

ML Problem

In this project, I will use the attributes (fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol, and color) of red and white wine to predict the quality of wine, so this is a regression problem

Import methods

```
In [1]: import pandas as pd
import matplotlib.pyplot as plt
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.model_selection import train_test_split
from sklearn.model_selection import cross_val_score
import numpy as np
```

Read Dataset

```
In [2]: white = pd.read_csv('winequality-white.csv', sep = ';')
white.head()
# white wine has 4898 rows
```

```
Out[2]:
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	6
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	6
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	6
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6

```
In [3]: red = pd.read_csv('winequality-red.csv', sep = ';')
red.head()
# red wine has 1599 rows
```

```
Out[3]:
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	5
1	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.8	5
2	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.8	5
3	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.8	6
4	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	5

Prepare the data

```
In [4]: print(white.isnull().any())
```

```
fixed acidity      False
volatile acidity   False
citric acid        False
residual sugar     False
chlorides          False
free sulfur dioxide False
total sulfur dioxide False
density           False
pH                False
sulphates          False
alcohol            False
quality            False
dtype: bool
```

```
In [5]: print(red.isnull().any())
```

```
fixed acidity      False
volatile acidity   False
citric acid        False
residual sugar     False
chlorides          False
free sulfur dioxide False
total sulfur dioxide False
density           False
pH                False
sulphates          False
alcohol            False
quality            False
dtype: bool
```

As you can see, from these two datasets, there is no missing information, so I will skip to find if there are any outliers in the dataset. According to the research, I found that the residual sugar in wines is rarely less than 1 gram/liter, and most wines' pH are between 3-4. Besides, the quality of wine is between 0 and 10.

```
In [6]: # First, let's check the residual sugar
less_than_zero_white = 0
less_than_one_white = 0
for i in white['residual sugar']:
    if i < 0:
        less_than_zore_white += 1
    elif i <= 1 and i > 0:
        less_than_one_white += 1
    else:
        continue
print('Outliers in residual sugar in white wine: ', less_than_zero_white)
print('residual sugar in white wine less than 1 gram/liter: ', less_than_one_white)

less_than_zero_red = 0
less_than_one_red = 0
for i in red['residual sugar']:
    if i < 0:
        less_than_zore_red += 1
    elif i <= 1 and i > 0:
        less_than_one_red += 1
    else:
        continue
print('Outliers in residual sugar in red wine: ', less_than_zero_red)
print('residual sugar in red wine less than 1 gram/liter: ', less_than_one_red)
```

```
Outliers in residual sugar in white wine: 0
residual sugar in white wine less than 1 gram/liter: 170
Outliers in residual sugar in red wine: 0
residual sugar in red wine less than 1 gram/liter: 2
```

As you can see, there is no outliers in both red wine and white wines' residual sugar. And the residual sugar which less than 1gm/liter in red wine is less than in white wine

```
In [7]: # Second, let's check the pH, the range of pH is 0 to 14
outliers_white = 0
for i in white['pH']:
    if i < 0 or i > 14:
        outliers_white += 1
    else:
        continue
print('Outliers in pH in white wine: ',outliers_white)

outliers_red = 0
for i in red['pH']:
    if i < 0 or i > 14:
        outliers_red += 1
    else:
        continue
print('Outliers in pH in red wine: ',outliers_red)
```

```
Outliers in pH in white wine: 0
Outliers in pH in red wine: 0
```

```
In [8]: # Third, quality
quality_white = 0
for i in white['quality']:
    if i > 10 or i < 0 :
        outliers_white += 1
    else:
        continue
print('Outliers in pH in white wine: ',quality_white)

quality_red = 0
for i in red['quality']:
    if i > 10 or i < 0 :
        outliers_red += 1
    else:
        continue
print('Outliers in pH in red wine: ',quality_red)
```

