CSE572-Lab10-key

November 4, 2022

1 CSE 572: Lab 10

In this lab, you will practice implementing techniques for model selection including cross validation and grid search.

To execute and make changes to this notebook, click File > Save a copy to save your own version in your Google Drive or Github. Read the step-by-step instructions below carefully. To execute the code, click on each cell below and press the SHIFT-ENTER keys simultaneously or by clicking the Play button.

When you finish executing all code/exercises, save your notebook then download a copy (.ipynb file). Submit the following **three** things: 1. a link to your Colab notebook, 2. the .ipynb file, and 3. a pdf of the executed notebook on Canvas.

To generate a pdf of the notebook, click File > Print > Save as PDF.

```
[1]: # Import libraries
import numpy as np
import pandas as pd

# Set the random seed for reproducibility
seed = 0
np.random.seed(0)
```

1.0.1 Load the iris dataset

```
[2]:
          sepal length
                         sepal width petal length petal width
                                                                                class
                    5.8
                                  2.8
                                                 5.1
                                                                      Iris-virginica
     114
                                                               2.4
                                                                     Iris-versicolor
     62
                    6.0
                                  2.2
                                                 4.0
                                                               1.0
     33
                    5.5
                                  4.2
                                                 1.4
                                                               0.2
                                                                         Iris-setosa
                    7.3
                                  2.9
                                                 6.3
     107
                                                               1.8
                                                                      Iris-virginica
     7
                    5.0
                                  3.4
                                                 1.5
                                                               0.2
                                                                         Iris-setosa
```

```
[3]: data.shape
```

[3]: (150, 5)

Standardize the data by subtracting the feature-wise mean and dividing by the feature-wise standard deviation for each sample.

```
[4]: # YOUR CODE HERE

data[data.columns[:-1]] = (data[data.columns[:-1]] - data[data.columns[:-1]].

mean(axis=0)) / data[data.columns[:-1]].std(axis=0)
```

```
[5]: data.sample(5, random_state=seed)
```

```
[5]:
          sepal length sepal width petal length petal width
                                                                             class
     114
             -0.052331
                           -0.585801
                                          0.760212
                                                                   Iris-virginica
                                                        1.574155
     62
              0.189196
                           -1.969583
                                          0.136778
                                                       -0.260321
                                                                  Iris-versicolor
     33
             -0.414621
                            2.643024
                                         -1.336794
                                                       -1.308593
                                                                       Iris-setosa
     107
              1.759119
                           -0.355171
                                          1.440322
                                                        0.787951
                                                                   Iris-virginica
     7
             -1.018437
                            0.797981
                                         -1.280118
                                                       -1.308593
                                                                       Iris-setosa
```

1.0.2 k-fold Cross validation

We will use 5-fold cross validation to train and evaluate our classifier. We will not do any model selection/hyperparameter tuning in this step, so we need to split our data into a training and test set.

To split the data into 5 folds we will shuffle the rows and then split them into k equal groups.

```
[6]: k = 5

# Note: np.split raises error if indices_or_sections is
# an integer and doesn't result in equal size splits
folds = np.split(data.sample(frac=1, random_state=seed), indices_or_sections=k)
```

Use a for loop to print the number of samples and number of samples from each class in each fold.

```
Fold 1 has 30 instances (11 setosa, 6 virginica, 13 versicolor)
Fold 2 has 30 instances (5 setosa, 15 virginica, 10 versicolor)
Fold 3 has 30 instances (10 setosa, 10 virginica, 10 versicolor)
Fold 4 has 30 instances (14 setosa, 10 virginica, 6 versicolor)
Fold 5 has 30 instances (10 setosa, 9 virginica, 11 versicolor)
```

1.0.3 Train a k Nearest Neighbors classifier

We will use the KNeighborsClassifier in sklearn for our classification model. Use cross validation to train and evaluate the model. Set hyperparameters to n_neighbors=5, metric='12', and weights='uniform'.

Implement a for loop to iterate through each fold, training a new kNN model each iteration with one fold assigned to validation and the remaining folds assigned to training. Compute the validation accuracy for each iteration and append it to the accuracies list.

```
[8]: from sklearn.neighbors import KNeighborsClassifier
    from sklearn.metrics import accuracy_score

accuracies = []

# YOUR CODE HERE

for i in range(len(folds)):
        # assign the folds to training and validation
        val = folds[i]
        train = pd.concat(folds[0:i] + folds[i+1:])
        # train the classifier
        knn = KNeighborsClassifier(n_neighbors=5, metric='12', weights='uniform')
        knn.fit(train[train.columns[:-1]], train['class'])
        # predict test set
        pred_val = knn.predict(val[val.columns[:-1]])
        # append accuracy to list
        accuracies.append(accuracy_score(val['class'], pred_val))
```

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Print the mean and standard deviation of the accuracy from cross validation (across all k folds).

```
[9]: print('Mean accuracy: {:.2f}'.format(np.mean(accuracies)))
print('Standard deviation of accuracy: {:.2f}'.format(np.std(accuracies)))
```

Mean accuracy: 0.95

Standard deviation of accuracy: 0.06

Question 1: If you increased the number of folds, do you expect the standard deviation of the accuracy across k folds to increase or decrease? Why?

