bonus

April 18, 2023

1 Bonus: Wine Quality Classification Model

In this bonus, we will build a classification model to predict the quality of wine.

2 Import Library

[1008]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

3 Import Dataset

[1009]:
```
df = pd.read_csv("../data/anggur.csv")
df.head()
```

[1009]:
```
   fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0           5.90            0.4451       0.1813        2.049401   0.070574
1           8.40            0.5768       0.2099        3.109590   0.101681
2           7.54            0.5918       0.3248        3.673744   0.072416
3           5.39            0.4201       0.3131        3.371815   0.072755
4           6.51            0.5675       0.1940        4.404723   0.066379

   free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0            16.593818                 42.27   0.9982  3.27       0.71
1            22.555519                 16.01   0.9960  3.35       0.57
2             9.316866                 35.52   0.9990  3.31       0.64
3            18.212300                 41.97   0.9945  3.34       0.55
4             9.360591                 46.27   0.9925  3.27       0.45

   alcohol  quality
0     8.64        7
1    10.03        8
2     9.23        8
3    14.07        9
4    11.49        8
```

4 Split Training and Test set

We will split the training and test set to determine the performance of a classification model.

[1010]:
```
from sklearn.model_selection import train_test_split

train_set, test_set = train_test_split(df, test_size=0.2,␣
↪stratify=df['quality'], random_state=42)
```

[1011]:
```
X_train = train_set.drop(['quality'], axis=1)
y_train = train_set['quality']
X_test = test_set.drop(['quality'], axis=1)
y_test = test_set['quality']
```

[1012]:
```
X_train
```

[1012]:
```
     fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
244           7.72            0.5451       0.1264        2.801338   0.091782
917           8.27            0.7417       0.2181        2.339661   0.063838
895           7.49            0.4576       0.2252        3.177156   0.075400
66            7.25            0.5545       0.2535        1.721984   0.089206
331           9.44            0.5490       0.2622        5.210260   0.054500
..             …               …            …              …          …
732           6.72            0.4886       0.2933        2.178067   0.085630
547           5.30            0.5220       0.3049        1.130890   0.089340
569           8.18            0.3570       0.1931        1.693136   0.077684
155           7.40            0.4505       0.2401        2.798932   0.069678
52            9.29            0.5590       0.2734        3.404153   0.098335

     free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
244            20.567663                 38.42   0.9963  3.29       0.72
917             8.221410                 55.40   0.9950  3.29       0.61
895            18.603452                 55.58   0.9922  3.25       0.68
66             21.507712                 43.33   0.9921  3.35       0.46
331            24.021371                 39.76   0.9998  3.25       0.55
..                   …                    …       …     …          …
732            15.476538                 45.15   0.9973  3.20       0.51
547            13.756951                 48.34   0.9976  3.32       0.55
569             7.751049                 38.81   0.9952  3.46       0.63
155            23.568005                 48.41   0.9965  3.44       0.55
52             13.935516                 46.79   0.9943  3.22       0.47

     alcohol
244    10.56
917    11.20
895     8.97
66     11.19
331    10.97
```

```
..       …
732    13.87
547    11.32
569    10.11
155    13.58
52     12.66

[800 rows x 11 columns]
```

[1013]:
```
y_train
```

[1013]:
```
244     8
917     9
895     7
66      8
331     9
       ..
732     9
547     8
569     8
155    10
52     10
Name: quality, Length: 800, dtype: int64
```

