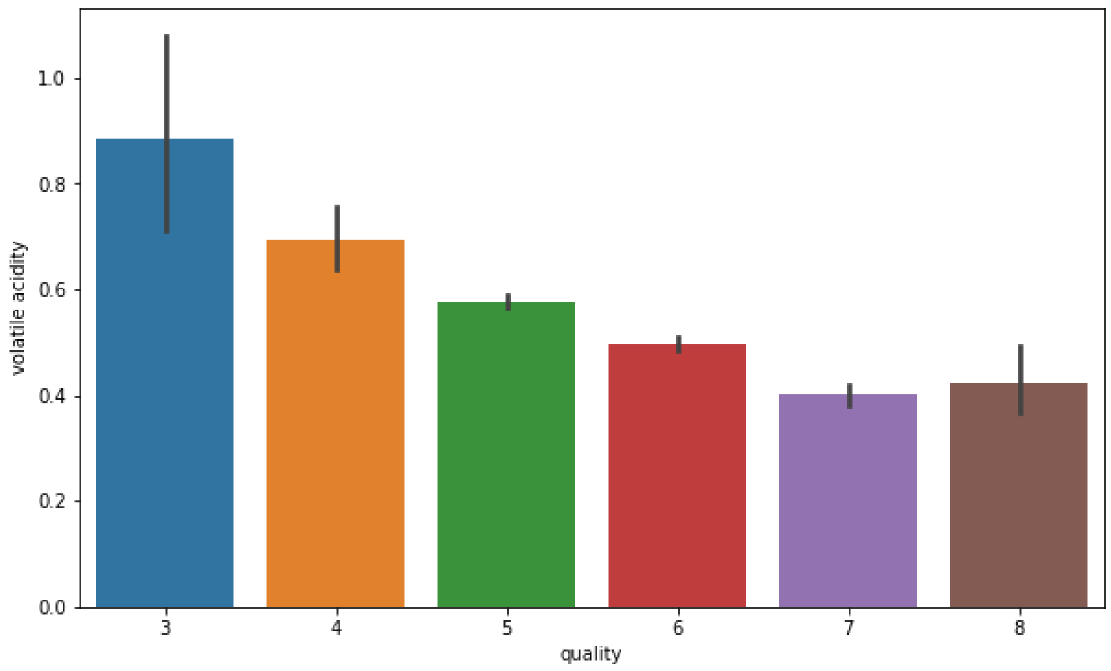
4.1 Let's do some plotting to know how the data columns are distributed in the dataset

```
In [9]: #Here we see that fixed acidity does not give any specification to classify the qualit
        fig = plt.figure(figsize = (10,6))
        sns.barplot(x = 'quality', y = 'fixed acidity', data = wine)
```

