Assignment 4: Performance Metrics, and Optimisation

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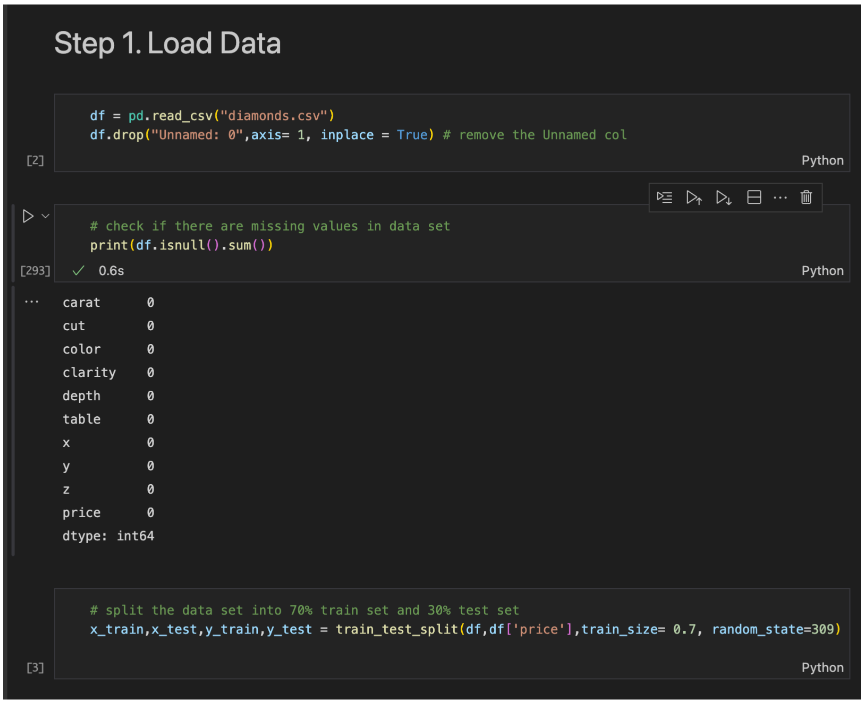
Part 1: Performance Metrics in Regression [30 marks]

Requirements

Based on exploratory data analysis, discuss what preprocessing that you need to do before regression, and provide evidence and justifications.

- Step1. Load Data && split the dataset



Step 1. Load Data

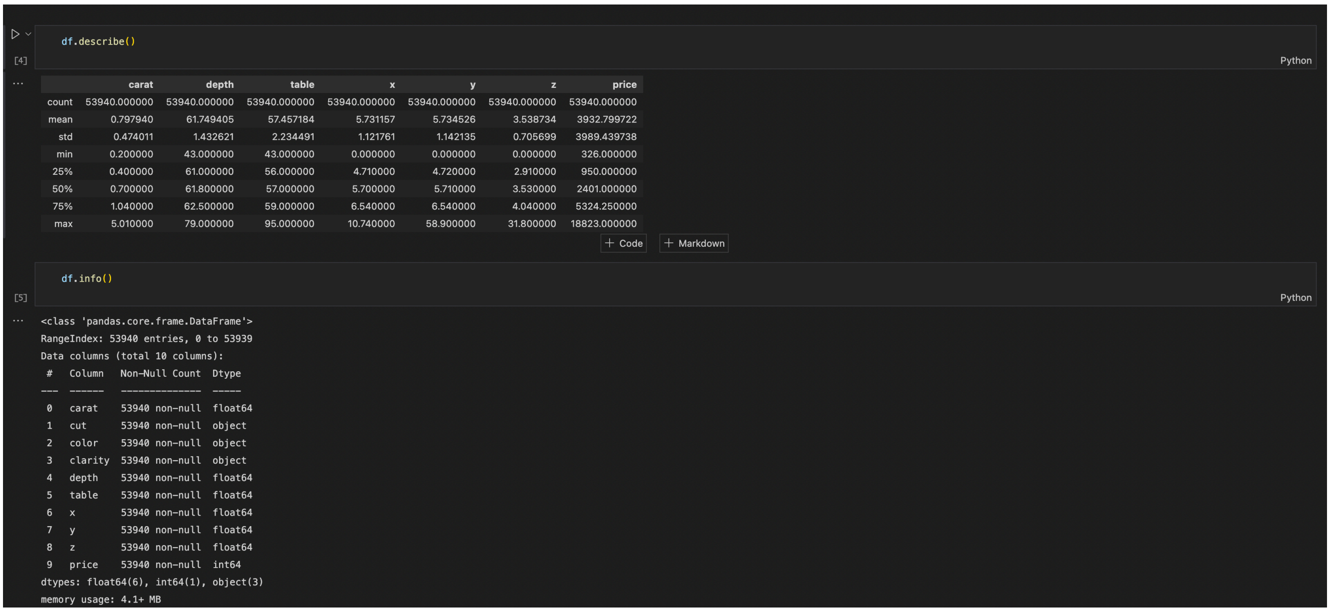
```
df = pd.read_csv("diamonds.csv")
df.drop("Unnamed: 0",axis= 1, inplace = True) # remove the Unnamed col
```

```
# check if there are missing values in data set
print(df.isnull().sum())
```

```
carat      0
cut        0
color      0
clarity    0
depth      0
table      0
x          0
y          0
z          0
price      0
dtype: int64
```

```
# split the data set into 70% train set and 30% test set
x_train,x_test,y_train,y_test = train_test_split(df,df['price'],train_size= 0.7, random_state=309)
```