[1014]:
```
X_test
```

[1014]:
```
     fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
643           9.37            0.4153       0.2638        3.430787   0.056311
612           7.90            0.4026       0.2746        2.791431   0.082855
822           6.82            0.5197       0.3358        2.408717   0.100882
982           8.25            0.5035       0.2690        1.573458   0.105009
588           7.91            0.6452       0.2551        3.074861   0.123317
..             …                …           …              …          …
748           6.32            0.4472       0.2593        3.599399   0.069487
957           7.88            0.4736       0.2887        4.380263   0.055661
884           6.88            0.4912       0.2175        1.992063   0.082524
688           7.44            0.6484       0.2596        3.196452   0.038998
170           5.94            0.5876       0.2906        2.584408   0.081678

     free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
643            16.719396                 24.74   0.9979  3.38       0.54
612             6.172613                 28.34   0.9987  3.27       0.54
822            13.210217                 41.16   0.9958  3.17       0.56
982             7.389244                 38.75   0.9956  3.42       0.66
588            15.755803                 33.95   0.9992  3.28       0.50
..                   …                     …      …     …         …
748            11.033585                 28.55   0.9955  3.19       0.56
```

```
957            21.633450                 45.21   0.9963  3.30        0.52
884             9.005354                 33.34   0.9966  3.50        0.71
688            21.260241                 34.14   0.9962  3.38        0.62
170            14.324538                 31.92   0.9935  3.24        0.59

     alcohol
643    12.41
612    11.16
822     8.96
982    10.48
588    12.20
..       …
748    12.40
957     9.18
884    11.31
688     7.19
170     7.82

[200 rows x 11 columns]
```

[1015]:
```
y_test
```

[1015]:
```
643    10
612     8
822     7
982     8
588     9
       ..
748     9
957     8
884     8
688     6
170     6
Name: quality, Length: 200, dtype: int64
```

5 Data Preprocessing

In this section, we will process the data before feeding it into a classifier.

5.1 Handle Missing Values

[1016]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1000 entries, 0 to 999
Data columns (total 12 columns):
 #   Column                Non-Null Count  Dtype
```

```
---  ------                --------------  -----
 0   fixed acidity         1000 non-null   float64
 1   volatile acidity      1000 non-null   float64
 2   citric acid           1000 non-null   float64
 3   residual sugar        1000 non-null   float64
 4   chlorides             1000 non-null   float64
 5   free sulfur dioxide   1000 non-null   float64
 6   total sulfur dioxide  1000 non-null   float64
 7   density               1000 non-null   float64
 8   pH                    1000 non-null   float64
 9   sulphates             1000 non-null   float64
 10  alcohol               1000 non-null   float64
 11  quality               1000 non-null   int64
dtypes: float64(11), int64(1)
memory usage: 93.9 KB
```

There are no missing values to be handled.

6 Encode Target Variable

The values in the target variable range from 5 to 10, which may work for some classification models but other models may require the target variable to have values starting from 0 and incrementing by 1.

[1017]:
```
from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
y_train = le.fit_transform(y_train)
y_test = le.transform(y_test)
```

7 Generate Synthetic Data

The data to be trained is relatively small, therefore we will perform resampling to balance the class distribution, then generate synthetic data using augmentation with Gaussian noise.

[1018]:
```
from imblearn.over_sampling import SMOTE

# Perform oversampling to balance the classes
y_counts = np.bincount(y_train)
min_sample = np.min(y_counts[np.nonzero(y_counts)]) - 1
sm = SMOTE(random_state=42, k_neighbors=min_sample)
X_train, y_train = sm.fit_resample(X_train, y_train)
```

[1019]:
```
# Set the standard deviation of the Gaussian noise to add
std_dev = 0.1

# Generate new data points with Gaussian noise added
n_iter = 5
```

```
fold = len(X_train)

for i in range(n_iter):
    for j in range(fold):
        synthetic_data = X_train.iloc[j].values + np.random.normal(loc=0,␣
 ↪scale=std_dev, size=X_train.shape[1])
        synthetic_data_df = pd.DataFrame(synthetic_data.reshape(1, -1),␣
 ↪columns=X_train.columns)
        X_train = pd.concat([X_train, synthetic_data_df], axis=0)
        y_train = np.append(y_train, y_train[j])
```

[1020]:
```
print(len(X_train), len(y_train))
```

```
12924 12924
```

8 Feature Scaling

In this section, we aim to perform feature scaling by transforming the numerical columns of our data into a normal standard distribution. The purpose of this transformation is to make the data comparable across different features, as well as to improve the performance of linear-based classification models. This way, the classifiers can more effectively recognize patterns in the data and make accurate predictions, regardless of the range of values in the original data.

[1021]:
```
from sklearn.preprocessing import StandardScaler