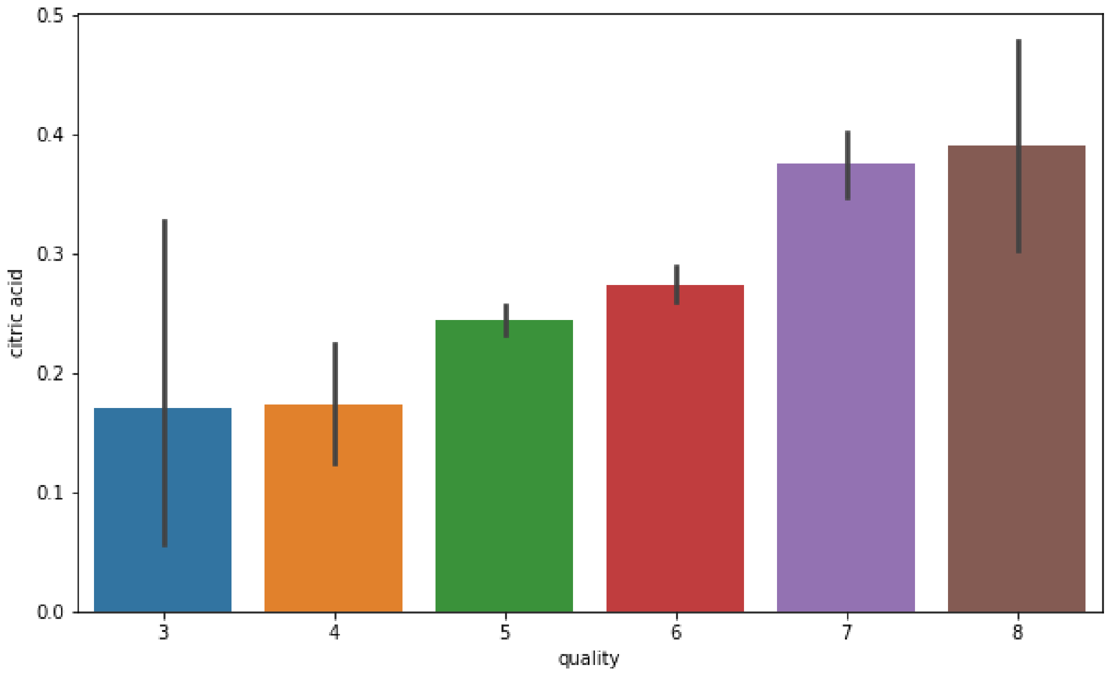
```
Out[9]: <matplotlib.axes._subplots.AxesSubplot at 0x7f7135278940>
```



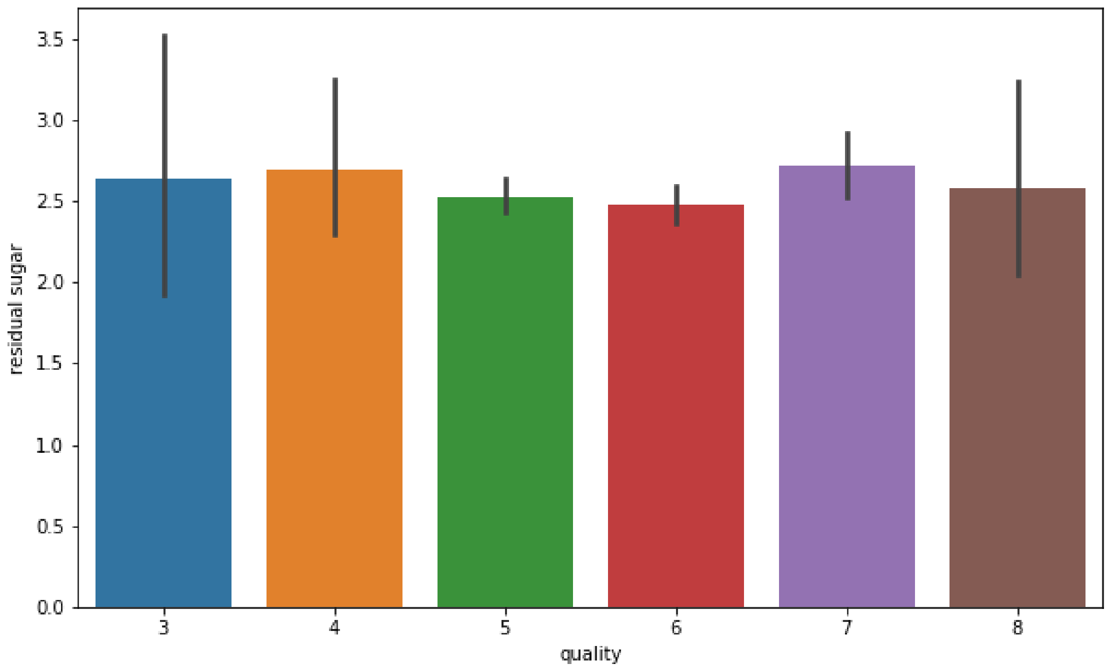
```
In [10]: #Here we see that its quite a downing trend in the volatile acidity as we go higher th
         fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'volatile acidity', data = wine)

Out[10]: <matplotlib.axes._subplots.AxesSubplot at 0x7f71316a3860>
```



