Machine Learning Homework 2

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[1]:
```
# toc
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import cross_val_score, GridSearchCV,␣
 ↪train_test_split
from sklearn.metrics import ConfusionMatrixDisplay, precision_score,␣
 ↪recall_score, accuracy_score
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.svm import SVC

plt.style.use('../maroon_ipynb.mplstyle')

cancer = load_breast_cancer()
features = cancer.data
target = cancer.target
```

Contents

Problem 1

The sklearn library includes a set of data containing image information on fine needle aspirates used to identify breast cancer. The dataset contains information gathered from the images as well as whether the mass was malignant (target=0) or benign (target=1). The included python template shows how to make arrays of the features and targets.

What is the split of malignant vs benign for the dataset? What issues might you forsee using a dataset with this split?

Solution

[2]:
```
benign = np.where(target == 1)
malignant = np.where(target == 0)

benign_count = len(benign[0])
malignant_count = len(malignant[0])
total = len(target)

assert benign_count + malignant_count == total

benign_ratio = benign_count/total
malignant_ratio = malignant_count/total
print(f'Benign: {benign_ratio:.2%} ({benign_count})')
print(f'Malignant: {malignant_ratio:.2%} ({malignant_count})')
```

```
Benign: 62.74% (357)
Malignant: 37.26% (212)
```

Though it is not severe, the imbalance between benign and malignant cases might cause issues. The dataset's imbalance, with benign samples making up about 63% and malignant samples about 37%, could cause a machine learning model to favor predicting the benign class. This bias may lead to underperformance in identifying malignant cases, which is particularly concerning in medical diagnostics where both classes are critical.

Problem 2

Generate a support vector classifier (SVC) to determine if the input data indicates a malignant or benign cancer. Use the linear kernel and varying values of C. Plot the accuracy score as a function of C. Use cross validation. What value of C gives the best results?

Solution

First off, let's understand what data we are dealing with. The features data looks like this:

[3]:
```
feature_names = cancer.feature_names
temp_df = pd.DataFrame(features, columns=feature_names)
temp_df.head(n=4).transpose()
```

[3]:

	0	1	2	3
mean radius	17.990000	20.570000	19.690000	11.420000
mean texture	10.380000	17.770000	21.250000	20.380000
mean perimeter	122.800000	132.900000	130.000000	77.580000
mean area	1001.000000	1326.000000	1203.000000	386.100000
mean smoothness	0.118400	0.084740	0.109600	0.142500
mean compactness	0.277600	0.078640	0.159900	0.283900
mean concavity	0.300100	0.086900	0.197400	0.241400
mean concave points	0.147100	0.070170	0.127900	0.105200
mean symmetry	0.241900	0.181200	0.206900	0.259700
mean fractal dimension	0.078710	0.056670	0.059990	0.097440
radius error	1.095000	0.543500	0.745600	0.495600
texture error	0.905300	0.733900	0.786900	1.156000
perimeter error	8.589000	3.398000	4.585000	3.445000
area error	153.400000	74.080000	94.030000	27.230000
smoothness error	0.006399	0.005225	0.006150	0.009110
compactness error	0.049040	0.013080	0.040060	0.074580
concavity error	0.053730	0.018600	0.038320	0.056610
concave points error	0.015870	0.013400	0.020580	0.018670
symmetry error	0.030030	0.013890	0.022500	0.059630
fractal dimension error	0.006193	0.003532	0.004571	0.009208
worst radius	25.380000	24.990000	23.570000	14.910000
worst texture	17.330000	23.410000	25.530000	26.500000
worst perimeter	184.600000	158.800000	152.500000	98.870000
worst area	2019.000000	1956.000000	1709.000000	567.700000
worst smoothness	0.162200	0.123800	0.144400	0.209800
worst compactness	0.665600	0.186600	0.424500	0.866300
worst concavity	0.711900	0.241600	0.450400	0.686900
worst concave points	0.265400	0.186000	0.243000	0.257500
worst symmetry	0.460100	0.275000	0.361300	0.663800
worst fractal dimension	0.118900	0.089020	0.087580	0.173000

This data needs to be normalized using the variance method.

