KNN-Classification

October 27, 2019

1 KNN for Classification

We can use K nearest neighbors for classification the same way we used KNN to approximate a function with continuous outputs. Our goal for KNN with continuous outputs was to estimate $P(y|X)$. The goal of KNN for classification is the same. We wish to estimate $P(y|X)$ except our y data can only take to values, 0 or 1.

The mechanics needed to estimate $P(y|X)$ are also the same between KNN for continuous outputs and classification. We need: a distance function in order to defined neighborhoods, and our estimate of $P(y|X)$ will be an average over the y values in our neighborhood.

1.1 Distance function

A distance function takes two vectors as input and outputs a non-negative real number. Given two vectors a and b, a valid distance function:

(i) must produce non-negative outputs,

$$d(a, b) \geq 0$$

(ii) must equal zero when the same vector is input

$$d(a, a) = 0$$

and must be symmetric

$$d(a, b) = d(b, a)$$

1.2 Neighborhood

A distance function in-hand, we can define a neighborhood. A neighborhood around x of radius r is the set of points whose distance from x is less than or equal to r

$$N_r(x) = \{x_i | d(x, x_i) \leq r\}$$

For KNN, we are interested in the K **nearest** neighbors. Or the K points x_i that have the smallest distances from our target x. In some sense, the K nearest neighbors defines a Neighborhood around x with a finite r.

1.3 Formula to estimate $P(y|X)$

Given y data $y_1, y_2, \cdots, y_n$ and corresponding x **vectors** of length m $x_1, x_2, \cdots, x_n$ we can estimate $P(y|X)$ using a distance function and neighborhood.

$$P(y = 1|x) = \frac{1}{|N|} \sum_{x_i \in N_r(x)} y_i$$

The y values take only two values: 0 or 1. The average over a set of binary y values is equal to the percentage of "1"s. The above formula looks at a neighborhood of x, y pairs and estimates $P(y = 1|x)$ as the percentage of y_i that equal 1.

1.4 Example by hand

Suppose I collected a small set of data

y	x1	x2	x3
1	0.25	1.1	1
0	0.85	0.1	3
1	1.25	-2.1	2
0	0.68	0.3	3
0	3.15	0.4	4
1	-0.25	0.1	-5

The goal is to approximate $P(y = 1|x = [0, 1, 0])$ (remember, x is a **vector**). I'll pre-specify my distance function and radius.

The distance function I want to use is

$$d(a, b) = \sum_i |a_i - b_i|$$

with a K equal to $r = 3$. I want to find the **3** nearest neighbors to estimate $P(y = 1|x = [0, 1, 0])$

To approximate $P(y = 1|x = [0, 1, 0])$ I need to compute the distance between my x training data and the vector $[0, 1, 0]$

y	x1	x2	x3	distance from x	Top 3 closest
1	0.25	1.1	1	1.35	yes
0	0.85	0.1	3	4.75	yes
1	1.25	-2.1	2	6.35	no
0	0.68	0.3	3	4.38	yes

y	x1	x2	x3	distance from x	Top 3 closest
0	3.15	0.4	4	7.75	no
1	-0.25	0.1	-5	6.15	no

We see that this corresponds to a Neighborhood of radius 4.75 around our vector $[0, 1, 0]$

Then my estimate of $P(y = 1|x = [0, 1, 0])$ equals

$$P(y = 1|x = [0, 1, 0]) \approx \frac{1}{3}(1 + 0 + 0) = 1/3 = 0.33$$

1.5 Example code

[43]:
```
library(ElemStatLearn)
require(class)

x <- mixture.example$x # example x data every x-vector has two entries.
y <- mixture.example$y # example y data [0 or 1]

d = cbind(x,y)
print(head(d))
```

