### Exercicio 3

#### Diego Fernandez Merjildo

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## 1 Descrição do exercicio

Use os dados do dataset SECOM do UCI O arquivo secom.data contem os dados. O arquivo secom labels.data contem (na 1a coluna) a classe de cada dado.

Usando um 5-fold externo para calcular a accuracia, e um 3-fold interno para a escolha dos hyperparametros, determine qual algoritimo entre kNN, SVM com kernel RBF, redes neurais, Random Forest, e Gradient Boosting Machine tem a maior acuracia.

- 1. Preprocesse os dados do arquivo: Substitua os dados faltantes pela media da coluna (imputação pela média). Finalmente padronize as colunas para media 0 e desvio padrao
- 2. Para o kNN, faça um PCA que mantem 80% da variancia. Busque os valores do k entre os valores 1, 5, 11, 15, 21, 25...
- 3. Para o SVM RBF teste para C=2\*\*(-5), 2\*\*(0), 2\*\*(5), 2\*\*(10) e gamma= 2\*\*(-15) 2\*\*(-10) 2\*\*(-5) 2\*\*(0) 2\*\*(5).
- 4. Para a rede neural, teste com 10, 20, 30 e 40 neuronios na camada escondida.
- 5. Para o RF, teste com mtry ou  $n_{f}eatrues = 10, 15, 20, 25$  e ntrees = 100, 200, 300 e 400.
- 6. Para o GBM (ou XGB) teste para numero de *arvores* = 30, 70, e 100, com learning rate de 0.1 e 0.05, e profundidade da *arvore* = 5. Voce pode tanto usar alguma versao do gbm para R ou SKlearn, ou usar o XGBoost (para ambos).
- 7. Voce nao precisam fazer os loops da validação cruzada explicitamente. Pode usar as funções como tunegrid (do caret) ou tuneParams (do mlr) ou GridSearchCV do SKlearn..
- 8. Reporte a acuracia de cada algoritmo calculada pelo 5-fold CV externo...

#### 2 Resultados

Os resultados foram obtidos rodando o script apresentado na seção 3. No script usamos um k-fold estratificado de 5 externo (para obter a acuracia) e um outro k-fold estratificado de 3 interno (para obter os parametros).

Rodando o script em python obtemos os seguintes resultados:

```
1
   --- kNN--
2
3
  Acuracia:0.93359083412
  Valor final K (K=25)
   --- SVM ---
6
  Acuracia:0.929117990669
   Valor final hiperparametros (C=0.03125, Gamma=3.0517578125e-05)
10
  --- Neural Network ---
  Acuracia:0.797816161135
12 Valor final parametros (Neurons=40)
  --- RF ---
14
15 Acuracia: 0.929765095103
16
  Valor final parametros (Feats=15, Trees=100)
17
  --- GBM ---
18
19 Acuracia: 0.845037435449
20 Valor final parametros (Learn Rate=0.1, Trees=100)
```