[4]:
```
pipline = make_pipeline(StandardScaler(), SVC(kernel='linear'))
scores = cross_val_score(pipline, features, target, cv=5)
scores
```

[4]:
```
array([0.96491228, 0.98245614, 0.96491228, 0.96491228, 0.98230088])
```

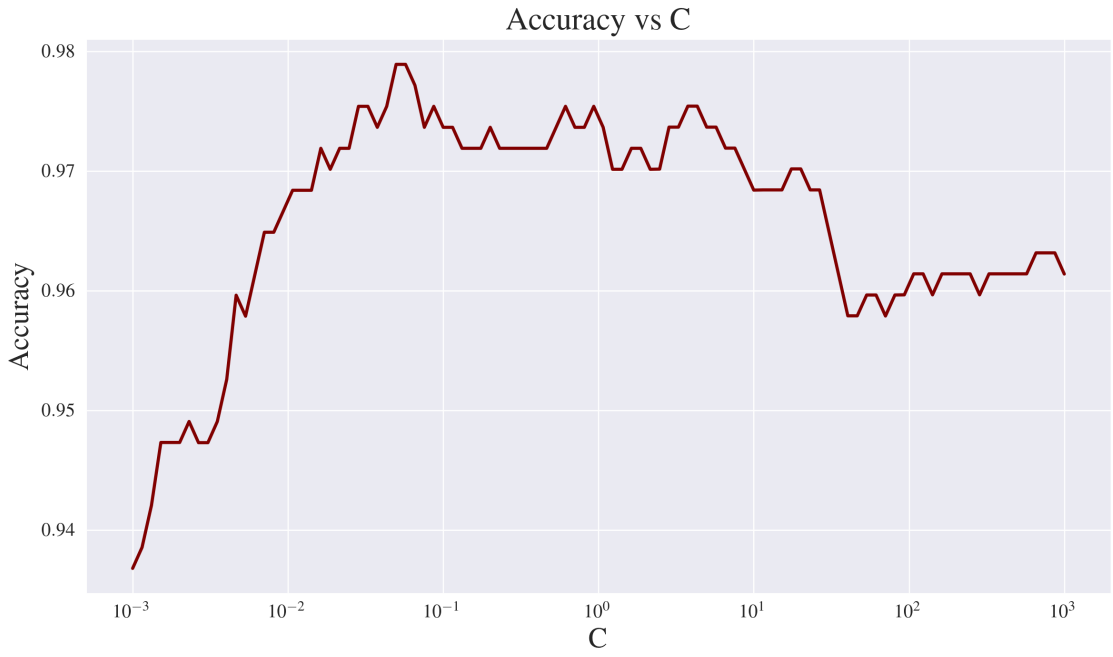
In this snippet above, the model is normalized with the variance method, and an SVC model with the regularization parameter, `C`, is 1 by default. The `cross_val_score` function will divide the data into 5 parts, train the model on 4 parts, and test it on the 5th part. It will then record the accuracy over the testing portion of the data:

$$Accuracy = \frac{Correct\ Predictions}{Total\ Predictions}$$

It does this procedure of dividing 5 times, choosing a different 4/5 to train, and a different 1/5 to test. We can make a loop that will see how adjusting the `C` parameter will change the accuracy of the model.

[5]:
```
c_values = np.logspace(-3, 3, 100)  # use logspace to get a wider range of C␣
↪values
cv_scores = []
for c in c_values:
    pipline = make_pipeline(StandardScaler(), SVC(kernel='linear', C=c))
    scores = cross_val_score(pipline, features, target, cv=5)
    cv_scores.append(np.mean(scores))

fig, ax = plt.subplots()
ax.semilogx(c_values, cv_scores)
ax.set_xlabel('C')
ax.set_ylabel('Accuracy')
ax.set_title('Accuracy vs C')
plt.show()
```



[6]:
```
# Best C value
best_index = np.argmax(cv_scores)
best_c = c_values[best_index]
float(best_c)
```

[6]: 0.049770235643321115

[7]:
```
# the highest score
float(cv_scores[best_index])
```

[7]: 0.9789163173420278

As seen above, a `C` value of around 0.05 gives the best results. You can even notice the overfitting that occurs after `C` values of around 30.

Problem 3

Using the radial basis function kernel (RBF), determine the hyperparameters (C and γ) that result in the best model.

Solution

You can use the `GridSearchCV` class to find the best hyperparameters for the model.

[8]:
```
pipline = make_pipeline(StandardScaler(), SVC(kernel='rbf'))
N = 20
param_grid = {
    'svc__C': np.logspace(-3, 3, N),
    'svc__gamma': np.logspace(-3, 3, N)
}

grid_search = GridSearchCV(pipline, param_grid, cv=5, scoring='accuracy')
grid_search.fit(features, target)

# Best parameters
grid_search.best_params_
```

[8]:
```
{'svc__C': np.float64(6.158482110660261),
 'svc__gamma': np.float64(0.018329807108324356)}
```