- Step 2. Initial Data Analysis



```
df.describe()
```

	carat	depth	table	x	y	z	price
count	53940.000000	53940.000000	53940.000000	53940.000000	53940.000000	53940.000000	53940.000000
mean	0.797940	61.749405	57.457184	5.731157	5.734526	3.538734	3932.799722
std	0.474011	1.432621	2.234491	1.121761	1.142135	0.705699	3989.439738
min	0.200000	43.000000	43.000000	0.000000	0.000000	0.000000	326.000000
25%	0.400000	61.000000	56.000000	4.710000	4.720000	2.910000	950.000000
50%	0.700000	61.800000	57.000000	5.700000	5.710000	3.530000	2401.000000
75%	1.040000	62.500000	59.000000	6.540000	6.540000	4.040000	5324.250000
max	5.010000	79.000000	95.000000	10.740000	58.900000	31.800000	18823.000000

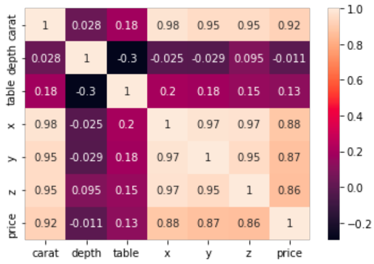
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 53940 entries, 0 to 53939
Data columns (total 10 columns):
 #   Column   Non-Null Count  Dtype  
---  ------   --------------  -----  
 0   carat    53940 non-null  float64
 1   cut      53940 non-null  object 
 2   color    53940 non-null  object 
 3   clarity  53940 non-null  object 
 4   depth    53940 non-null  float64
 5   table    53940 non-null  float64
 6   x        53940 non-null  float64
 7   y        53940 non-null  float64
 8   z        53940 non-null  float64
 9   price    53940 non-null  int64  
dtypes: float64(6), int64(1), object(3)
memory usage: 4.1+ MB
```

Conclusion: In this stage we can know there are 10 features in this dataset. We need to predict the value of price based on other 9 features. Also, there is no missing value in this dataset.

- correlation analysis

  Heat map



	Correlation
carat	0.921591
x	0.884435
y	0.865421
z	0.861249
price	1.000000

- Step 3. Preprocess Data && Step 4. Exploratory Data Analysis
  - First, use histogram to display features, if the feature is numeric type then plot the hist according to the value of feature. If the feature is category type then plot the hist according to the frequency of the value.

carat	cut	Color	Clarity	Depth

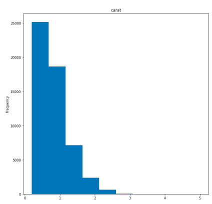
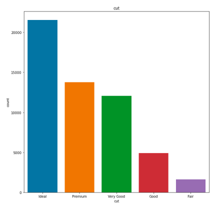
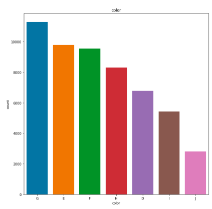
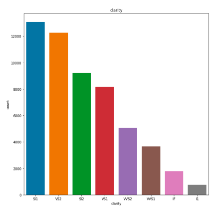
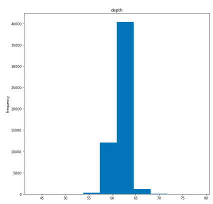
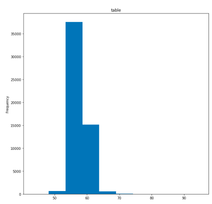
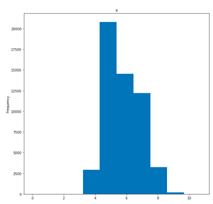
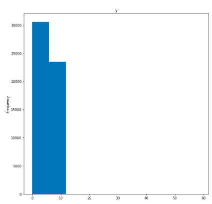
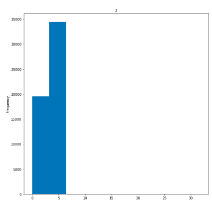
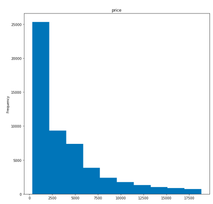
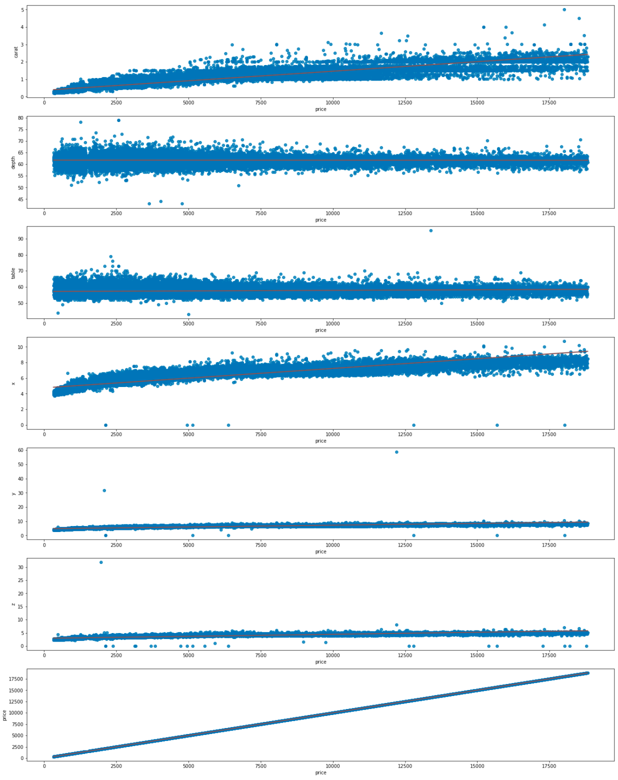
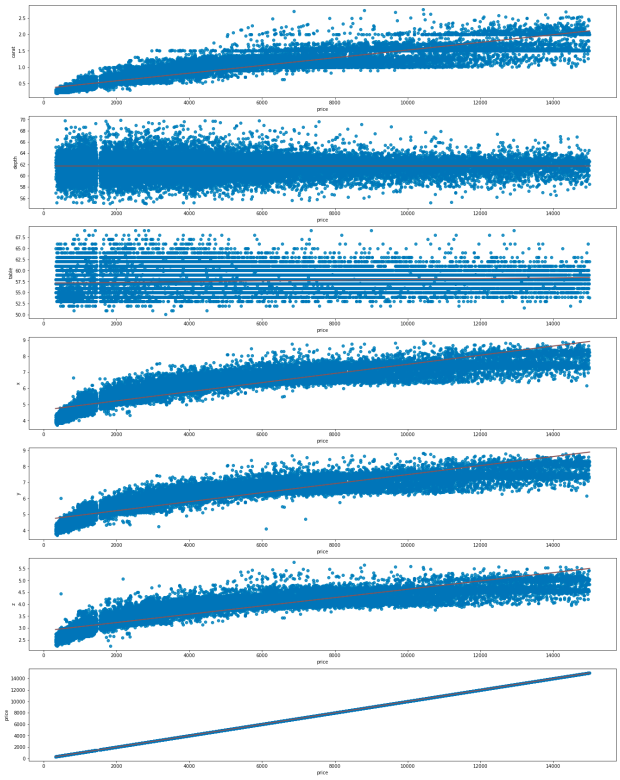

				

table	**x**	**y**	**z**	**price**
				

- Remove outliers
  1. In carat plot, remove the points - carat > 2.9
  2. In depth plot, remove the points - depth > 70 || depth <= 55
  3. In table plot, remove the points - table >= 70 || table <= 50
  4. In x plot, remove the points - x >= 9 && price >= 15000
  5. In y plot, remove the points - y >= 20 || y == 0
  6. in z plot, remove the points - z >= 6 || z <= 1
- Right(origin), Left(after removing outliers)





- Encode categorical features based on diamond documentation
    - cut

Ideal	Predium	Very Good	Good	Fair
100	80	60	40	20

    - color
        - One Hot Encode
    - clarity

I1	SI2	SI1	VS2	VVS2	VVS1	IF
30	40	50	60	70	80	90

    - Standardization

```
# standardization
scaler = StandardScaler()
standard_train = scaler.fit_transform(preprocess_train)
standard_test = scaler.fit_transform(preprocess_test)
```

- Step 5. Build classification (or regression) models using the training data && Step 7. Assess model on the test data.

Model	Parameters	MSE	RMSE	RSE	MAE	excution time
linear regression	positive = True	1647909.22(7)	1283.71(7)	0.13(7)	816.89(7)	0.02s(2)
k-neighbors regression	Default	1339014.10(6)	1157.16(6)	0.12(6)	554.29(6)	1.49s(5)
Ridge regression	Default	2190847.01(9)	1480.15(9)	0.21(8)	848.85(8)	0.004s(1)
decision tree regression	Max_depth = None	825284.43(4)	908.45(4)	0.06(4)	413.07(4)	0.02s(3)
random forest regression	n_estimators = 1000	632325.04(2)	795.19(2)	0.05(2)	336.00(1)	1m50.00s(8)
gradient Boosting regression	Max_depth = none	791343.44(3)	889.57(3)	0.06(3)	401.06(3)	17.83s(7)
SGD regression	Default	2178494.94(8)	1475.97(8)	0.22(10)	864.34(10)	0.20s(4)
support vector regression (SVR)	C=1500	998458.52(5)	999.23(5)	0.09(5)	524.38(5)	3m6.66s(9)
linear SVR	max_iter=50000, C = 5.0, loss = 'squared_epsilon_insensitive' ,dual = True	2201090.06(10)	1483.61(10)	0.21(9)	848.94(9)	10.78s(6)
multi-layer perceptron regression	max_iter=5000	570093.37(1)	755.05(1)	0.04(1)	391.20(2)	3m22.46s(10)

Discussion

From the table, we can find that multi-layer-preceptron regression, random forest, and gradient boosting regression have a good performance in diamond dataset, but there are some simple model doesn't suitable for this datset(SGD, linear SVR). Although those simple model take short time in excution stage, they still can't get a great performance. MLP and random forest model takes a long time in excution, but those two model won't be influenced by similar linear features and they will analysis the relationship between features(which help those two model have a better performance than other models).

Part 2: Performance Metrics in Classification [30 marks]

Requirement

- Based on exploratory data analysis, discuss what preprocessing that you need to do before classification, and provide evidence and justifications.
  - Initial data exploration
    - Use Pandas Profilling Report
    - **Dataset statistics**

Number of variables	15
Number of observations	32561
Missing cells	0
Missing cells (%)	0.0%
Duplicate rows	23
Duplicate rows (%)	0.1%
Total size in memory	3.7 MiB
Average record size in memory	120.0 B

      Variable types

Numeric	6
Categorical	9

    So we can find that there are missing value in train dataset, I desided to drop all instanced with missing values in both train and test set.

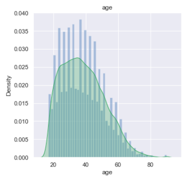
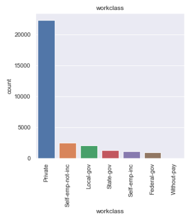
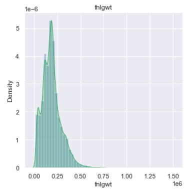
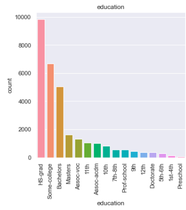
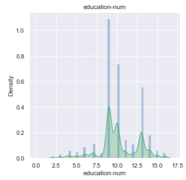
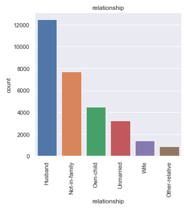
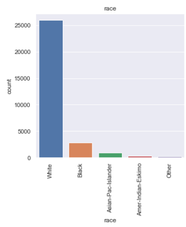
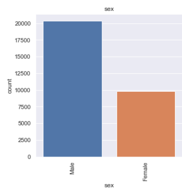
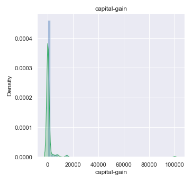
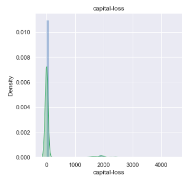
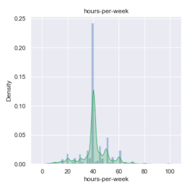
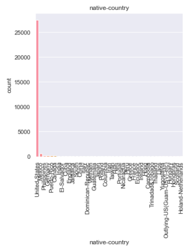
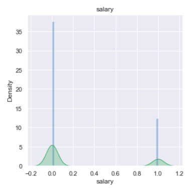
```python
# replace " ?" value with np.nan
train.replace({"?": np.nan}, inplace = True)
test.replace({"?": np.nan}, inplace = True)

# Drop the instance with missing value
train.dropna(inplace = True)
test.dropna(inplace = True)
```

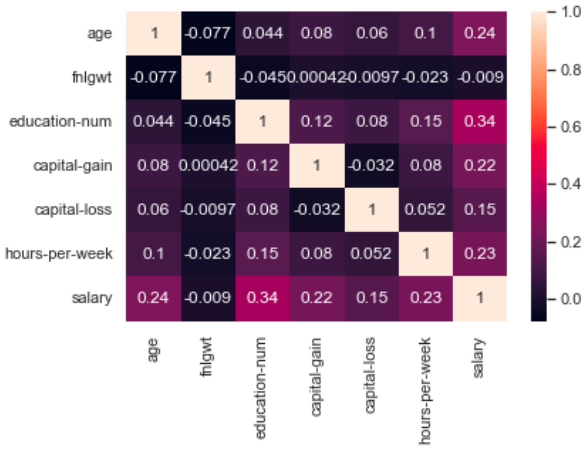
- Result

  The shape of train set: (32561, 15) $\longrightarrow$ (30162, 15)
  The shape of test set: (16281, 15) $\longrightarrow$(15060, 15)

- Plot the histogram of each features

Age	Work class	Fnglwt	Education	Education-num
				
Relationship	**Race**	**sex**	**Capital-gain**	**Capital-loss**
				
Hours-per-week	**Native-country**	**Salary**		
				

  - From the plot we can find that there are:
    - numeric features: ['age', 'fnlgwt', 'education-num', 'capital-gain', 'capital-loss', 'hours-per-week', 'salary']
    - category features: ['workclass', 'education', 'marital-status', 'occupation', 'relationship', 'race', 'sex', 'native-country']
- Correlation Heatmap



- **One-hot encoding category features**

```
def onehotencode(train,test,cols):
    for col in cols:
        setA = set(train[col])
        setB = set(test[col])

        # replace artist name
        test[col] = test[col].replace(setA.difference(setB),'null')
        train[col] = train[col].replace(setB.difference(setA),'null')

        test[col] = test[col].replace(setB.difference(setA),'null')
        train[col] = train[col].replace(setA.difference(setB),'null')

        train.drop(train[train[col] == 'null'].index,inplace= True,axis=0)
        test.drop(test[test[col] == 'null'].index,inplace= True,axis=0)

        train = pd.concat([train,pd.get_dummies(train[col])],axis = 1)
        train = train.drop(col,axis = 1)

        test = pd.concat([test,pd.get_dummies(test[col])],axis = 1)
        test = test.drop(col,axis = 1)

    return train,test

coded_train,coded_test = onehotencode(train.copy(),test.copy(),cat_col)
# print the shape of train set and test set
print("The shape of train set: ", coded_train.shape)
print("The shape of test set: ", coded_test.shape)
```

The shape of train set: (30161, 104)

The shape of test set: (15060, 104)

- Find the high correlation features with salary

```
corrMatrix = coded_train.corr(method="pearson")

# find the features have high correlation with salary
salary_corr = coded_train.corr()[['salary']]
high_salary_corr = salary_corr.loc[abs(salary_corr['salary']) > 0.1] # pick the feature
which has more than 10% correlation
high_corrFeature_list = high_salary_corr.index.to_list()
high_salary_corr.sort_values(by="salary",ascending=False)
```

	salary
salary	1.000000
Married-civ-spouse	0.445409
Husband	0.401227
education-num	0.335287
age	0.241991
hours-per-week	0.229480
capital-gain	0.221195
Male	0.216680
Exec-managerial	0.213436
Prof-specialty	0.181452
Bachelors	0.178840
Masters	0.174122
Prof-school	0.156471
capital-loss	0.150222
Self-emp-inc	0.137643
Doctorate	0.129160
Wife	0.125122
Private	-0.117208
Divorced	-0.132038
HS-grad	-0.136152
Unmarried	-0.145807
Other-service	-0.165942
Not-in-family	-0.193271
Female	-0.216680
Own-child	-0.226196
Never-married	-0.320038

- Demension reduction based on correlation

```
# Dimension reduction
high_corrFeature_list
reduced_train = coded_train[high_corrFeature_list]
reduced_test = coded_test[high_corrFeature_list]
```

origin features number: 104 $\longrightarrow$ **now: 25**

- Report the results (keep 2 decimals) of all the 10 classification algorithms on the given test data in terms of classification accuracy, precision, recall, F1-score, and AUC. You should report them in a table.

  In this part, I use default parameters in every model

Model name	Accuracy	Precision	Recall	F1-score	AUC
KNN	0.84(4)	0.70(6)	0.62(2)	0.66(3)	0.77(3)
Naive Bayes	0.83(7)	0.66(8)	0.64(1)	0.65(4)	0.77(4)
SVM	0.80(10)	0.73(4)	0.27(10)	0.39(10)	0.62(10)
Decision Tree	0.82(8)	0.64(9)	0.59(6)	0.61(8)	0.74(7)
Random Forest	0.84(5)	0.70(7)	0.61(4)	0.65(5)	0.76(5)
AdaBoost	0.86(2)	0.76(2)	0.60(5)	0.67(2)	0.77(2)
Gradient Boosting	0.86(1)	0.79(1)	0.61(3)	0.69(1)	0.78(1)
Linear discriminant analysis	0.84(6)	0.71(5)	0.55(8)	0.62(7)	0.74(8)
Multi-layer perceptron	0.84(3)	0.75(3)	0.55(9)	0.63(6)	0.74(6)
Logistic regression	0.81(9)	0.63(10)	0.55(7)	0.59(9)	0.72(9)

- Find the two best algorithms according to each of the four performance metrics, Are they the same? Explain why.
  - Accuracy

        - Definition: Predicted correct results as a percentage of the total sample
        - $Accuracy = \frac{TP+TN}{TP+FP+TN+FN}$
        - Best two models: Gradient Boosting, AdaBoost
    - Precision
        - Definition: The probability that all predicted positive samples are actually positive
        - $Precision = \frac{TP}{TP+FP}$
        - Best two models: Gradient Boosting, AdaBoost
    - Recall
        - The probability of being predicted to be positive among the actual positive samples
        - $Recall = \frac{TP}{TP+FN}$
        - Best two models: KNN, Naive Bayes
    - F1-Score
        - Harmonic mean of precision and recall
        - $F_1 = 2\frac{Precission \cdot Recall}{Precission+Recall}$
        - Best two models: Gradient Boosting, AdaBoost
    - AUC(Area Under the ROC curve)
        - Gives an overall measure of a classifier's performance
        - Best two models: Gradient Boosting, AdaBoost

The best models in **Accuracy, Precision, F1-score and AUC** are **same**(Gradient Boosting, AdaBoost), but the best model in Recall are KNN and Naive Bayes.

Why are they mostly the same?

Accuracy by quantifying the correct rate predicted by the model provides an intuitive way for us to evaluate the model.

precision represents the accuracy of the model for positive samples.

Recall describes the ability of the model to predict the correct rate of positive samples.

However, the F1-score is a hamonic mean of precision and recall, so its result will be simillar with precision and recall.

AUC is a better measure than accuracy based on formal definitions of discriminancy and consistency.

To sum up, the F1 score is based on precision and recall, and F1, AUC, and accuracy can all be used to evaluate the model generally, which is why the results are almost the same (because Gradient Boosting, AdaBoost, while maintaining high precision, It also maintains recall at a moderately high level, which results in a high composite score for both models relative to the other models)

From accuracy and AUC, we can have a general evaluation on models. But if we want to apply our model on some specific condition, we have to evaluate our model by Precision and Recall.