Outliers in pH in white wine: 0
 Outliers in pH in red wine: 0

After checking data that may have outliers, I found that these two datasets are already cleaned, so I can directly use these two datasets.

```
In [9]: white.describe()
```

Out[9]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	
count	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.
mean	6.854788	0.278241	0.334192	6.391415	0.045772	35.308085	138.360657	0.
std	0.843868	0.100795	0.121020	5.072058	0.021848	17.007137	42.498065	0.
min	3.800000	0.080000	0.000000	0.600000	0.009000	2.000000	9.000000	0.
25%	6.300000	0.210000	0.270000	1.700000	0.036000	23.000000	108.000000	0.
50%	6.800000	0.260000	0.320000	5.200000	0.043000	34.000000	134.000000	0.
75%	7.300000	0.320000	0.390000	9.900000	0.050000	46.000000	167.000000	0.
max	14.200000	1.100000	1.660000	65.800000	0.346000	289.000000	440.000000	1.

```
In [10]: red.describe()
```

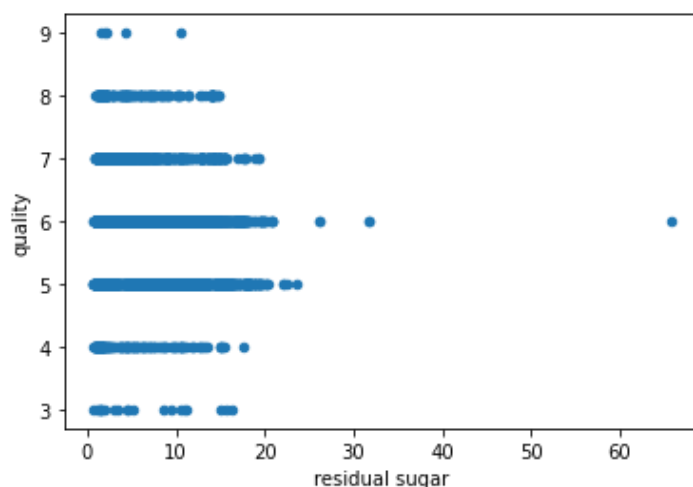
```
Out[10]:
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	
count	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.
mean	8.319637	0.527821	0.270976	2.538806	0.087467	15.874922	46.467792	0.
std	1.741096	0.179060	0.194801	1.409928	0.047065	10.460157	32.895324	0.
min	4.600000	0.120000	0.000000	0.900000	0.012000	1.000000	6.000000	0.
25%	7.100000	0.390000	0.090000	1.900000	0.070000	7.000000	22.000000	0.
50%	7.900000	0.520000	0.260000	2.200000	0.079000	14.000000	38.000000	0.
75%	9.200000	0.640000	0.420000	2.600000	0.090000	21.000000	62.000000	0.
max	15.900000	1.580000	1.000000	15.500000	0.611000	72.000000	289.000000	1.

We can also directly find from these two tables, there is no outlier in thses two datasets.

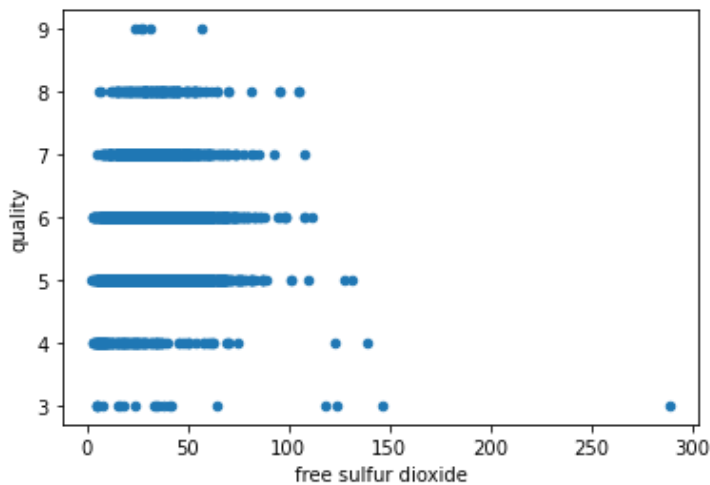
Visualize the data

```
In [11]: # relationship between white winde's residual sugar and quality
white.plot(kind = 'scatter', x = 'residual sugar', y = 'quality')
plt.show()
```



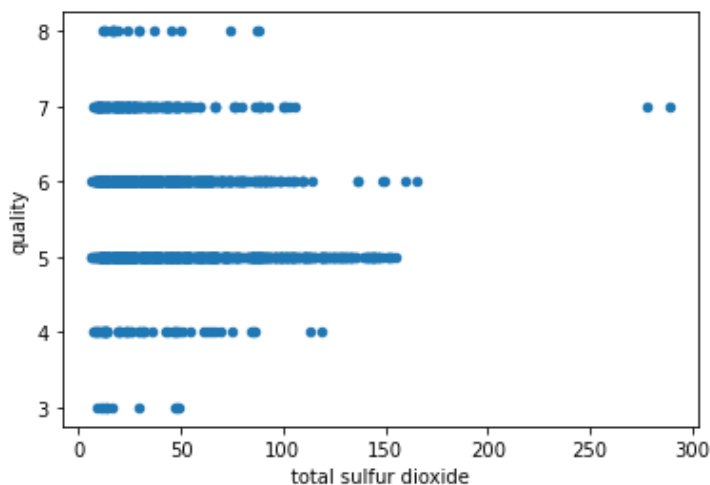
Although I haven't found outliers beyond, after creating the scatter plot with residual sugar and quality, I find there is only one white wine which the residual sugar is much higher than others, it contains more than 60.

```
In [12]: # relationship between white wine's free sulfur dioxide and quality
white.plot(kind = 'scatter', x = 'free sulfur dioxide', y = 'quality')
plt.show()
```



Through creating all scatter plots to find the relationship between quality and attributes. I found there is one wine that the free sulfur dioxide is wired, which is twice higher than other white wines.

```
In [13]: # relationship between red wine's total sulfur dioxide and quality
red.plot(kind = 'scatter', x = 'total sulfur dioxide', y = 'quality')
plt.show()
```



After comparing all red wine scatter plots, I found there are two red wines in which the total sulfur dioxide is higher than the others

After visualizing two datasets, there are a few data I found should be removed from the dataset, so I will

process the datasets again below.

Prepare data II

After creating a few graphics, I found a few outliers, so I will process data to remove those data and merge the white wine and red wine tables. Besides, I will add color as an additional attribute to predict the quality of the wine. 0 is white wine, and 1 is red wine.

White wine

```
In [14]: # cleaned outliers in residual sugar and free sulfur dioxide
rs_white = white.drop(white[white['residual sugar'] > 60].index)
cleaned_white = rs_white.drop(rs_white[rs_white['free sulfur dioxide']>300].index)
cleaned_white.insert(11, 'color', 0)
cleaned_white
```

Out[14]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	color
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.00100	3.00	0.45	8.8	0
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.99400	3.30	0.49	9.5	0
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.99510	3.26	0.44	10.1	0
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.99560	3.19	0.40	9.9	0
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.99560	3.19	0.40	9.9	0
...
4893	6.2	0.21	0.29	1.6	0.039	24.0	92.0	0.99114	3.27	0.50	11.2	0
4894	6.6	0.32	0.36	8.0	0.047	57.0	168.0	0.99490	3.15	0.46	9.6	0
4895	6.5	0.24	0.19	1.2	0.041	30.0	111.0	0.99254	2.99	0.46	9.4	0
4896	5.5	0.29	0.30	1.1	0.022	20.0	110.0	0.98869	3.34	0.38	12.8	0
4897	6.0	0.21	0.38	0.8	0.020	22.0	98.0	0.98941	3.26	0.32	11.8	0

4897 rows × 13 columns

Red wine

```
In [15]: ## cleaned two outliers in red wine's total sulfur dioxide
cleaned_red = red.drop(red[red['total sulfur dioxide']>250].index)
cleaned_red.insert(11, 'color', 1)
cleaned_red
```

Out[15]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	color
0	7.4	0.700	0.00	1.9	0.076	11.0	34.0	0.99780	3.51	0.56	9.4	1
1	7.8	0.880	0.00	2.6	0.098	25.0	67.0	0.99680	3.20	0.68	9.8	1
2	7.8	0.760	0.04	2.3	0.092	15.0	54.0	0.99700	3.26	0.65	9.8	1
3	11.2	0.280	0.56	1.9	0.075	17.0	60.0	0.99800	3.16	0.58	9.8	1
4	7.4	0.700	0.00	1.9	0.076	11.0	34.0	0.99780	3.51	0.56	9.4	1
...
1594	6.2	0.600	0.08	2.0	0.090	32.0	44.0	0.99490	3.45	0.58	10.5	1
1595	5.9	0.550	0.10	2.2	0.062	39.0	51.0	0.99512	3.52	0.76	11.2	1
1596	6.3	0.510	0.13	2.3	0.076	29.0	40.0	0.99574	3.42	0.75	11.0	1
1597	5.9	0.645	0.12	2.0	0.075	32.0	44.0	0.99547	3.57	0.71	10.2	1
1598	6.0	0.310	0.47	3.6	0.067	18.0	42.0	0.99549	3.39	0.66	11.0	1

1597 rows × 13 columns

Combine two tables

```
In [16]: frames = [cleaned_red, cleaned_white]
cleaned_wine = pd.concat(frames)
cleaned_wine
```

Out[16]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	color
0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.99780	3.51	0.56	9.4	1
1	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.99680	3.20	0.68	9.8	1
2	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.99700	3.26	0.65	9.8	1
3	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.99800	3.16	0.58	9.8	1
4	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.99780	3.51	0.56	9.4	1
...
4893	6.2	0.21	0.29	1.6	0.039	24.0	92.0	0.99114	3.27	0.50	11.2	0
4894	6.6	0.32	0.36	8.0	0.047	57.0	168.0	0.99490	3.15	0.46	9.6	0
4895	6.5	0.24	0.19	1.2	0.041	30.0	111.0	0.99254	2.99	0.46	9.4	0
4896	5.5	0.29	0.30	1.1	0.022	20.0	110.0	0.98869	3.34	0.38	12.8	0

Create train and test sets

In this project, I will use all attributes of wine to predict the quality. I split the dataset to two groups 80% of them are training data, 20% are testing data.

```
In [17]: train_ratio = 0.8 # 80% for training, 30% for validation
random_seed = 42

train_dataframe = cleaned_wine.sample(frac=train_ratio, random_state=random_seed)
valid_dataframe = cleaned_wine.drop(train_dataframe.index)
print('training set size:', len(train_dataframe))
print('validation set size:', len(valid_dataframe))

training set size: 5195
validation set size: 807
```

```
In [19]: train_X = train_dataframe.drop(columns=['quality'])
valid_X = valid_dataframe.drop(columns=['quality'])
```

```
In [20]: train_y = train_dataframe.drop(columns=['fixed acidity', 'volatile acidity', 'citric
        'total sulfur dioxide', 'density', 'pH', 'sulphates
valid_y = valid_dataframe.drop(columns=['fixed acidity', 'volatile acidity', 'citric
        'total sulfur dioxide', 'density', 'pH', 'sulphates
```

First Model

My first model is linear regression. Linear regression is the basic method to make a prediction.

```
In [21]: def display_scores(scores):
        print("Scores:", scores)
        print("Mean:", scores.mean())
        print("Standard deviation:", scores.std())
```

```
In [53]: from sklearn.linear_model import LinearRegression

lin_reg = LinearRegression()
lin_reg.fit(train_X, train_y)
```

Out[53]: LinearRegression()

In a Jupyter environment, please rerun this cell to show the HTML representation or trust the notebook.

On GitHub, the HTML representation is unable to render, please try loading this page with nbviewer.org.

```
In [56]: lin_scores = cross_val_score(lin_reg, train_X, train_y,
                                     scoring="neg_mean_squared_error", cv=10)
lin_rmse_scores = np.sqrt(-lin_scores)
display_scores(lin_rmse_scores)
lin_r_score = cross_val_score(lin_reg, train_X, train_y,
                             scoring="r2", cv=10)
lin_r_score
```

```
Scores: [0.76470848 0.75033062 0.70127051 0.72233122 0.75759131 0.75729597
 0.71350671 0.70332116 0.73641529 0.71338266]
Mean: 0.7320153948555037
Standard deviation: 0.022954345560951522
```

```
Out[56]: array([0.24285946, 0.24372999, 0.29272982, 0.32637246, 0.34127641,
 0.27017454, 0.30103023, 0.31689538, 0.32083351, 0.29080455])
```

For the first linear regression model, the mean MSE is 0.7320153948555037. And the highest R square in ten sets is 0.32083351. This model is not good enough because MSE is too high and R square is too low, so we need to find another model to get a better output.

Second Model

My second model is random forest because it is a popular method to make a prediction, and it introduces randomness and avoids overfitting. And I use mean-square error to calculate the accuracy of this model. The lower the score, the better the result.

```
In [89]: from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_squared_error
from sklearn.metrics import r2_score
forest = RandomForestRegressor(n_estimators=100, random_state=42)
forest.fit(train_X, train_y)
```

```
/var/folders/gx/14ygghxd5psd114n4d94lws0000gn/T/ipykernel_3001/209574164.py:
5: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
forest.fit(train_X, train_y)
```

```
Out[89]: RandomForestRegressor(random_state=42)
```

In a Jupyter environment, please rerun this cell to show the HTML representation or trust the notebook.

On GitHub, the HTML representation is unable to render, please try loading this page with nbviewer.org.

```
In [77]: forest_scores = cross_val_score(forest, train_X, train_y,
                                         scoring="neg_mean_squared_error", cv=10)
forest_rmse_scores = np.sqrt(-forest_scores)
display_scores(forest_rmse_scores)
forest_r_score = cross_val_score(forest, train_X, train_y,
                                scoring="r2", cv=10)
forest_r_score
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

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/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

Scores: [0.62779958 0.66448274 0.55825019 0.59189883 0.66407802 0.64532064

```
0.58336807 0.56260627 0.62817717 0.60436052]
Mean: 0.6130342019928237
Standard deviation: 0.03699789602379698
```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
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```
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```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
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```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
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```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
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```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
Out[77]: array([0.48969865, 0.40688495, 0.55179991, 0.54768392, 0.49385907,
                0.4700452 , 0.53275186, 0.56289176, 0.50580888, 0.4910056 ])
```

Then I will use grid search to find a better combination of parameters than the period one

```
In [70]: from sklearn.model_selection import GridSearchCV
rf = RandomForestRegressor(random_state=0)
rf_params = {
    'n_estimators': [100, 150],
    'criterion': ['squared_error', 'poisson'],
}
# Define the gridsearchCV
rf_grid = GridSearchCV(rf, rf_params)
# fit with the tranformed sparse matrix
rf_grid.fit(train_X, train_y)
print('Best Score:', rf_grid.best_score_)
# assign the best estimator to a .0variable
best_rf = rf_grid.best_estimator_
print('Best Params:', rf_grid.best_params_)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

```

/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
    estimator.fit(X_train, y_train, **fit_params)
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/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
    estimator.fit(X_train, y_train, **fit_params)
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
    estimator.fit(X_train, y_train, **fit_params)
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    estimator.fit(X_train, y_train, **fit_params)
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    estimator.fit(X_train, y_train, **fit_params)
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
    estimator.fit(X_train, y_train, **fit_params)
/Users/juangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_search.py:910: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
    self.best_estimator_.fit(X, y, **fit_params)