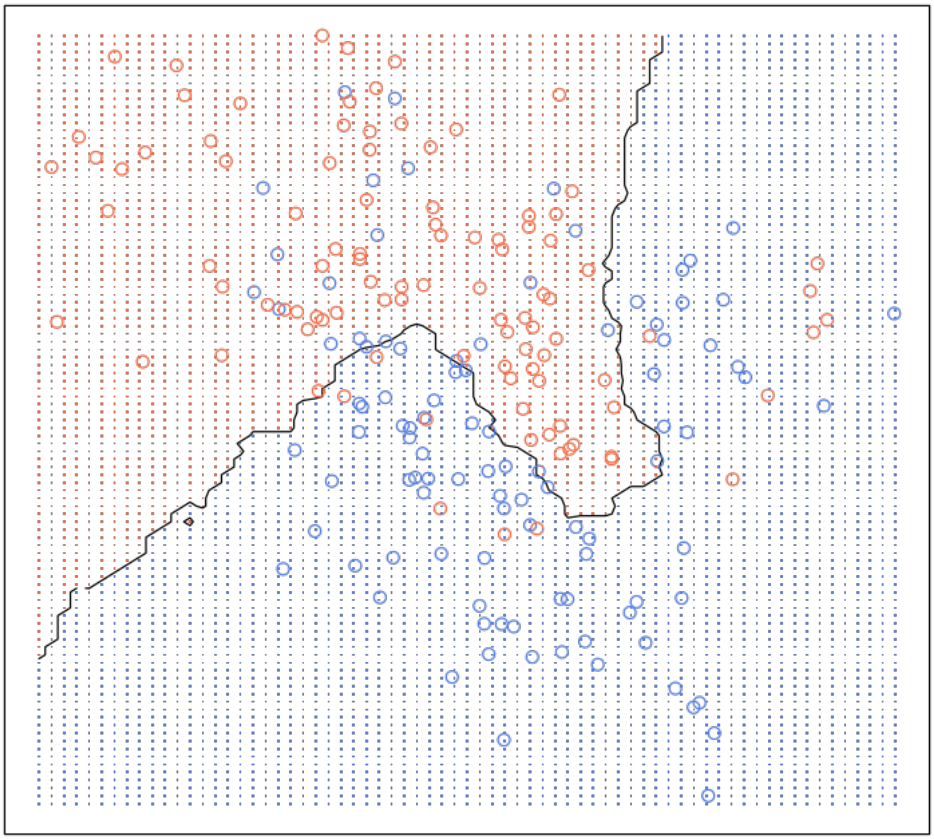
```
                          y
[1,]  2.52609297  0.3210504 0
[2,]  0.36695447  0.0314621 0
[3,]  0.76821908  0.7174862 0
[4,]  0.69343568  0.7771940 0
[5,] -0.01983662  0.8672537 0
[6,]  2.19654493 -1.0230141 0
```

[45]:
```
xTest <- mixture.example$xnew # example test x data. The test data also has 2␣
 ↪dimensions.
print(head(xTest))
```

```
    x1 x2
1 -2.6 -2
2 -2.5 -2
3 -2.4 -2
4 -2.3 -2
5 -2.2 -2
6 -2.1 -2
```

[48]:
```
# The KNN function.
# This function takes the training X data, test X data, and training y data.
# Next, the KNN function requires you to specify a number of neighbors
# and the prob=TRUE means we're using KNN for classifcation
```

```r
oneAndZeroPredictionsOnTestSet <- knn(x, xTest, y, k=15, prob=TRUE)

#The below extracts the probabilites for each x test point
probOnTest <- attr(oneAndZeroPredictionsOnTestSet, "prob")

# This function builds a vector by evaluating the first argument.
# If true, then set the vector value to probOnTest otherwise set to 1-probOnTest.
probOnTest <- ifelse(oneAndZeroPredictionsOnTestSet=="1", probOnTest,1-probOnTest)

# create a grid of x values
px1 = seq( min(x[,1]) -0.1 ,max(x[,1])+0.1,0.1)
px2 = seq( min(x[,2]) -0.05 ,max(x[,2]),0.05)

# create a grid of X1 by X2 and fill in the corresponding probabilities
prob15 <- matrix(probOnTest, length(px1), length(px2))

contour(px1, px2, prob15, levels=0.5, labels="", xlab="", ylab="", main=
        "15-nearest neighbour", axes=FALSE)
points(x, col=ifelse(g==1, "coral", "cornflowerblue"))
gd <- expand.grid(x=px1, y=px2)
points(gd, pch=".", cex=1.2, col=ifelse(prob15>0.5, "coral", "cornflowerblue"))
box()
```


15-nearest neighbour

[ ]: