

Exercise 5

Applications of Data Analysis

Marco Willgren 502606 mahewi@utu.fi

Jarno Vuorenmaa 503618 jkivuo@utu.fi

1 DATA PREPROCESSING AND CREATING DEPENDENCIES MATRIX

We read feature data into variable x and labels into y. Dependencies matrix is created in generateIndexDep – method. Matrix has information about dependencies between objects. One column has every index of pairs where object (responding to the column) is one of the member.

```
basepath = os.path.dirname(__file__)
featurepath = os.path.abspath(os.path.join(basepath,
    "../Data5/proteins.features"))
labelpath = os.path.abspath(os.path.join(basepath,
    "../Data5/proteins.labels"))

x = np.genfromtxt(featurepath, delimiter=',')
y = np.genfromtxt(labelpath, delimiter=',')

def generateIndexDep():
    indexDeps = []
    for i in range(20):
        iDep = []
        for j in range(i*20, i*20+20):
            iDep.append(j)
        k = i
        while(k < 400):
            iDep.append(k)
            k = k + 20
        indexDeps.append(iDep)

    return indexDeps

dependencies = generateIndexDep()
```

2 UNMODIFIED LEAVE-ONE-OUT CROSS-VALIDATION

Method takes each instance of the training set and uses it as a test instance. For every test instance method predicts the label using 1-nearest-neighbor. In inferNeighbors - method, the euclidean distance between test instance and each training instance is calculated and sorted into distances – array. The method returns 1-nearest neighbors.

```

def LooCV(modified):
    yPredictions = []
    for i in range(len(x)):
        if modified:
            trainSet,trainLabels = filterTrainSet(i)
            trainSet.append(x[i])
            trainLabels.append(y[i])
        else:
            trainSet = x
            trainLabels = y
        yPredictions.append(inferNeighbors(trainSet,x[i],trainLabels))

    return yPredictions

def inferNeighbors(trainSet,testInstance,labels):
    distances = []
    for i in range(len(trainSet)):
        distances.append((ssd.euclidean(trainSet[i], testInstance),
labels[i]))

    distances.sort(key=operator.itemgetter(0))
    return distances[1][1]

```

3 MODIFIED LEAVE-ONE-OUT CROSS-VALIDATION

Modified leave-one-out cross-validation is similar as unmodified except the training set is filtered. Method `filterTrainSet()` gets index of the pair as an argument. The method calculates members of this pair and uses dependencies matrix to filter shared objects out of training set.

```
def filterTrainSet(index):
    lowerBound = (index/10)*10

    if lowerBound % 20 != 0:
        lowerBound = lowerBound - 10

    indexOfSecondPair = lowerBound / 20
    indexOfFirstPair = index - lowerBound
    print indexOfFirstPair

    testIndexes = dependencies[indexOfFirstPair] +
dependencies[indexOfSecondPair]
    #CREATE TRAINING SET AND LABELS
    trainSet = []
    trainLabels = []
    for i in range(len(x)):
        if not i in testIndexes:
            trainSet.append(x[i])
            trainLabels.append(y[i])

    return trainSet,trainLabels
```

4 CALCULATING C-INDEX

```
def calculateCIndex(predictions, labels):
    n = 0
    h_sum = 0
    for i in range(len(labels)):
        t = labels[i]
        p = predictions[i]
        for j in range(i+1, len(labels)):
            nt = labels[j]
            np = predictions[j]
            if t != nt:
                n = n + 1
                if (p < np and t < nt) or (p > np and t > nt):
                    h_sum = h_sum + 1
                elif (p < np and t > nt) or (p > np and t < nt):
                    h_sum = h_sum + 0
                elif (p == np):
                    h_sum = h_sum + 0.5

    if n == 0:
        return 0
    else:
        return h_sum/n
```

C-index is calculated as shown in Ileana Montoya's presentation slides (I.Montoya, Prediction of the metal ion content from multi-parameter data, 2015).

5 RESULTS

Concordance index of unmodified CV
0.98820754717

Concordance index of modified CV
0.524287434765

6 CODE

```
'''
Authors: Marco Willgren, 502606
         Jarno Vuorenmaa, 503618
'''

import os
import numpy as np
import operator
import scipy.spatial.distance as ssd

if __name__ == '__main__':
    pass

basepath = os.path.dirname(__file__)
featurepath = os.path.abspath(os.path.join(basepath, "../Data5/proteins.features"))
labelpath = os.path.abspath(os.path.join(basepath, "../Data5/proteins.labels"))

x = np.genfromtxt(featurepath, delimiter=',')
y = np.genfromtxt(labelpath, delimiter=',')

def generateIndexDep():
    indexDeps = []
    for i in range(20):
        iDep = []
        for j in range(i*20, i*20+20):
            iDep.append(j)
        k = i
        while(k < 400):
            iDep.append(k)
            k = k + 20
        indexDeps.append(iDep)

    return indexDeps

dependencies = generateIndexDep()

def filterTrainSet(index):
    lowerBound = (index/10)*10

    if lowerBound % 20 != 0:
        lowerBound = lowerBound - 10

    indexOfSecondPair = lowerBound / 20
    indexOfFirstPair = index - lowerBound

    testIndexes = dependencies[indexOfFirstPair] + dependencies[indexOfSecondPair]
    #CREATE TRAINING SET AND LABELS
    trainSet = []
```

```

trainLabels = []
for i in range(len(x)):
    if not i in testIndexes:
        trainSet.append(x[i])
        trainLabels.append(y[i])

return trainSet,trainLabels

def LooCV(modified):
    yPredictions = []
    for i in range(len(x)):
        if modified:
            trainSet,trainLabels = filterTrainSet(i)
            trainSet.append(x[i])
            trainLabels.append(y[i])
        else:
            trainSet = x
            trainLabels = y
        yPredictions.append(inferNeighbors(trainSet,x[i],trainLabels))

    return yPredictions

def inferNeighbors(trainSet,testInstance,labels):
    distances = []
    for i in range(len(trainSet)):
        distances.append((ssd.euclidean(trainSet[i], testInstance), labels[i]))

    distances.sort(key=operator.itemgetter(0))
    return distances[1][1]

def calculateCIndex(predictions, labels):
    n = 0
    h_sum = 0
    for i in range(len(labels)):
        t = labels[i]
        p = predictions[i]
        for j in range(i+1,len(labels)):
            nt = labels[j]
            np = predictions[j]
            if t != nt:
                n = n + 1
                if (p < np and t < nt) or (p > np and t > nt):
                    h_sum = h_sum + 1
                elif (p < np and t > nt) or (p > np and t < nt):
                    h_sum = h_sum + 0
                elif (p == np):
                    h_sum = h_sum + 0.5

    if n == 0:
        return 0
    else:
        return h_sum/n

```

```
def main():
    predictedLabels = LooCV(False)
    print 'Concordance index of unmodified CV'
    print calculateCIndex(predictedLabels, y)
    print
    predictedLabels = LooCV(True)
    print 'Concordance index of modified CV'
    print calculateCIndex(predictedLabels, y)

main()
```