sc = StandardScaler()
X_train = sc.fit_transform(X_train)
X_test = sc.transform(X_test)
```

[1022]:
```
X_train
```

[1022]:
```
array([[ 0.65066188,  0.22472489, -1.33732389, …,  0.04638432,
         0.99118125,  0.22716987],
       [ 1.05039913,  1.67835607, -0.44315074, …,  0.04638432,
         0.15164928,  0.48779326],
       [ 0.48349903, -0.42223711, -0.37391814, …, -0.24398311,
         0.6858969 , -0.42031635],
       …,
       [ 0.16082745, -1.52734396,  0.98722   , …,  0.96227328,
         0.55311443,  1.64866168],
       [ 0.56565969,  0.84972886, -1.64360931, …, -0.16819   ,
        -0.97252942,  1.36956385],
       [ 1.54875651,  0.56386636, -0.41566247, …,  0.79181839,
         0.36833465,  0.87357648]])
```

[1023]:
```
X_test
```

[1023]:
```
array([[ 1.84987364e+00, -7.34997022e-01,  2.47317665e-03, …,
         6.99711025e-01, -3.82598333e-01,  9.80534350e-01],
       [ 7.81484980e-01, -8.28898934e-01,  1.07784737e-01, …,
        -9.87993946e-02, -3.82598333e-01,  4.71504299e-01],
       [-3.45362807e-03,  3.69210615e-02,  7.04550244e-01, …,
        -8.24717958e-01, -2.29956157e-01, -4.24388591e-01],
       …,
       [ 4.01540724e-02, -1.73803703e-01, -4.49001382e-01, …,
         1.57081330e+00,  9.14860164e-01,  5.32587905e-01],
       [ 4.47159277e-01,  9.88509733e-01, -3.84813190e-02, …,
         6.99711025e-01,  2.27970371e-01, -1.14517514e+00],
       [-6.43033235e-01,  5.38963570e-01,  2.63801863e-01, …,
        -3.16574964e-01, -9.92892647e-04, -8.88623998e-01]])
```

9 Implement Classifiers

In this section, we will fit multiple models to the processed training data.

9.1 Logistic Regression

[1024]:
```python
from sklearn.linear_model import LogisticRegression

lr = LogisticRegression(random_state=42, max_iter=10000)
lr.fit(X_train, y_train)
```

[1024]:
```
LogisticRegression(max_iter=10000, random_state=42)
```

9.2 Support Vector Machine

[1025]:
```python
from sklearn.svm import SVC

svc = SVC(random_state=42)
svc.fit(X_train, y_train)
```

[1025]:
```
SVC(random_state=42)
```

9.3 XGBoost

[1026]:
```python
from xgboost import XGBClassifier

xgb = XGBClassifier()
xgb.fit(X_train, y_train)
```

[1026]:
```
XGBClassifier(base_score=None, booster=None, callbacks=None,
              colsample_bylevel=None, colsample_bynode=None,
              colsample_bytree=None, early_stopping_rounds=None,
```

```
                enable_categorical=False, eval_metric=None, feature_types=None,
                gamma=None, gpu_id=None, grow_policy=None, importance_type=None,
                interaction_constraints=None, learning_rate=None, max_bin=None,
                max_cat_threshold=None, max_cat_to_onehot=None,
                max_delta_step=None, max_depth=None, max_leaves=None,
                min_child_weight=None, missing=nan, monotone_constraints=None,
                n_estimators=100, n_jobs=None, num_parallel_tree=None,
                objective='multi:softprob', predictor=None, …)
```

9.4 Voting Classifier

[1027]:
```python
from sklearn.ensemble import VotingClassifier

vote = VotingClassifier(estimators=[('lr', LogisticRegression(random_state=42,␣
 ↪max_iter=10000)),
                                    ('xgb', XGBClassifier())], voting='hard')
vote.fit(X_train, y_train)
```

[1027]:
```
VotingClassifier(estimators=[('lr',
                              LogisticRegression(max_iter=10000,
                                                 random_state=42)),
                             ('xgb',
                              XGBClassifier(base_score=None, booster=None,
                                            callbacks=None,
                                            colsample_bylevel=None,
                                            colsample_bynode=None,
                                            colsample_bytree=None,
                                            early_stopping_rounds=None,
                                            enable_categorical=False,
                                            eval_metric=None,
                                            feature_types=None, gamma=None,
                                            gpu_id=None, grow_policy=None,
                                            importance_type=None,
                                            interaction_constraints=None,
                                            learning_rate=None, max_bin=None,
                                            max_cat_threshold=None,
                                            max_cat_to_onehot=None,
                                            max_delta_step=None, max_depth=None,
                                            max_leaves=None,
                                            min_child_weight=None, missing=nan,
                                            monotone_constraints=None,
                                            n_estimators=100, n_jobs=None,
                                            num_parallel_tree=None,
                                            predictor=None, random_state=None,
…))])
```

10 Evaluation

In this section, we will determine the performance of each model towards the test set.

10.1 Test set Performance

[1028]:
```python
from sklearn.metrics import classification_report

y_pred_lr = lr.predict(X_test)
print(classification_report(y_test, y_pred_lr, zero_division=0))
```

```
              precision    recall  f1-score   support

           0       0.50      1.00      0.67         1
           1       1.00      0.88      0.93         8
           2       0.91      1.00      0.95        50
           3       0.96      0.81      0.88        90
           4       0.76      0.86      0.81        44
           5       0.70      1.00      0.82         7

    accuracy                           0.88       200
   macro avg       0.80      0.92      0.84       200
weighted avg       0.89      0.88      0.88       200
```

[1029]:
```python
y_pred_svc = svc.predict(X_test)
print(classification_report(y_test, y_pred_svc, zero_division=0))
```

```
              precision    recall  f1-score   support

           0       0.00      0.00      0.00         1
           1       0.67      0.75      0.71         8
           2       0.92      0.88      0.90        50
           3       0.90      0.86      0.88        90
           4       0.79      0.86      0.83        44
           5       0.88      1.00      0.93         7

    accuracy                           0.86       200
   macro avg       0.69      0.72      0.71       200
weighted avg       0.86      0.86      0.86       200
```

[1030]:
```python
y_pred_xgb = xgb.predict(X_test)
print(classification_report(y_test, y_pred_xgb, zero_division=0))
```

```
              precision    recall  f1-score   support

           0       0.00      0.00      0.00         1
```

```
           1       0.86      0.75      0.80         8
           2       0.90      0.90      0.90        50
           3       0.84      0.86      0.85        90
           4       0.73      0.75      0.74        44
           5       0.80      0.57      0.67         7

    accuracy                           0.82       200
   macro avg       0.69      0.64      0.66       200
weighted avg       0.83      0.82      0.82       200
```

[1031]:
```
y_pred_vote = vote.predict(X_test)
print(classification_report(y_test, y_pred_vote, zero_division=0))
```

```
              precision    recall  f1-score   support

           0       0.50      1.00      0.67         1
           1       1.00      0.88      0.93         8
           2       0.89      1.00      0.94        50
           3       0.89      0.86      0.87        90
           4       0.77      0.75      0.76        44
           5       0.80      0.57      0.67         7

    accuracy                           0.86       200
   macro avg       0.81      0.84      0.81       200
weighted avg       0.86      0.86      0.86       200
```

10.2 One-Versus-Rest ROC Curve

[1032]:
```
from sklearn.metrics import roc_curve, auc

def plot_ovr_roc_curve(y_true, y_prob):
    n_classes = y_prob.shape[1]
    fpr = dict()
    tpr = dict()
    roc_auc = dict()
    for i in range(n_classes):
        fpr[i], tpr[i], _ = roc_curve(y_true[:, i], y_prob[:, i])
        roc_auc[i] = auc(fpr[i], tpr[i])