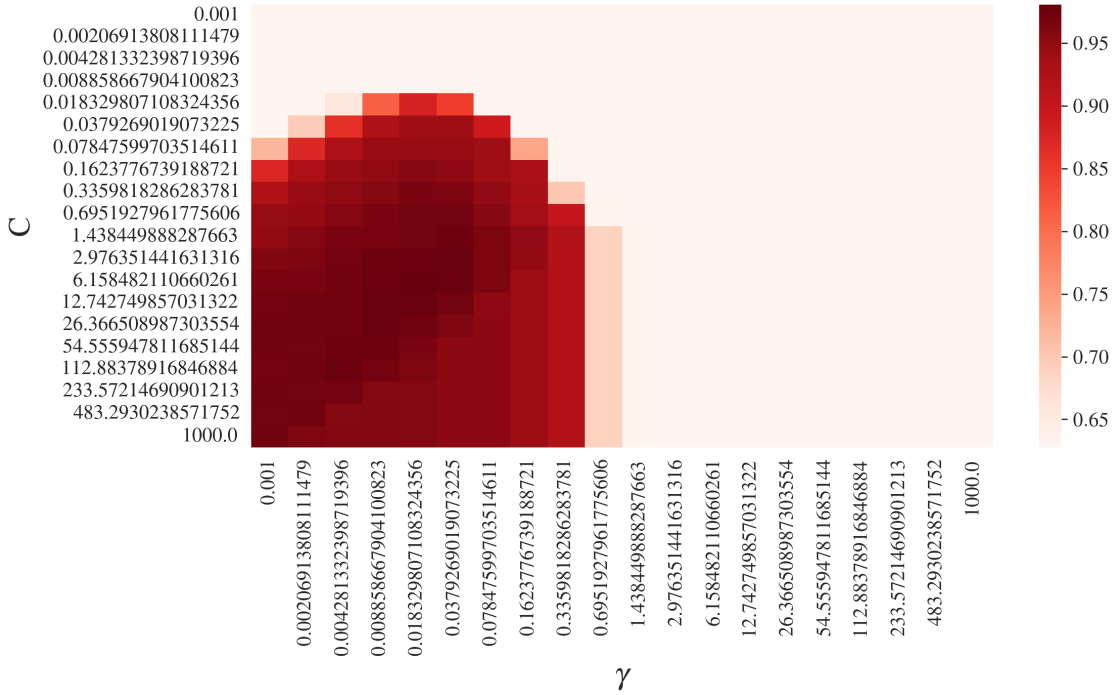
[9]:
```
# Best score
float(grid_search.best_score_)
```

[9]:
```
0.9806862288464524
```

As seen above, the best parameters are $C = 6.16$ and $\gamma = 0.018$. These parameters result in a cross-validated accuracy score of 0.98. Here is a heatmap of the grid:

[10]:
```
results_df = pd.DataFrame(grid_search.cv_results_)
scores_pivot = results_df.pivot(index='param_svc__C',␣
 ↪columns='param_svc__gamma', values='mean_test_score')

fig, ax = plt.subplots()
sns.heatmap(scores_pivot, fmt='.3f', cmap='Reds')
ax.set_xlabel(r'$\gamma$')
ax.set_ylabel('C')
plt.show()
```


C
0.001
0.00206913808111479
0.00428133239871940
0.00885866790410082
0.01832980710832436
0.03792690190732250
0.07847599703514611
0.16237767391887210
0.33598182862837810
0.69519279617756060
1.43844988828766300
2.97635144163131600
6.15848211066026100
12.74274985703132200
26.36650898730355400
54.55594781168514400
112.88378916846884000
233.57214690901213000
483.29302385717520000
1000.0
γ
0.95
0.90
0.85
0.80
0.75
0.70
0.65

Problem 4

Generate the most accurate SVC model you can (feel free to use other kernels and varying hyperparameters). What is the precision and recall of this model? Use a train/test split and give the precision and recall for the test data. Show the confusion matrix for both the training and test data.

Solution

I'm going to redo the hyperparameter search using a finer grid around the best parameters found above.