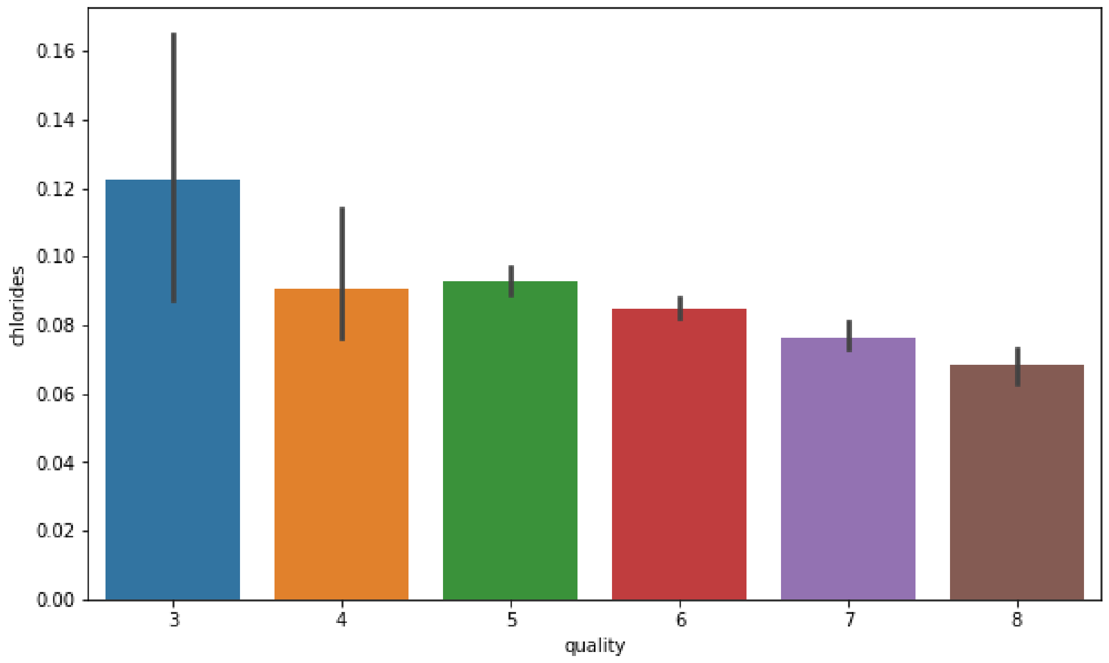
```
In [11]: #Composition of citric acid go higher as we go higher in the quality of the wine
         fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'citric acid', data = wine)

Out[11]: <matplotlib.axes._subplots.AxesSubplot at 0x7f713166f0b8>
```



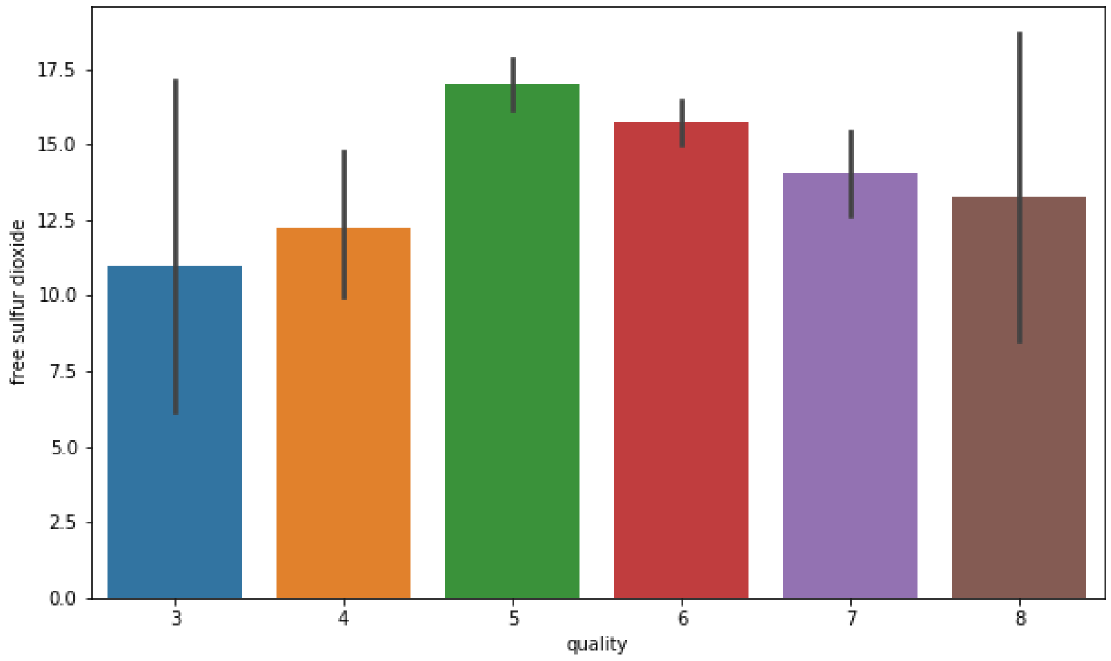
```
In [12]: fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'residual sugar', data = wine)

Out[12]: <matplotlib.axes._subplots.AxesSubplot at 0x7f71315e5438>
```



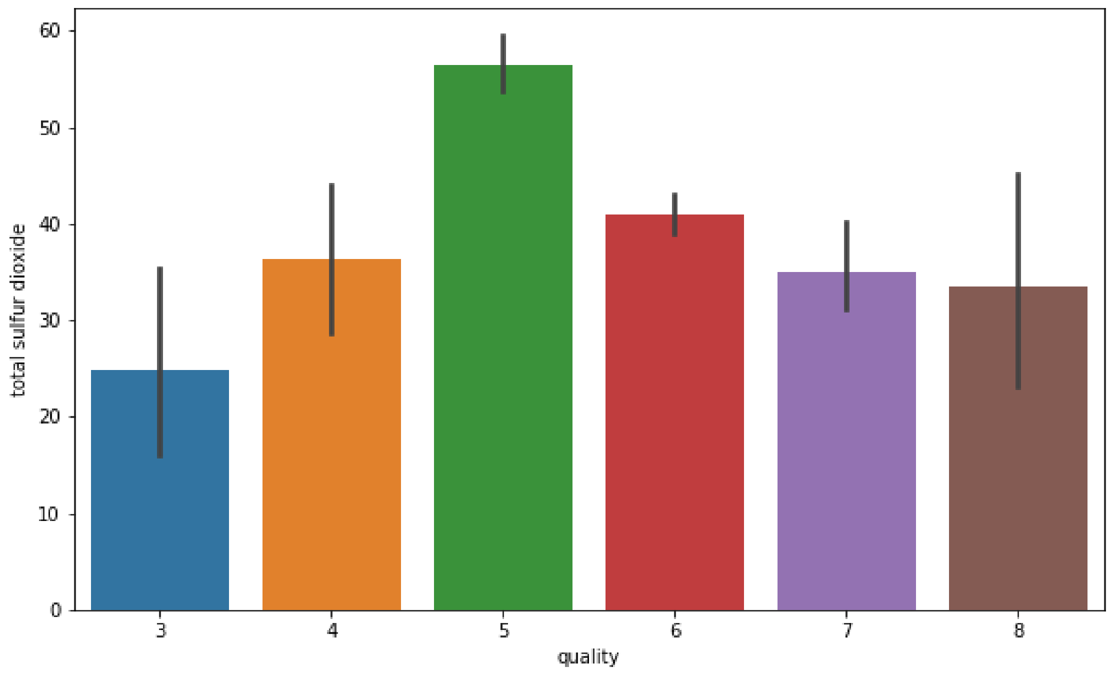
```
In [13]: #Composition of chloride also go down as we go higher in the quality of the wine
         fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'chlorides', data = wine)

Out[13]: <matplotlib.axes._subplots.AxesSubplot at 0x7f7131588a20>
```



```
In [14]: fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'free sulfur dioxide', data = wine)

Out[14]: <matplotlib.axes._subplots.AxesSubplot at 0x7f7131502be0>
```

