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1 import pandas as pd
2 import numpy as np
3 from sklearn.neural_network import MLPClassifier
4 from sklearn.model_selection import GridSearchCV
5 from sklearn.metrics import accuracy_score, f1_score, roc_auc_score,
precision_score, recall_score
6 from bootstrap import bootstrap
7
8 def run_ann(X, y, n_trials=5):
9     """
10     Runs artificial neural network for a dataset
11     5 trials of ANN with 5-fold cross validation and a gridsearch over
hyperparameters:
12         hidden_layer_sizes, momentum
13     and computes mean accuracy over metrics
14         accuracy, f1, roc, precision, recall
15
16     parameters
17     -----
18     X: feature vector
19     y: target vector
20     n_trials: number of trials to run
21
22     returns
23     -----
24     train_metrics: average of each metric on training set across 5 trials
25     test_metrics: average of each metric on test set across 5 trials
26
27     """
28
29     # hyperparameters
30     layers = [[50], [50, 50], [50, 50, 50, 50, 50], [50, 50, 50, 50, 50, 50, 50, 50], [100],
[100, 100], [100, 100, 100, 100, 100],
31               [100, 100, 100, 100, 100, 100, 100, 100], [200], [200, 200],
[200, 200, 200, 200, 200],
32               [200, 200, 200, 200, 200, 200, 200, 200]]
33     momentums = [0, 0.2, 0.5, 0.9]
34     params = {'hidden_layer_sizes': layers, 'momentum': momentums}
35
36     # metric evaluation scores
37     scores = ['accuracy', 'f1', 'roc_auc', 'precision', 'recall']
38
39     # to hold calculated metric performances
40     train_metrics = []
41     test_metrics = []
42
43     for trial in range(n_trials):
44
45         # initialize model for cross validation grid search
ANN = MLPClassifier(solver='adam', learning_rate='adaptive')

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46 ANN = MLPClassifier(solver='sgd', learning_rate='adaptive',
47 GS = GridSearchCV(ANN, params, scoring=scores, refit=False)
48
49 # bootstrap training and testing sets
50 X_train, X_test, y_train, y_test = bootstrap(X,y)
51 GS.fit(X_train, y_train)
52
53 # collect results
54 res = GS.cv_results_
55
56 # collect/store hyperparameters for visualization
57 hyperp = pd.DataFrame(res['params'])
58 hyperp['acc'] = res['mean_test_accuracy']
59 hyperp['f1'] = res['mean_test_f1']
60 hyperp['roc'] = res['mean_test_roc_auc']
61 hidden_layers = []
62 # rename hidden layer sizes column from list to str
63 for i,row in hyperp.iterrows():
64     if 50 in row['hidden_layer_sizes']:
65
66 hidden_layers.append('{}x50'.format(len(row['hidden_layer_sizes'])))
67     elif 100 in row['hidden_layer_sizes']:
68
69 hidden_layers.append('{}x100'.format(len(row['hidden_layer_sizes'])))
70     elif 200 in row['hidden_layer_sizes']:
71
72 hidden_layers.append('{}x200'.format(len(row['hidden_layer_sizes'])))
73 hyperp['hidden_layer_sizes'] = hidden_layers
74
75 test_per = [] # test set performances
76 train_per = [] # train set performances
77
78 # get best hyperparameters for each metric and use on test set
79 for s in scores:
80
81     # train rf with best hyperparameters for metric
82     best_p = res['params'][np.argmax(res['mean_test_{}'.format(s)])]
83     ANN = MLPClassifier(solver='sgd', learning_rate='adaptive',
84
85 hidden_layer_sizes=best_p['hidden_layer_sizes'],
86 momentum=best_p['momentum'])
87 ANN.fit(X_train, y_train)
88
89 # predictions for train and test sets
90 y_pred = ANN.predict(X_test)
91 y_pred_train = ANN.predict(X_train)
92
93 # evaluate metric on test set
94 if s == 'accuracy':
95     test_per.append(accuracy_score(y_test, y_pred))

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91         train_per.append(accuracy_score(y_train, y_pred_train))
92     elif s == 'f1':
93         test_per.append(f1_score(y_test, y_pred))
94         train_per.append(f1_score(y_train, y_pred_train))
95     elif s == 'roc_auc':
96         test_per.append(roc_auc_score(y_test, y_pred))
97         train_per.append(roc_auc_score(y_train, y_pred_train))
98     elif s == 'precision':
99         test_per.append(precision_score(y_test, y_pred))
100        train_per.append(precision_score(y_train, y_pred_train))
101     elif s == 'recall':
102         test_per.append(recall_score(y_test, y_pred))
103         train_per.append(recall_score(y_train, y_pred_train))
104
105     train_metrics.append(train_per)
106     test_metrics.append(test_per)
107
108     print('Trial {} done'.format(trial+1))
109
110     # take mean of each metric across 5 trials
111     train_metrics = np.mean(np.array(train_metrics), axis=0)
112     test_metrics = np.mean(np.array(test_metrics), axis=0)
113
114     return train_metrics, test_metrics, hyperp
```