[11]:
```
pipline = make_pipeline(StandardScaler(), SVC(kernel='rbf'))
N = 20
param_grid = {
    'svc__C': np.linspace(1, 10, N),
    'svc__gamma': np.linspace(0.005, 0.05, N)
}

grid_search = GridSearchCV(pipline, param_grid, cv=5, scoring='accuracy')
grid_search.fit(features, target)

# Best parameters
grid_search.best_params_
```

[11]:
```
{'svc__C': np.float64(4.789473684210526),
 'svc__gamma': np.float64(0.023947368421052634)}
```

[12]:
```
# Best score
float(grid_search.best_score_)
```

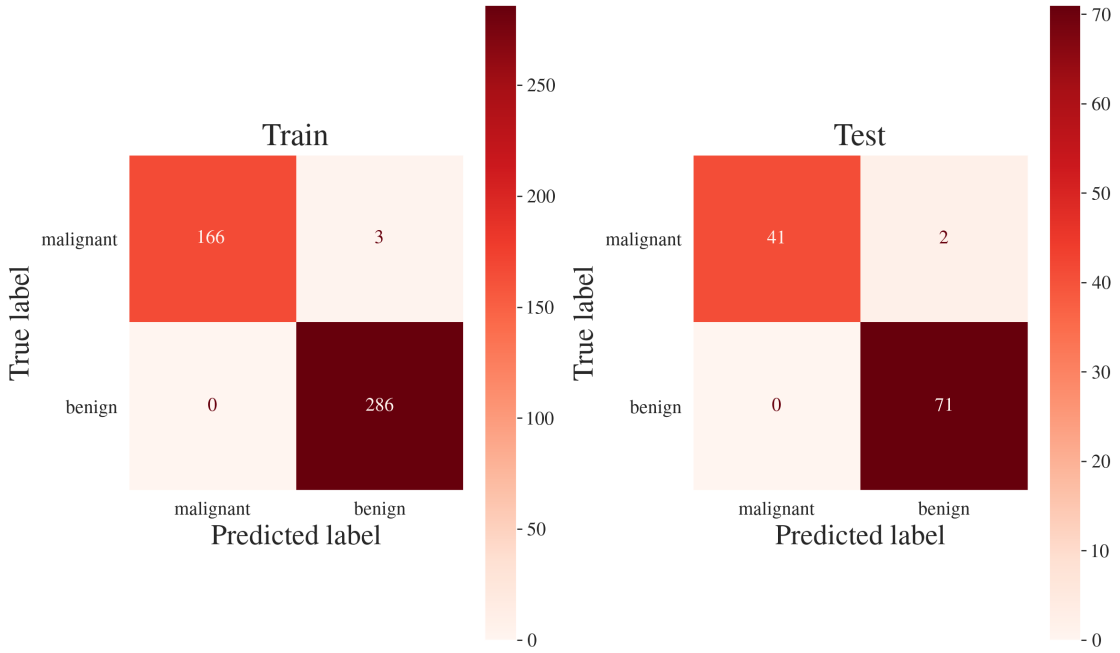
[12]:
```
0.9824561403508772
```

[13]:
```
# Making a new model with this hyperparameter set
x_train, x_test, y_train, y_test = train_test_split(features, target,␣
 ↪test_size=0.2, random_state=42)
final_pipe = make_pipeline(StandardScaler(), SVC(kernel='rbf', C=4.7895,␣
 ↪gamma=0.02395))
final_pipe.fit(x_train, y_train)

y_pred = final_pipe.predict(x_test)
accuracy = accuracy_score(y_test, y_pred)
precision = precision_score(y_test, y_pred)
recall = recall_score(y_test, y_pred)
print(f'Accuracy: {accuracy:.2%}')
print(f'Precision: {precision:.2%}')
print(f'Recall: {recall:.2%}')
```

```
Accuracy: 98.25%
Precision: 97.26%
Recall: 100.00%
```

[14]:
```
# Confusion matrix for test data
fig, ax = plt.subplots(ncols=2)
ConfusionMatrixDisplay.from_estimator(final_pipe, x_train, y_train, ax=ax[0],␣
 ↪display_labels=cancer.target_names, cmap='Reds')
ConfusionMatrixDisplay.from_estimator(final_pipe, x_test, y_test, ax=ax[1],␣
 ↪display_labels=cancer.target_names, cmap='Reds')
ax[0].set_title('Train')
ax[1].set_title('Test')
ax[0].grid(False)
ax[1].grid(False)
plt.show()
```



Problem 5

If your trained model from question 4 is given a novel set of inputs and determines that the cancer is benign, what is the chance that it is wrong? How does this relate to your answer for question 1?

Solution

From the calculation above, the precision is 97.26%. This is the ratio of the correctly predicted benign cases to the total predicted benign cases. Going off only the test data, this means that there is a 2.74% chance that the model will predict benign, but it is actually malignant.

In relation to the first question, we predicted that the model would bias the benign cases because there were far more benign cases in the data. These results reflect this bias, and it is a bad bias because it is more dangerous to predict benign and it actually be malignant.

[15]:
```
# You can do this to shift the positive class
# This would find the precision of the malignant class
malignant_precision = precision_score(y_test, y_pred, pos_label=0)
malignant_precision*100
```

[15]:
```
100.0
```