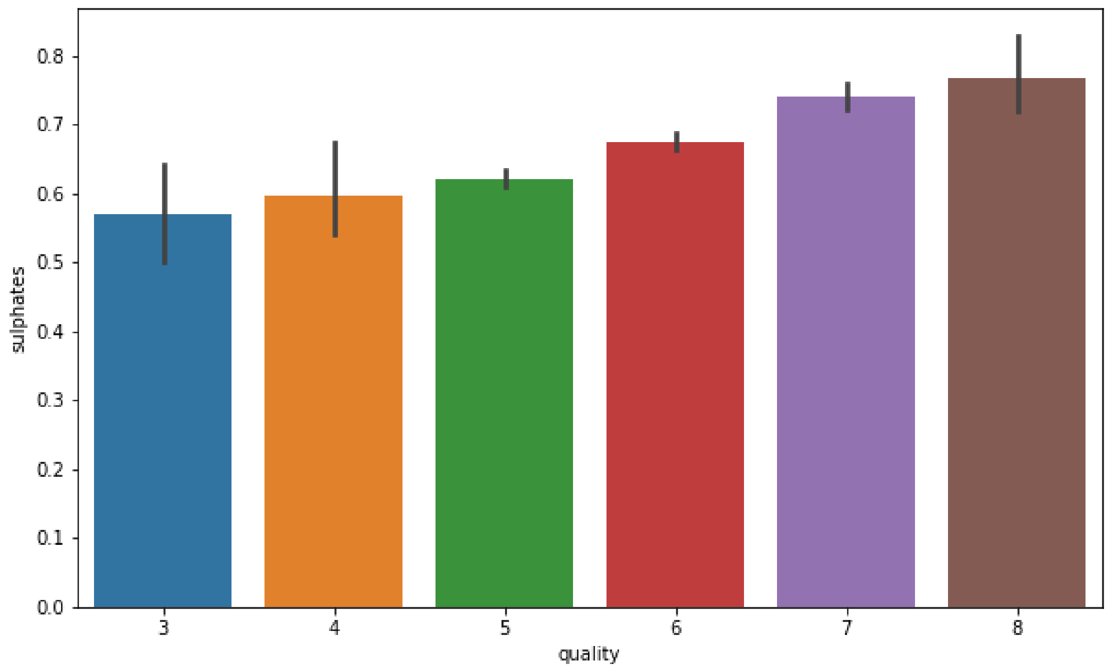


```
In [15]: fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'total sulfur dioxide', data = wine)

Out[15]: <matplotlib.axes._subplots.AxesSubplot at 0x7f71314db5f8>
```