    # Compute macro-average ROC curve
    all_fpr = np.unique(np.concatenate([fpr[i] for i in range(n_classes)]))
    mean_tpr = np.zeros_like(all_fpr)
    for i in range(n_classes):
        mean_tpr += np.interp(all_fpr, fpr[i], tpr[i])
    mean_tpr /= n_classes
    fpr["macro"] = all_fpr
```

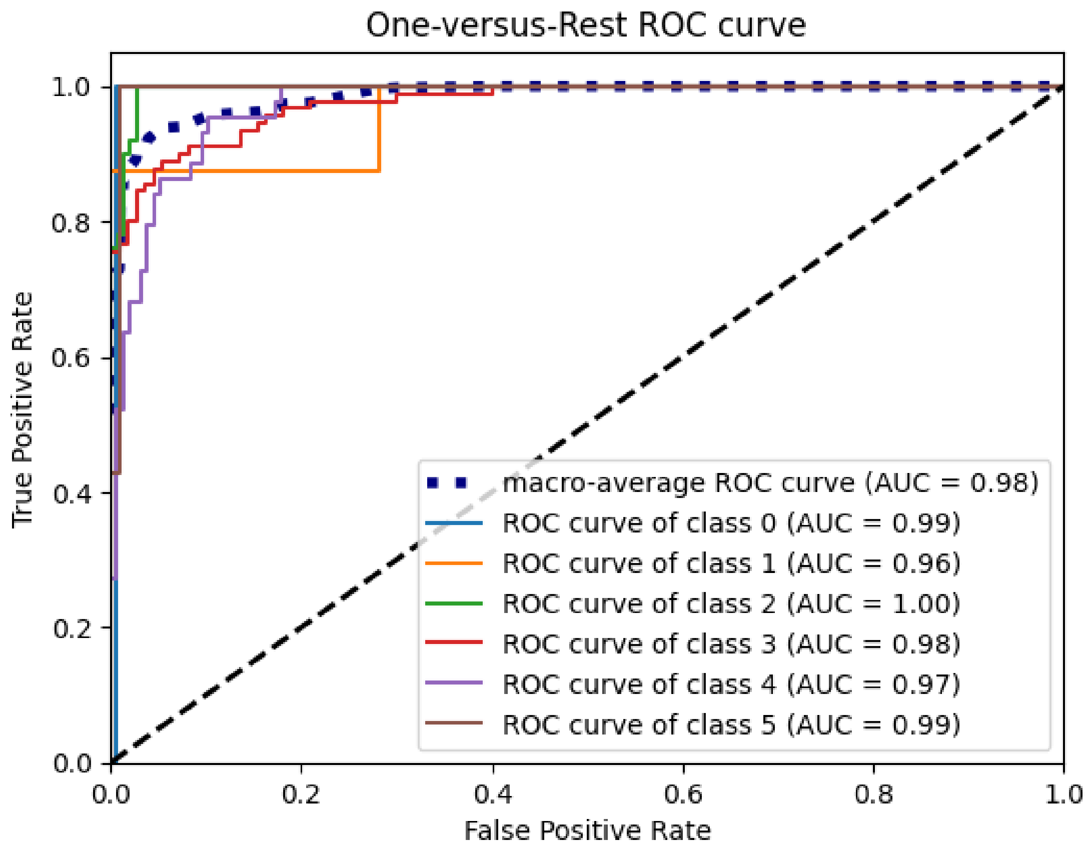
```
    tpr["macro"] = mean_tpr
    roc_auc["macro"] = auc(fpr["macro"], tpr["macro"])

    # Plot ROC curves
    plt.figure()
    plt.plot(fpr["macro"], tpr["macro"],
             label='macro-average ROC curve (AUC = {0:0.2f})'
                   ''.format(roc_auc["macro"]),
             color='navy', linestyle=':', linewidth=4)
    for i in range(n_classes):
        plt.plot(fpr[i], tpr[i], label='ROC curve of class {0} (AUC = {1:0.2f})'
                                       ''.format(i, roc_auc[i]))
    plt.plot([0, 1], [0, 1], 'k--', lw=2)
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('One-versus-Rest ROC curve')
    plt.legend(loc="lower right")
    plt.show()
```

[1033]:
```
# Predict probabilities for test set
y_prob = lr.predict_proba(X_test)

# Get true labels for test set
n_samples = y_prob.shape[0]
n_classes = lr.classes_.shape[0]
y_true = np.zeros((n_samples, n_classes))
for i in range(n_samples):
    true_label = y_test[i]
    y_true[i, true_label] = 1
```

[1034]:
```
plot_ovr_roc_curve(y_true, y_prob)
```



After conducting multiple trials, we can conclude that the **Logistic Regression model outperformed other models on the test data**. This could be attributed to the strong correlation between the `alcohol` feature and the target variable, where the average `alcohol` values for each class showed a linear relationship with the target variable. Logistic Regression is particularly suitable for datasets with linear relationships between input and output variables, which could explain why it performed the best in this case.