# 3 Codigo fonte em python

Listing 1: Codigo em Python

```
1
2 #!/usr/bin/python
3
4 import sys,os,csv
5 import pandas
6 import numpy as np
7 import math
8 from sklearn.model_selection import StratifiedKFold
9 from sklearn import sym as SVM
10 from sklearn.neighbors import KNeighborsClassifier
```

```
11 from sklearn.ensemble import RandomForestClassifier
12 from sklearn.ensemble import GradientBoostingClassifier
13 from sklearn.neural_network import MLPClassifier
14
15 datFileName="secom.data"
16 labelsFileName="secom_labels.data"
17 dirPath=os.path.dirname(os.path.realpath(__file__))
18 classList=[]
19 data=[]
20
21
  def load_data(fileName):
22
       raw_data = open(fileName, 'rb')
23
       rawData = pandas.read_csv(raw_data, delimiter=" ")
24
       return rawData.values
25
26
   def getData(rawData):
27
       #print "\n--- Getting data from File ----"
28
       lineNum = rawData.shape[0]
29
       colNum = rawData.shape[1]
30
       data = np.array(rawData[0:lineNum, 0:colNum-1])
31
       for i in range(lineNum):
32
            classList.append(rawData[i][colNum - 1])
33
       return [data, np.array(classList) ]
34
35
   def getLabels(fileName):
36
       labelData = load_data(dirPath + "/" + fileName)
37
       labels = labelData[:,0].clip(min=0)
38
       return np.array(labels)
39
40
   def svm_intern_folds(data_train, data_test, labelsTrain, labelsTest←)
      ):
       acxmax = 0
41
42
       c_{max}=0
43
       gamma_max=0
44
       for c in [2**(-5), 1, 2**(5), 2**(10)]:
            for gamm in [2**(-15), 2**(-10), 2**(-5), 1, 2**5]:
45
46
                svm = SVM.SVC(C = c, gamma = gamm)
47
                svm.fit(data_train, labelsTrain)
48
                accuracy = svm.score(data_test, labelsTest)
49
                if accuracy > acxmax:
50
                    acxmax = accuracy
51
                    c_{max} = c
52
                    gamma_max = gamm
53
       return [acxmax, c_max, gamma_max]
54
   {\tt def} knn_intern_folds(data_train, data_test, labels_train, \hookleftarrow
      labels_test):
56
       acxmax = 0
```

```
57
       cores = 4
58
       k_value = 0
59
       for k in [1, 5, 11, 15, 21, 25]:
60
            knn = KNeighborsClassifier(n_neighbors = k, n_jobs = cores)
61
            knn.fit(data_train, labels_train)
62
            accuracy = knn.score(data_test, labels_test)
63
            if accuracy > acxmax:
64
                acxmax = accuracy
65
                k_value = k
66
       return [acxmax, k]
67
68
   def neural_intern_folds(data_train, data_test, labels_train, ←
       labels_test):
69
       # 10, 20, 30 e 40 neuronios na camada escondida.
70
       acxmax = 0
71
       cores = 4
72
       n_value = 0
73
       for n in [10, 20, 30, 40]:
74
            clf = MLPClassifier(hidden_layer_sizes=(n,), solver='lbfgs'←
               )
            clf.fit(data_train, labels_train)
75
76
            accuracy = clf.score(data_test, labels_test)
77
            if accuracy > acxmax:
78
                acxmax = accuracy
79
                n_value = n
80
       return [acxmax, n]
81
82
   def rf_intern_folds(data_train, data_test, labels_train, ←
       labels_test):
       # teste com mtry ou n_featrues = 10, 15, 20, 25 e ntrees = 100, \leftarrow
83
            200, 300 e 400
       acxmax = 0
84
85
       n_feats = 0
86
       n_{trees} = 0
87
       for feat in [10, 15, 20, 25]:
            for trees in [100, 200, 300, 400]:
88
89
                clf = RandomForestClassifier (max_features = feat, \hookleftarrow
                   n_{estimators} = trees)
90
                clf.fit(data_train, labels_train)
91
                accuracy = clf.score(data_test, labels_test)
92
                #print "first acc:", accuracy
93
                if accuracy > acxmax:
94
                    acxmax = accuracy
95
                    n_feats = feat
96
                    n_trees = trees
97
       return [acxmax, n_feats, n_trees]
98
```

```
def gbm_intern_folds(data_train, data_test, labels_train, ←
       labels_test):
100
        ## numero de arvores = 30, 70, e 100, com learning rate de 0.1\leftarrow
             e 0.05, e profundidade da arvore=5.
101
        acxmax = 0
102
        n_learn_rate = 0
103
        n_{trees} = 0
104
        depth_tree = 5
105
        for trees in [30, 70, 100]:
             for learn_rate in [0.1, 0.05]:
106
107
                 clf = GradientBoostingClassifier (n_estimators = trees,\hookleftarrow
                     learning_rate = learn_rate, max_depth = depth_tree ←
                    )
108
                 clf.fit(data_train, labels_train)
109
                 accuracy = clf.score(data_test, labels_test)
110
                 #print "first acc:", accuracy
111
                 if accuracy > acxmax:
112
                     acxmax = accuracy
113
                     n_trees = trees
114
                     n_learn_rate = learn_rate
115
        return [acxmax, n_learn_rate, n_trees]
116
117
    ## Data preprocessing
    def data_preprocess(fileName):
118
119
        rawdata = load_data(dirPath + "/" + fileName)
120
        ## column mean
121
        column_mean = np.nanmean(np.array(rawdata), axis=0)
122
        ## Nan values index
123
        nan_indexes = np.where(np.isnan(rawdata))
124
        ## Replace Nan values
125
        rawdata[nan_indexes] = np.take(column_mean, nan_indexes[1])
126
        ## Standarize each column individually
127
        rawdata = (rawdata - np.mean(rawdata, axis=0)) / np.std(rawdata↔
            , axis=0)
128
        rawdata = np.nan_to_num(rawdata)
129
        return rawdata
130
131
    def run_folds( alg, data, labels):
132
        print "--- %s --- " % alg
133
        final_accuracy = 0
134
        params_final = [0.0, 0.0]
135
        skf = StratifiedKFold(n_splits=5)
136