```

Best Score: 0.49331472512959607

Best Params: {'criterion': 'poisson', 'n_estimators': 150}

```
In [73]: forest1 = RandomForestRegressor(criterion='poisson', n_estimators=150)
         forest1.fit(train_X, train_y)
```

```
/var/folders/gx/14ygghxd5psd114n4d94lws0000gn/T/ipykernel_3001/60622051.py:2:
DataConversionWarning: A column-vector y was passed when a 1d array was expect
ed. Please change the shape of y to (n_samples,), for example using ravel().
```

```
forest1.fit(train_X, train_y)
```

```
Out[73]: RandomForestRegressor(criterion='poisson', n_estimators=150)
```

In a Jupyter environment, please rerun this cell to show the HTML representation or trust the notebook.

On GitHub, the HTML representation is unable to render, please try loading this page with nbviewer.org.

Next, we can evaluate the Random Forest model using cross validation.


```
In [74]: forest1_scores = cross_val_score(forest1, train_X, train_y,
                                         scoring="neg_mean_squared_error", cv=10)
forest1_rmse_scores = np.sqrt(-forest1_scores)
display_scores(forest1_rmse_scores)
forest1_r_score = cross_val_score(forest1, train_X, train_y,
                                  scoring="r2", cv=10)
forest1_r_score
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```

/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().

```
estimator.fit(X_train, y_train, **fit_params)
```



```
Scores: [0.6165399 0.66735657 0.55710025 0.59378051 0.65653129 0.64244055
0.59110223 0.56359567 0.62809578 0.60413717]
Mean: 0.6120679909109545
Standard deviation: 0.03527194926005537
```

```
/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
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```

```
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```

```
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```

```
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```

```
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```

```
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```

```
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```

```
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```

```
/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
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```

```
/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
/Users/yuangyang/opt/anaconda3/lib/python3.9/site-packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
```

```
estimator.fit(X_train, y_train, **fit_params)
```

```
Out[74]: array([0.50590433, 0.39398007, 0.55808603, 0.54558815, 0.51030094,
0.47222075, 0.52438539, 0.56543646, 0.50966855, 0.49157614])
```

Evaluate Second Model

For the random forest, I first ran this model without adding any parameters, and after cross-fold validation, I got the baseline result the mean of MSE is 0.6130342019928237.The highest R square is 0.56289176. Then I used the grid search to find a better combination of parameters, and the result of cross-validation is the mean of MSE is 0.6119037272368506. The highest R square is 0.5633744. As we can see, the mean MSE of the model with parameters is lower than the baseline,which is better than the model without any parameters.

Compare the performance of model 1 and model 2

After training two models, linear regression and random forest, I found that random forest is better than the linear regression. The MSE of random forest is lower than the linear regression, and the R sequare is also higher than it. Hence, I wil use random forest model to continuly solve problems in this project.

Final Model

For the final model, I will add a new computed feature that calculate the ratio between fixed acidity and residual sugar. And I will still use random forest regressor.

In [79]:

```
train_X['Fixed_acidity_Sugar_ratio'] = train_X['fixed acidity'] / train_X['residual sugar']
train_X
```