Answer:

YOUR ANSWER HERE

The standard deviation would be expected to increase because more folds means smaller datasets in each fold, which means there will be more variability from fold to fold and the model will be less likely to generalize to the held-out fold.

1.0.4 Hyperparameter selection using cross validation and grid search

In this exercise, we will use the KNeighborsClassifier again but this time we will perform hyperparameter selection using k-fold cross validation and Grid Search.

We have three model choices (hyperparameters) for our kNN model: - Number of neighbors (k or n_neighbors). We will consider all integer values $k \in [1, 10]$. - Whether to treat all neighbors equally when taking majority vote, or weight them according to their distance from the query point (weights='uniform' or weights='distance'). - The distance metric for computing distance between query point and neighbors (metric argument). We will consider three options for metric: '11', '12', and 'cosine'.

Question 2: How many total combinations of the above hyperparameter choices are there?

Answer:

YOUR ANSWER HERE

10 values for neighbors * 2 values for weights * 3 values for distance metric = 60

Instead of implementing cross validation manually as we did in the previous example, we will use the GridSearchCV class in sklearn to perform grid search and cross validation simultaneously.

First, we will split the data into a training (70%) and test (30%) test.

We will then use the training set for cross validation and grid search to select the optimal hyperparameter settings.

Next, we define the values for grid search using a dictionary in which the keys are the parameter names to be passed to the model function and each corresponding value is a list of possible values to try in grid search.

Next, we instantiate a kNeighborsClassifier but do not specify the hyperparameter settings yet.

```
[12]: knn = KNeighborsClassifier()
```

We can then pass this classifier and our parameter grid to a new GridSearchCV object and fit the GridSearchCV using our training data.

```
[13]: from sklearn.model_selection import GridSearchCV

clf = GridSearchCV(knn, param_grid)

clf.fit(X_train, y_train)
```

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packages/sklearn/neighbors/_classification.py:228: FutureWarning: Unlike other reduction functions (e.g. `skew`, `kurtosis`), the default behavior of `mode` typically preserves the axis it acts along. In SciPy 1.11.0, this behavior will change: the default value of `keepdims` will become False, the `axis` over which the statistic is taken will be eliminated, and the value None will no longer be accepted. Set `keepdims` to True or False to avoid this warning.

mode, _ = stats.mode(_y[neigh_ind, k], axis=1)

/Users/hkerner/anaconda3/envs/cse572/lib/python3.9/site-

packages/sklearn/neighbors/_classification.py:228: FutureWarning: Unlike other reduction functions (e.g. `skew`, `kurtosis`), the default behavior of `mode` typically preserves the axis it acts along. In SciPy 1.11.0, this behavior will change: the default value of `keepdims` will become False, the `axis` over which the statistic is taken will be eliminated, and the value None will no longer be accepted. Set `keepdims` to True or False to avoid this warning.

mode, _ = stats.mode(_y[neigh_ind, k], axis=1)

/Users/hkerner/anaconda3/envs/cse572/lib/python3.9/site-

packages/sklearn/neighbors/_classification.py:228: FutureWarning: Unlike other reduction functions (e.g. `skew`, `kurtosis`), the default behavior of `mode` typically preserves the axis it acts along. In SciPy 1.11.0, this behavior will change: the default value of `keepdims` will become False, the `axis` over which the statistic is taken will be eliminated, and the value None will no longer be accepted. Set `keepdims` to True or False to avoid this warning.

The cross validation results are stored as an attribute of the GridSearchCV object as a dictionary with keys as column headers and values as columns, that can be imported into a pandas DataFrame.

```
[14]: cv_results = pd.DataFrame(clf.cv_results_)
cv_results
```

[14]:	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_metric	\
0	0.001475	0.000152	0.002119	0.000167	11	
1	0.001329	0.000067	0.001411	0.000067	11	
2	0.001382	0.000052	0.001990	0.000085	11	
3	0.001293	0.000062	0.001385	0.000037	11	
4	0.001205	0.000079	0.001714	0.000062	11	
5	0.001129	0.000026	0.001241	0.000037	11	
6	0.001105	0.000016	0.001552	0.000013	11	
7	0.001099	0.000007	0.001190	0.000025	11	
8	0.001082	0.000005	0.001564	0.000045	11	
9	0.001086	0.000006	0.001166	0.000004	11	
10	0.001079	0.000009	0.001729	0.000347	11	
11	0.001164	0.000119	0.001345	0.000185	11	
12	0.001962	0.000652	0.002491	0.000484	11	
13	0.001341	0.000048	0.001573	0.000206	11	
14	0.001498	0.000091	0.002180	0.000205	11	
15	0.001323	0.000082	0.001447	0.000068	11	
16	0.001283	0.000040	0.001882	0.000074	11	
17	0.001242	0.000048	0.001316	0.000036	11	
18	0.001214	0.000075	0.001696	0.000082	11	
19	0.001069	0.000005	0.001178	0.000029	11	
20	0.001067	0.000004	0.001538	0.000075	12	
21	0.001080	0.000020	0.001147	0.000031	12	
22	0.001114	0.000096	0.001526	0.000017	12	
23	0.001084	0.000045	0.001252	0.000215	12	
24	0.001101	0.000014	0.001755	0.000099	12	
25	0.001098	0.000044	0.001145	0.000024	12	
26	0.001199	0.000159	0.001827	0.000263	12	
27	0.001140	0.000123	0.001253	0.000177	12	
28	0.001115	0.000094	0.001771	0.000281	12	
29	0.001251	0.000270	0.001269	0.000131	12	
30	0.001066	0.000042	0.001594	0.000214	12	
31	0.001150	0.000135	0.001260	0.000179	12	
32	0.001072	0.000037	0.001520	0.000020	12	
33	0.001058	0.000008	0.001163	0.000049	12	

0.4			0 004400		
34	0.001038	0.000003	0.001492	0.000019	12
35	0.001055	0.000037	0.001142	0.000028	12
36	0.001034	0.000004	0.001487	0.000020	12
37	0.001037	0.000003	0.001128	0.000007	12
38	0.001045	0.000014	0.001485	0.000018	12
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59	0.000952	0.000053	0.001193	0.000042	cosine

param_n_neighbors param_weights \ uniform distance uniform

```
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20
                    1
                             uniform
                    1
21
                            distance
                    2
22
                             uniform
23
                    2
                            distance
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                    3
                            distance
26
                    4
                             uniform
27
                    4
                            distance
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                    5
                             uniform
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                    5
                            distance
30
                    6
                             uniform
                    6
31
                            distance
32
                    7
                             uniform
33
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                            distance
34
                    8
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                    8
35
                            distance
36
                    9
                             uniform
37
                    9
                            distance
38
                   10
                             uniform
39
                   10
                            distance
40
                    1
                             uniform
41
                    1
                            distance
42
                    2
                             uniform
                    2
43
                            distance
                    3
44
                             uniform
45
                    3
                            distance
46
                    4
                             uniform
47
                    4
                            distance
48
                    5
                             uniform
49
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50
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                             uniform
51
                    6
                            distance
                    7
52
                             uniform
53
                    7
                            distance
54
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                             uniform
55
                    8
                            distance
56
                    9
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                   10
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                                              split3_test_score
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	0.002001	0.923810	0.048562	37
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				37
2	0.952381	0.914286	0.055533	37 44
2 3	0.952381 0.952381	0.914286 0.923810	0.055533 0.048562	37 44 37
2 3 4	0.952381 0.952381 0.952381	0.914286 0.923810 0.942857	0.055533 0.048562 0.055533	37 44 37 10
2 3 4 5	0.952381 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381	0.055533 0.048562 0.055533 0.042592	37 44 37 10 2
2 3 4 5 6	0.952381 0.952381 0.952381 0.952381 1.000000	0.914286 0.923810 0.942857 0.952381 0.952381	0.055533 0.048562 0.055533 0.042592 0.060234	37 44 37 10 2
2 3 4 5 6 7	0.952381 0.952381 0.952381 0.952381 1.000000 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533	37 44 37 10 2 2
2 3 4 5 6 7 8	0.952381 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270	37 44 37 10 2 2 10 27
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2 3 4 5 6 7 8 9 10	0.952381 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 1.000000 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.933333 0.961905 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.071270 0.055533	37 44 37 10 2 2 10 27 27 1
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2 3 4 5 6 7 8 9 10 11 12 13	0.952381 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.933333 0.961905 0.942857 0.933333 0.933333	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.055533 0.055533 0.071270 0.071270	37 44 37 10 2 2 10 27 27 1 10 27 27
2 3 4 5 6 7 8 9 10 11 12 13 14	0.952381 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.961905 0.942857 0.933333 0.933333 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.055533 0.055533 0.071270 0.071270 0.071270 0.071270	37 44 37 10 2 2 10 27 27 1 10 27 27 10
2 3 4 5 6 7 8 9 10 11 12 13 14 15	0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.933333 0.961905 0.942857 0.933333 0.933333 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.055533 0.055533 0.071270 0.071270 0.071270 0.055533	37 44 37 10 2 2 10 27 27 1 10 27 27 10 10 10
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	0.952381 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.933333 0.961905 0.942857 0.933333 0.933333 0.942857 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.055533 0.055533 0.071270 0.055533 0.071270 0.055533 0.055533	37 44 37 10 2 2 10 27 27 1 10 27 27 10 10 10
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 0.952381 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.961905 0.942857 0.933333 0.933333 0.942857 0.942857 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.055533 0.055533 0.071270 0.071270 0.071270 0.055533 0.055533 0.055533	37 44 37 10 2 2 10 27 27 1 10 27 27 10 10 10 10
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 1.000000 0.952381 0.952381 0.952381 0.952381 0.952381 0.952381 0.952381	0.914286 0.923810 0.942857 0.952381 0.952381 0.942857 0.933333 0.933333 0.961905 0.942857 0.933333 0.942857 0.942857 0.942857	0.055533 0.048562 0.055533 0.042592 0.060234 0.055533 0.071270 0.055533 0.055533 0.071270 0.055533 0.055533 0.055533 0.055533 0.055533	37 44 37 10 2 2 10 27 27 1 10 27 27 10 10 10 10 10

21	0.952381	0.933333	0.038095	27
22	0.952381	0.933333	0.048562	25
23	0.952381	0.933333	0.038095	27
24	0.952381	0.933333	0.064594	25
25	0.952381	0.942857	0.055533	10
26	1.000000	0.952381	0.060234	2
27	0.952381	0.952381	0.042592	2
28	1.000000	0.952381	0.073771	2
29	1.000000	0.952381	0.073771	2
30	1.000000	0.952381	0.073771	2
31	0.952381	0.933333	0.071270	27
32	0.952381	0.933333	0.071270	27
33	0.952381	0.933333	0.071270	27
34	0.952381	0.942857	0.055533	10
35	0.952381	0.942857	0.055533	10
36	0.952381	0.942857	0.055533	10
37	0.952381	0.942857	0.055533	10
38	0.952381	0.952381	0.052164	2
39	0.952381	0.942857	0.055533	10
40	0.857143	0.847619	0.076190	57
41	0.857143	0.847619	0.076190	57
42	0.857143	0.838095	0.064594	60
43	0.857143	0.847619	0.076190	57
44	0.952381	0.904762	0.060234	48
45	0.952381	0.904762	0.085184	48
46	0.952381	0.895238	0.069985	52
47	0.952381	0.904762	0.085184	48
48	0.904762	0.904762	0.052164	48
49	0.952381	0.914286	0.081927	44
50	0.952381	0.914286	0.055533	44
51	0.952381	0.914286	0.063174	44
52	0.904762	0.866667	0.069985	56
53	0.952381	0.923810	0.064594	37
54	0.952381	0.885714	0.083027	53
55	0.952381	0.923810	0.064594	37
56	0.952381	0.876190	0.064594	54
57	0.952381	0.923810	0.064594	37
58	0.952381	0.876190	0.077372	54
59	0.952381	0.923810	0.064594	37

Look at the GridSearchCV documentation to read about the other attributes stored after fitting. Print the value of the attribute that gives the parameter settings for the best results on the hold out data.

```
[15]: # YOUR CODE HERE

clf.best_params_
```

```
[15]: {'metric': 'l1', 'n_neighbors': 6, 'weights': 'uniform'}
```

Train a new kNN classifier using the hyperparameter settings that were found to give the best results on the hold out data from GridSearchCV (the values printed in the last cell). Train it on the full training set.

```
[16]: # YOUR CODE HERE

knn_best = KNeighborsClassifier(n_neighbors=6, weights='uniform', metric='11')
knn_best.fit(X_train, y_train)
```

[16]: KNeighborsClassifier(metric='l1', n_neighbors=6)

Apply the trained classifier to the test dataset and print the test accuracy.

```
[17]: # YOUR CODE HERE
print(accuracy_score(y_test, knn_best.predict(X_test)))
```

0.97777777777777

/Users/hkerner/anaconda3/envs/cse572/lib/python3.9/site-packages/sklearn/neighbors/_classification.py:228: FutureWarning: Unlike other reduction functions (e.g. `skew`, `kurtosis`), the default behavior of `mode` typically preserves the axis it acts along. In SciPy 1.11.0, this behavior will change: the default value of `keepdims` will become False, the `axis` over which the statistic is taken will be eliminated, and the value None will no longer be accepted. Set `keepdims` to True or False to avoid this warning.