        for train_index, test_index in skf.split(data, labels):
137
            new_data_train = data[train_index]
138
            new_data_test = data[test_index]
            new_labels_train = labels[train_index]
139
140
            new_labels_test = labels[test_index]
141
            acx = 0
```

```
142
             skf_intern = StratifiedKFold(n_splits=3)
143
             for intern_train_index, intern_test_index in skf_intern.←
                split(new_data_train, new_labels_train):
144
                 intern_data_train = new_data_train[intern_train_index]
145
                 intern_data_test = new_data_train[intern_test_index]
146
                 intern_labels_train = new_labels_train[←
                     intern_train_index]
147
                 intern_labels_test = new_labels_train[intern_test_index <--
148
                 params = get_intern_folds (alg, intern_data_train, ←
                     intern_data_test, intern_labels_train, \hookleftarrow
                     intern_labels_test)
149
                 if params[0] > acx:
150
                     acx = params[0]
151
                     params_final[0] = params[1]
152
                     if len(params) > 2:
153
                          params_final[1] = params[2]
154
155
             final_accuracy = final_accuracy + model_score(alg, \leftarrow
                params_final,
156
                                                               new_data_train \leftarrow
157
                                                               new_labels_train \leftarrow
158
                                                               \texttt{new\_data\_test} \leftarrow
159
                                                               new_labels_test \leftarrow
160
        final_accuracy = final_accuracy / 5
161
        print_results(alg, final_accuracy, params_final)
162
163
    def model_score(alg, params, new_data_train, new_labels_train, ←
        new_data_test, new_labels_test):
164
        if 'svm' == alg:
165
             svm_model = SVM.SVC(C = params[0], gamma = params[1])
             svm_model.fit(new_data_train, new_labels_train)
166
167
             return svm_model.score(new_data_test, new_labels_test)
168
        elif 'knn' == alg:
             knn = KNeighborsClassifier(n_neighbors = params[0], n_jobs \hookleftarrow
169
170
             knn.fit(new_data_train, new_labels_train)
171
             return knn.score(new_data_test, new_labels_test)
        elif 'neural' == alg:
172
173
             clf = MLPClassifier(hidden_layer_sizes=(params[0],), solver↔
                ='lbfgs')
174
             clf.fit(new_data_train, new_labels_train)
175
             return clf.score(new_data_test, new_labels_test)
176
        elif 'rf' == alg:
```

```
177
            clf = RandomForestClassifier (max_features = params[0], ←
                n_estimators = params[1])
178
            clf.fit(new_data_train, new_labels_train)
179
            return clf.score(new_data_test, new_labels_test)
180
        elif 'gbm' == alg:
181
            clf = GradientBoostingClassifier (learning_rate = params←)
                [0], n_estimators = params[1], max_depth = 5)
182
            clf.fit(new_data_train, new_labels_train)
183
            return clf.score(new_data_test, new_labels_test)
184
185
    def get_intern_folds (alg, data_train, data_test, labels_train, ←
       labels_test):
186
        if 'svm' == alg:
187
            return svm_intern_folds(data_train, data_test, labels_train ↔
                , labels_test)
188
        elif 'knn' == alg:
189
            return knn_intern_folds(data_train, data_test, labels_train ←
                , labels_test)
190
        elif 'neural' == alg:
            return neural_intern_folds(data_train, data_test, ←
191
                labels_train, labels_test)
192
        elif 'rf' == alg:
193
            return rf_intern_folds(data_train, data_test, labels_train, ←
                 labels_test)
194
        elif 'gbm' == alg:
195
            return gbm_intern_folds(data_train, data_test, labels_train↔
                , labels_test)
196
    def print_results(alg, final_accuracy, params):
197
        if 'svm' == alg:
198
199
            print("Acuracia:%s" % final_accuracy)
200
            print("Valor final hiperparametros (C=%s, Gamma=%s)" % (←
               params[0], params[1]) )
201
        elif 'knn' == alg:
202
            print("Acuracia:%s" % final_accuracy)
            print("Valor final K (K=%s)" % (params[0]))
203
204
        elif 'neural' == alg:
205
            print("Acuracia:%s" % final_accuracy)
206
            print("Valor final parametros (Neurons=%s)" % (params[0]) )
        elif 'rf' == alg:
207
208
            print("Acuracia:%s" % final_accuracy)
209
            print("Valor final parametros (Feats=%s, Trees=%s)" % (↔
                params[0], params[1]) )
210
        elif 'gbm' == alg:
211
            print("Acuracia:%s" % final_accuracy)
212
            print("Valor final parametros (Learn Rate=%s, Trees=%s)" % ↔
                (params [0], params [1]))
213
```

```
214
215
   def main(argv=None):
216
        if argv is None:
217
            arv = sys.argv
218
219
        ## Data pre-processing
220
        data = data_preprocess(datFileName)
221
        labels = getLabels(labelsFileName)
222
        labels = np.array(list(labels[:data.shape[0]]))
223
224
        ## kNN , PCA com 80% da variancia
225
        run_folds('knn', data, labels)
226
227
        ## SVM RBF
228
        run_folds('svm', data, labels)
229
        ## Neural network
230
        run_folds('neural', data, labels)
231
232
233
        ## RF
234
        run_folds('rf', data, labels)
235
236
        ## GBM
237
        run_folds('gbm', data, labels)
238
239
    if __name__ == "__main__":
        sys.exit(main())
240
```