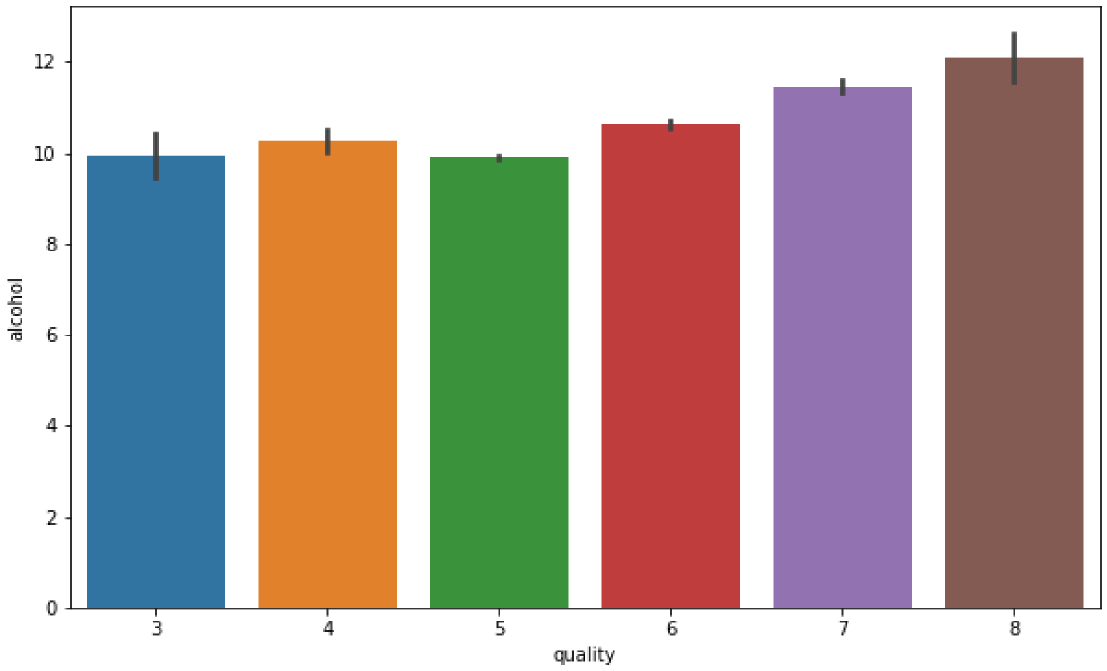


```
In [16]: #Sulphates level goes higher with the quality of wine
         fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'sulphates', data = wine)
```

```
Out[16]: <matplotlib.axes._subplots.AxesSubplot at 0x7f71313e27f0>
```



```
In [17]: #Alcohol level also goes higher as te quality of wine increases
         fig = plt.figure(figsize = (10,6))
         sns.barplot(x = 'quality', y = 'alcohol', data = wine)

Out[17]: <matplotlib.axes._subplots.AxesSubplot at 0x7f713144dac8>
```



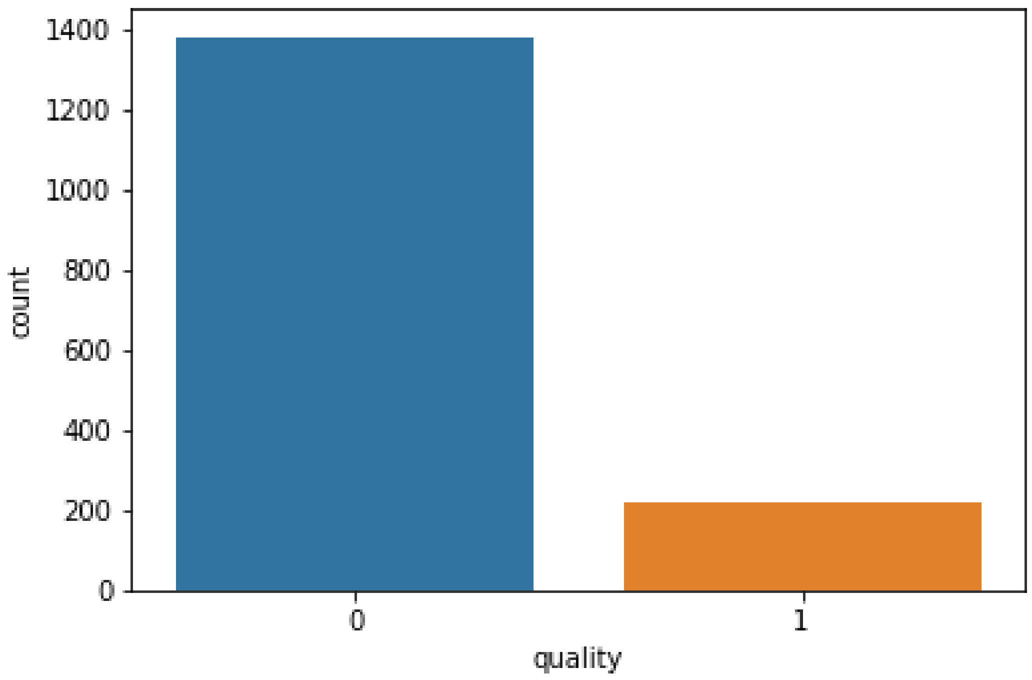
4.2 Preprocessing Data for performing Machine learning algorithms

```
In [18]: #Making binary classificaion for the response variable.
         #Dividing wine as good and bad by giving the limit for the quality
         bins = (2, 6.5, 8)
         group_names = ['bad', 'good']
         wine['quality'] = pd.cut(wine['quality'], bins = bins, labels = group_names)

In [19]: #Now lets assign a labels to our quality variable
         label_quality = LabelEncoder()

In [20]: #Bad becomes 0 and good becomes 1
         wine['quality'] = label_quality.fit_transform(wine['quality'])

In [21]: wine['quality'].value_counts()
```

```
Out[21]: 0    1382
         1     217
         Name: quality, dtype: int64
```

```
In [22]: sns.countplot(wine['quality'])
```

```
Out[22]: <matplotlib.axes._subplots.AxesSubplot at 0x7f713131ffd0>
```



```
In [23]: #Now seperate the dataset as response variable and feature variabes
         X = wine.drop('quality', axis = 1)
         y = wine['quality']
```

```
In [24]: #Train and Test splitting of data
         X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_sta
```

```
In [25]: #Applying Standard scaling to get optimized result
         sc = StandardScaler()
```

```
In [26]: X_train = sc.fit_transform(X_train)
         X_test = sc.fit_transform(X_test)
```

4.3 Our training and testing data is ready now to perform machine learning algorithm

4.3.1 Random Forest Classifier

```
In [27]: rfc = RandomForestClassifier(n_estimators=200)
         rfc.fit(X_train, y_train)
         pred_rfc = rfc.predict(X_test)
```

```
In [28]: #Let's see how our model performed
         print(classification_report(y_test, pred_rfc))

             precision    recall  f1-score   support

          0       0.91      0.96      0.93       273
          1       0.65      0.43      0.51        47

avg / total       0.87      0.88      0.87       320
```

Random forest gives the accuracy of 87%

```
In [29]: #Confusion matrix for the random forest classification
         print(confusion_matrix(y_test, pred_rfc))

[[262  11]
 [ 27  20]]
```

4.4 Stochastic Gradient Decent Classifier

```
In [30]: sgd = SGDClassifier(penalty=None)
         sgd.fit(X_train, y_train)
         pred_sgd = sgd.predict(X_test)

/home/prateek/anaconda3/envs/dltf/lib/python3.6/site-packages/sklearn/linear_model/stochastic_
  "and default tol will be 1e-3." % type(self), FutureWarning)
```

```
In [31]: print(classification_report(y_test, pred_sgd))

             precision    recall  f1-score   support

          0       0.89      0.93      0.91       273
          1       0.47      0.34      0.40        47

avg / total       0.83      0.85      0.84       320
```

84% accuracy using stochastic gradient descent classifier

```
In [32]: print(confusion_matrix(y_test, pred_sgd))

[[255  18]
 [ 31  16]]
```

4.5 Support Vector Classifier

```
In [33]: svc = SVC()
         svc.fit(X_train, y_train)
         pred_svc = svc.predict(X_test)

In [34]: print(classification_report(y_test, pred_svc))

             precision    recall  f1-score   support

          0       0.88      0.98      0.93       273
          1       0.71      0.26      0.37        47

avg / total       0.86      0.88      0.85       320
```

Support vector classifier gets 86%

4.6 Grid Search CV

Trying out a pipeline with PCA and standard scaler

```
In [45]: #Finding best parameters for our SVC model
         param = {
             'clf__C': [0.1,0.8,0.9,1,1.1,1.2,1.3,1.4],
             'clf__kernel':['linear', 'rbf'],
             'clf__gamma' :[0.1,0.8,0.9,1,1.1,1.2,1.3,1.4]
         }

         pipeline_svc = Pipeline([('scl', StandardScaler()),
                                  ('pca', PCA(n_components=3)),
                             ('clf', SVC())])

         grid_svc = GridSearchCV(estimator=pipeline_svc, param_grid=param, scoring='accuracy',

In [46]: grid_svc.fit(X_train, y_train)

Out[46]: GridSearchCV(cv=10, error_score='raise',
                estimator=Pipeline(memory=None,
              steps=[('scl', StandardScaler(copy=True, with_mean=True, with_std=True)), ('pca'
           svd_solver='auto', tol=0.0, whiten=False)), ('clf', SVC(C=1.0, cache_size=200, class
           decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
           max_iter=-1, probability=False, random_state=None, shrinking=True,
           tol=0.001, verbose=False))]),
                fit_params=None, iid=True, n_jobs=1,
                param_grid={'clf__C': [0.1, 0.8, 0.9, 1, 1.1, 1.2, 1.3, 1.4], 'clf__kernel': [
                pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
                scoring='accuracy', verbose=0)
```

```
In [47]: #Best parameters for our svc model
         grid_svc.best_params_

Out[47]: {'clf__C': 1.1, 'clf__gamma': 0.8, 'clf__kernel': 'rbf'}

In [48]: #Let's run our SVC again with the best parameters.
         svcp = SVC(C = 1.1, gamma =  0.8, kernel= 'rbf')
         svcp.fit(X_train, y_train)
         pred_svcp = svcp.predict(X_test)
         print(classification_report(y_test, pred_svcp))

             precision    recall  f1-score   support

          0       0.89      0.99      0.94       273
          1       0.88      0.32      0.47        47

avg / total       0.89      0.89      0.87       320



In [39]: #Finding best parameters for our SVC model
         param = {
             'clf__C': [0.1,0.8,0.9,1,1.1,1.2,1.3,1.4],
             'clf__kernel':['linear', 'rbf'],
             'clf__gamma' :[0.1,0.8,0.9,1,1.1,1.2,1.3,1.4]
         }

         pipeline_svc = Pipeline([('scl', StandardScaler()),
                                 ('clf', SVC())])

         grid_svc = GridSearchCV(estimator=pipeline_svc, param_grid=param, scoring='accuracy',

In [40]: grid_svc.fit(X_train, y_train)

Out[40]: GridSearchCV(cv=10, error_score='raise',
                estimator=Pipeline(memory=None,
              steps=[('scl', StandardScaler(copy=True, with_mean=True, with_std=True)), ('clf'
           decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
           max_iter=-1, probability=False, random_state=None, shrinking=True,
           tol=0.001, verbose=False))]),
                fit_params=None, iid=True, n_jobs=1,
                param_grid={'clf__C': [0.1, 0.8, 0.9, 1, 1.1, 1.2, 1.3, 1.4], 'clf__kernel': [
                pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
                scoring='accuracy', verbose=0)

In [41]: #Best parameters for our svc model
         grid_svc.best_params_

Out[41]: {'clf__C': 1.2, 'clf__gamma': 0.9, 'clf__kernel': 'rbf'}
```

```
In [42]: #Let's run our SVC again with the best parameters.
         svc2 = SVC(C = 1.2, gamma =  0.9, kernel= 'rbf')
         svc2.fit(X_train, y_train)
         pred_svc2 = svc2.predict(X_test)
         print(classification_report(y_test, pred_svc2))

             precision    recall  f1-score   support

          0       0.90      0.99      0.94       273
          1       0.89      0.34      0.49        47

avg / total       0.90      0.90      0.88       320
```

4.6.1 SVC without PCA improves from 86% to 90% using Grid Search CV hence we would go forward with that

4.7 Cross Validation Score for random forest and SGD

```
In [44]: #Now lets try to do some evaluation for random forest model using cross validation.
         rfc_eval = cross_val_score(estimator = rfc, X = X_train, y = y_train, cv = 10)
         rfc_eval.mean()

Out[44]: 0.9093073326771653
```

4.7.1 Random forest accuracy increases from 87% to 91 % using cross validation score