Out[79]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	color
1503	6.8	0.36	0.24	4.6	0.039	24.0	124.0	0.99090	3.27	0.34	12.6	0
654	6.5	0.21	0.37	2.5	0.048	70.0	138.0	0.99170	3.33	0.75	11.4	0
98	9.8	0.36	0.46	10.5	0.038	4.0	83.0	0.99560	2.89	0.30	10.1	0
1178	9.8	0.44	0.40	2.8	0.036	35.0	167.0	0.99560	2.97	0.39	9.2	0
1438	7.0	0.59	0.00	1.7	0.052	3.0	8.0	0.99600	3.41	0.47	10.3	1
...
4489	6.7	0.48	0.49	2.9	0.030	28.0	122.0	0.98926	3.13	0.40	13.0	0
3245	7.6	0.27	0.29	2.5	0.059	37.0	115.0	0.99328	3.09	0.37	9.8	0
1997	8.4	0.20	0.38	11.8	0.055	51.0	170.0	1.00040	3.34	0.82	8.9	0
323	6.8	0.28	0.44	9.3	0.031	35.0	137.0	0.99460	3.16	0.36	10.4	0

```
In [83]: valid_X['Fixed_acidity_Sugar_ratio'] = valid_X['fixed acidity'] / valid_X['residual_sugar']
```

Out[83]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	color
34	5.2	0.320	0.25	1.8	0.103	13.0	50.0	0.99570	3.38	0.55	9.2	1
66	7.5	0.520	0.11	1.5	0.079	11.0	39.0	0.99680	3.42	0.58	9.6	1
125	9.0	0.620	0.04	1.9	0.146	27.0	90.0	0.99840	3.16	0.70	9.4	1
127	8.1	1.330	0.00	1.8	0.082	3.0	12.0	0.99640	3.54	0.48	10.9	1
137	7.2	0.415	0.36	2.0	0.081	13.0	45.0	0.99720	3.48	0.64	9.2	1
...
4875	7.4	0.220	0.26	1.2	0.035	18.0	97.0	0.99245	3.12	0.41	9.7	C
4882	5.5	0.320	0.13	1.3	0.037	45.0	156.0	0.99184	3.26	0.38	10.7	C
4884	6.5	0.330	0.38	8.3	0.048	68.0	174.0	0.99492	3.14	0.50	9.6	C
4888	6.8	0.220	0.36	1.2	0.052	38.0	127.0	0.99330	3.04	0.54	9.2	C
4890	6.1	0.340	0.29	2.2	0.036	25.0	100.0	0.98938	3.06	0.44	11.8	C

807 rows × 13 columns

```
In [84]: forest2 = RandomForestRegressor(criterion='poisson', n_estimators=150)
forest2.fit(train_X, train_y)
```

```
/var/folders/gx/14ygghxd5psd114n4d941lsw0000gn/T/ipykernel_3001/4117239677.py:
2: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
forest2.fit(train_X, train_y)
```

Out[84]: RandomForestRegressor(criterion='poisson', n_estimators=150)

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```
In [85]: y_test_pred = forest2.predict(valid_X)
score = mean_squared_error(valid_y, y_test_pred)
score
```

Out[85]: 0.3338981137271101

```
In [90]: y_test_pred = forest2.predict(valid_X)
score1 = r2_score(valid_y, y_test_pred)
score1
```

Out[90]: 0.5496905878194984

Evaluate Final Model

After calculating, we can see that random forest regressor works not bad, the MSE is 0.3338981137271101, which is lower than the MSE of second model. It means the final model performs better when it make prediction. Besides, the highest R square is 0.5496905878194984, which reached the highest score in this project. Hence, this model perform pretty good.

Reflect on the performance of the final model

What other ideas do you have about possible ways to improve performance? What types of instances does it perform well on? Which does it not perform well on? What were the main challenges that you faced while working on this project?

To improve performance, I think I can try other regression models, like logistic regression and decision tree, and use grid search to try all parameters, and find the best combination. The logistic regression performs well when it used to predict the categorical dependent variable. And decision tree model is used for handling non-linear data sets. However, decision tree model is less effective in predicting the outcome of a continuous variable. In this project, I think the challenges is adjust parameters, I tried to set all parameters to find the best combination, but it cost me hours, even a day and did not get the answer. Hence, I delete some parameters and did not train them. So, the model doesn't perform best.

In []: