In [18]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

import plotly.express as px
import plotly.graph_objects as go
from plotly.subplots import make_subplots

from collections import Counter

from sklearn.metrics import f1_score,accuracy_score,precision_score,recall_score
from sklearn.model_selection import RandomizedSearchCV
from xgboost import XGBClassifier
#from hyperopt import STATUS_OK,Trials, fmin, hp, tpe
```

```
The history saving thread hit an unexpected error (OperationalError('attempt to writ
e a readonly database')).History will not be written to the database.
```

In [19]:
```
red_train = pd.read_csv("data/red_wine_train.csv",index_col=0)
red_test = pd.read_csv("data/red_wine_test.csv",index_col=0)
```

In [20]:
```
red_train.describe()
```

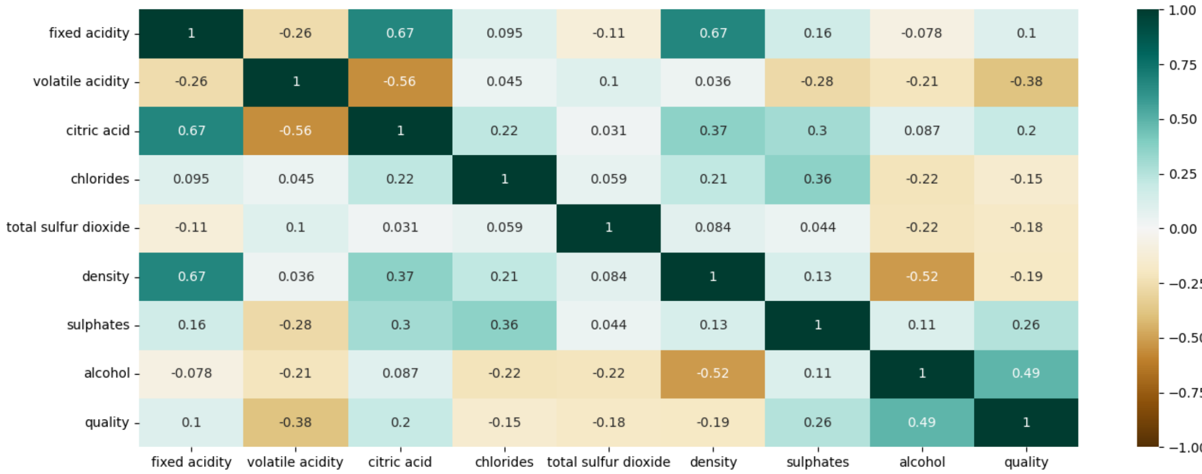
Out[20]:

	fixed acidity	volatile acidity	citric acid	chlorides	total sulfur dioxide	density	su
count	1279.000000	1279.000000	1279.000000	1279.000000	1279.000000	1279.000000	1279
mean	8.282877	0.531235	0.266059	0.087127	46.464816	0.996715	0
std	1.717760	0.176222	0.193606	0.047654	32.173470	0.001916	0
min	4.900000	0.120000	0.000000	0.012000	6.000000	0.990070	0
25%	7.100000	0.400000	0.090000	0.070000	23.000000	0.995545	0
50%	7.900000	0.520000	0.250000	0.079000	38.000000	0.996700	0
75%	9.100000	0.640000	0.420000	0.090000	62.000000	0.997800	0
max	15.900000	1.580000	1.000000	0.611000	278.000000	1.003690	2

First Attempt: outlier removal, and dropping fixed acidity and chlordies, and the two binary variables (no binning)

In [21]:
```
#dropping binary values that were created just
red_train = red_train.drop(["alcohol_higher", "va_high"], axis=1)
red_test= red_test.drop(["alcohol_higher", "va_high"], axis=1)
```

In [22]:
```
plt.figure(figsize=(16, 6))
heatmap = sns.heatmap(red_train.corr(), vmin=-1, vmax=1, annot=True, cmap='BrBG')
```



Preprocessing

For decision trees, there typically no reason to do much when it comes to altering the data. Decision trees do not have much problems with scaled, normalized, and other types continous data is not a big deal (especially with XGB). If we had categorical data, this would be different, espcially if we had to data cleanup, but other than outliers there is not much that can more be done that what is given.

In [23]:
```
def remove_outliers(df: pd.DataFrame, n :float, columns):
    #this is the Tukey ruel which gets the values that exists outside of the outer
    #This is valuable if outliers effect the data alot (typically regression), in c
    #From EDA it seems that we should not remove outliers as they can help point to
    total_outliers = []

    for col in columns:

        #generating the quantile ranges that will be used to determine outliers
        q1 = df[col].quantile(.25)
        q3 = df[col].quantile(.75)

        iqr = q3 - q1
        outer_fence = iqr * 1.5

        outliers = df[(df[col] < q1 - outer_fence) | (df[col] > q3 + outer_fence)].

        total_outliers.extend(outliers)

    #select the indexes (tuples) that have more than n attributes that are outliers
    #creates an object that has keys (index), with values (amount of apperences, wh
    outliers = Counter(total_outliers)

    #iterates over all items and reutrns the
    items_greater =[]
    for i in outliers.items():
        if(i[1] >= n):
            items_greater.append(i[0])
```

```
    return items_greater
```

In [24]:
```
#chose two as during Eda it seemed that individually there was not much outliers an
print("old len: " + str(len(red_train)))
outliers = remove_outliers(red_train, 2 , red_train.columns[:-1])
print("new len: " + str(len(red_train.drop(outliers, axis = 0).reset_index(drop=Tru
```

```
old len: 1279
new len: 1213
```

overall outliers are neglible

Model Testing

In [25]:
```
X_train = red_train.drop("quality" , axis=1)
y_train = red_train["quality"]
X_test = red_test.drop("quality" , axis=1).copy()
y_test = red_test["quality"]
```

In [26]:
```
#xgb expects only what is present, not the actual scale of the data relative to qua
#therefore, we have to map to values 0-5 for the scale
y_train = y_train.map({3: 0, 4: 1, 5:2, 6:3, 7:4, 8:5})
y_test = y_test.map({3: 0, 4: 1, 5:2, 6:3, 7:4, 8:5})
```

Hyperopt

```
-- uses bayesian optimization to find the best parameter for
machine learning algorithm, by using probablistic search of the
hyperparamters supplied
   Compared to exahustive search it is much faster and its
performance is only a bit lower

How to implement:
    1. intitalise the domain space (same as a grid search)
    2. define the objective function  that we want to minimze
(error rate) of the model that we are testing (XGBoost decision
trees in this case)
    3. Optimize alogirhtm choice (the method used to construct the
surrogate objective function)
    4. Results, the score or the value pairs that the algorithm
uses to build the model
```

Below the hyperopt stuff that I personally was messing around wiht, but I do not think that I am going to include it in final report. Just skip...

In [27]:
```
# space = {"max_depth":hp.quniform("max_depth",3,18,1), #the max dept with integer
#          "gamma" : hp.uniform('gamma',1,9), #the gamma values with values ranging
#         'colsample_bytree' : hp.uniform('colsample_bytree', 0.5,1), #ratio of col
#         'min_child_weight' : hp.quniform('min_child_weight', 0, 10, 1), #tuning t
#         'n_estimators': 180,
```

```
#         'seed': 0
#     }


# def ojective(space:dict):
#         #creating a classifer with the opametrs pulled from the space that has be
#         #Most explanation is above
#         clf=XGBClassifier(
#                 n_estimators =space['n_estimators'],
#                 max_depth = int(space['max_depth']),
#                 gamma = space['gamma'],
#                 min_child_weight=int(space['min_child_weight']),
#                 colsample_bytree=int(space['colsample_bytree']),
#                 objective="multi:softprob", #type of objective function that is u
#                 early_stopping_rounds=10, #sets the early stopping rounds if the
#                 eval_metric="auc") #the measure to determine within the gradient

#         #evalutation train set and test set for doing a fit, efficivly measuring
#         evaluation = [( X_train, y_train), ( X_test, y_test)]

#         clf.fit(X_train,
#                 y_train,
#                 eval_set=evaluation, #passed in for the set
#                 verbose=False)

#         # make a prediction
#         y_pred = clf.predict(X_test)

#         accuracy = f1_score(y_test,y_pred,average="weighted",zero_division=1)
#         print("SCORE:" + str(accuracy))
#         return {'loss' : -accuracy, "status" : STATUS_OK}

#trials = Trials()


# best_hyperparams = fmin(fn = ojective,
#                         space = space,
#                         algo = tpe.suggest,
#                         max_evals = 50,
#                         trials = trials)
```

Available optimizaiton algorithms: (oudated)

```
-- hp.choice(label,options) : returns a choice of one of the
options

-- hp.randint(label,upper) : returns a random integer better range
of 0 --> upper

-- hp.uniform(label,low, high) : returns a value uniformly between
the low and high

-- hp.uniform(label,low,high,q) : returns a value round to
(uniforn(low,high)/q) , and returns an integer
```

```
-- hp.normal(label,mean,std) : returns a real value that is
normally distributed with mean and standard deviation
```

Trials:

-- an object that contains or stores all the relevent information such as a hyperparameter. The loss functions for each type of parameter is stored here. Whenever doing iterations of training with current hyperparameters.

-- fmin is an optimization function that minimizes the loss function for each paramter inside of space.

-- algo: The type of the algorithm for finding best hyperparamter. Tpe is a type of decision tree, so effectively we are using a decision tree to do the hyperparamter choosing.

-- max evals: the amount of iterations that we choose to run through

Hyper parameters:

```
Booster: choose the type of booster to use (we will use tree in
this case)
    -- 3 options
    tree( gbtree,dart)
    linear(gblinear)

Booster Parameters: only the tree booster ones, only listing the
ones usuful to mulitlable imbalanced data (trees for the win)

    -- eta: the learning rat for Gradient boosting, and its range
typically is 0.01 - 0.2
    -- gamma: how the node is split in a tree, the larger the more
conservative a tree is, range(0 --> infinity)
    -- max_depth: maximum depth of a tree typical values are (3-
10), should use cv
    -- min_child_weight: tune using cv but range is 0-->infinite
    -- subsample: fraction of observations to be samples for tree,
lower values more conservative, typical values (0,1)
    -- colsample_bytree: ratio of columns when construction each
tree
    -- colsample_bylevel: ratio of columns at each level of the
tree
    -- tree method: constuction algorithm used in model (multiple
choices)
    -- max_leaves: is maximum number of nodes to be added

    Others
    -- alpha : used for lasso regression, increasing makes the
model more conservative
    -- lambda : used for ridge regression, increasing makes the
model more conservative
```

```
Learning Task: parameters used to define the optimization objective
for learning

    --objective: should use multi:softprob or multi: softmax
    --eval metric: should use auc, or merror
```

In [28]:
```python
space = {'max_depth': [3, 6, 10, 15, 20],
         'learning_rate': [0.01, 0.1, 0.2, 0.3, 0.4],
         'subsample': np.arange(0.5, 1.0, 0.1),
         'gamma' : np.arange(1,9,1),
         'colsample_bytree': np.arange(0.5, 1.0, 0.1),
         'colsample_bylevel': np.arange(0.5, 1.0, 0.1),
         'min_child_weight' : np.arange(1, 10, 1),
         'n_estimators': [100,180, 250, 500, 750],
        }
```

In [29]:
```python
#making the base model
#multi prob is a vector, containing all the classes
model = XGBClassifier(objective="multi:softprob",eval_metric="auc",)
clf = RandomizedSearchCV(estimator=model,
                         param_distributions=space, #assigning space
                         scoring="f1_weighted", #eval metric for the hyperparms, we
                         n_iter=25, #amount of iterations per cv (random combinatio
                         n_jobs=4, #amount of parralel processes to run
                         random_state=1)

clf.fit(X_train,y_train)
```

Out[29]:
```
▸ RandomizedSearchCV
▸ estimator: XGBClassifier
    ▸ XGBClassifier
```

In [30]:
```python
best_hyperparams = clf.best_params_
best_hyperparams
```

Out[30]:
```
{'subsample': 0.8999999999999999,
 'n_estimators': 750,
 'min_child_weight': 9,
 'max_depth': 15,
 'learning_rate': 0.1,
 'gamma': 2,
 'colsample_bytree': 0.8999999999999999,
 'colsample_bylevel': 0.6}
```

In [31]:
```python
accuracy_f1 = []
recall = []
precision = []
accuracy = []
for i in range(0,5):
    #creating model with best hyperparameters
    clf=XGBClassifier(
        n_estimators = best_hyperparams['n_estimators'],
```

```
        max_depth = int(best_hyperparams['max_depth']),
        learning_rate = best_hyperparams['learning_rate'],
        gamma = best_hyperparams['gamma'],
        min_child_weight=int(best_hyperparams['min_child_weight']),
        colsample_bytree=int(best_hyperparams['colsample_bytree']),
        colsample_bylevel=best_hyperparams['colsample_bylevel'],
        objective="multi:softprob", #type of objective function that is used, you h
        eval_metric="auc", #the measure to determine within the gradient boosting t
        seed=i)

    clf.fit(X_train,y_train)

    y_pred = clf.predict(X_test)

    #appending the scores from the particular rune to the list
    accuracy_f1.append(f1_score(y_test,y_pred,average="weighted",zero_division=1))
    recall.append(recall_score(y_test,y_pred,average="weighted",zero_division=1))
    precision.append(precision_score(y_test, y_pred,average="weighted",zero_divisio
    accuracy.append(accuracy_score(y_test,y_pred))
```

In [32]:

```
average_f1 = np.mean(accuracy_f1)
average_recall = np.mean(recall)
average_precision = np.mean(precision)
average_accuracy = np.mean(accuracy)
print("Average F1: " + str(average_f1))
print("Average Recall: " + str(average_recall))
print("Average Precision: " + str(average_precision))
print("Average Accuracy: " + str(average_accuracy))
```

```
Average F1: 0.5943817969672713
Average Recall: 0.62375
Average Precision: 0.653822962237242
Average Accuracy: 0.62375
```