KNNregression

October 3, 2019

0.1 KNN Regression

A main goal of regression is estimating

$$P(y|X)$$

Our previous approach to understanding this conditional probability was to define a linear regression model

$$P(y|X) \sim N[f(X), \sigma^2].$$

The above model had many advantages. The regression parameters (β) were easy to compute, the association between y and X followed a functional form f.

But there are disadvantages too. A model like the above makes strong assumption about the form of our model. We restrict the types of models we can fit by prespecifying f.

Nonparametric models broaden the class of models we can fit. These models do not assume our function f is the same everywhere, determined by a single set of parameters. Instead, our model and parameters that define the model are allowed to grow with the data.

K nearest neighbor (KNN) regression is one type of nonparametric model. KNN regression estimates f(x) by looking at data points close to the value x and then averaging the response values. For example, we can make a prediction given a point x by the following

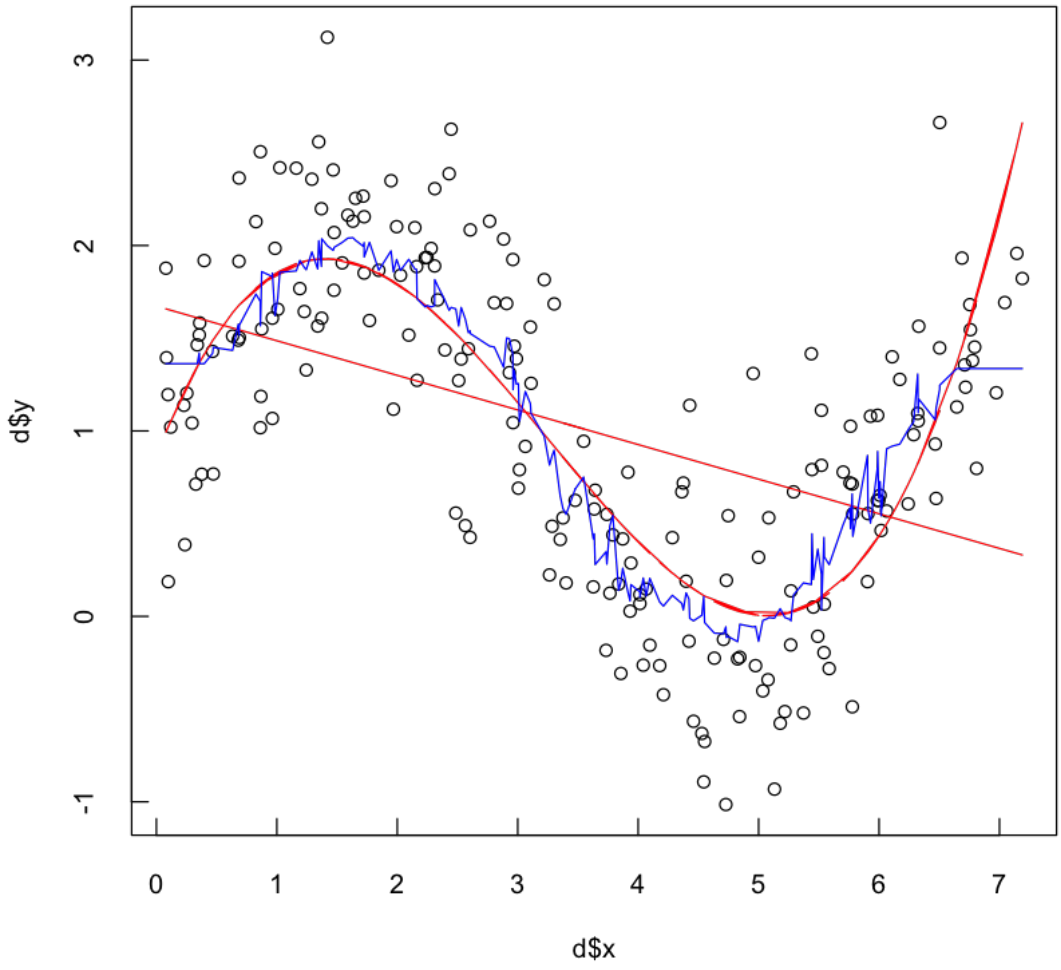
$$f(x) = \frac{1}{|N(x)|} \sum_{i \in N(x)} y_i$$

where $N(x)$ is a *neighborhood* of (x_{i},y_{i}) data points near the value x and $|N(x)|$ counts the total number of data points in the neighborhood.

We can compare simple linear, polynomial, and KNN regression by looking at a dataset.

[58]:
```
d = read.csv('./dataSet1.csv')
plot(d$x,d$y,tck=0.02)

#SLR
SLR = lm(y~x,data=d)
predictions = predict(SLR)
```

```
lines(d$x,predictions,col='red')

#PR
PR = lm(y~x+I(x^2)+I(x^3),data=d)
predictions = predict(PR)
lines(d$x,predictions,col='red')

#KNN regression
library(FNN)
d = d[order(d$x),] # sort the data frame by the variable X
KNN = knn.reg(train = d, test=d, y = d$y, k = 25) #FIT KNN MODEL
lines(d$x,KNN$pred,col='blue')
```



0.2 Neighborhood

A neighborhood at a point x defines a set of points that are considered close to x. In order to define close, we will need to define a distance metric.

A distance metric is a function $d(x, y)$ that takes two points and returns a number on the real line. The distance between a a point and itself $d(x, x)$ must equal 0. The distance should also be symmetric or $d(x, y) = d(y, x)$. Intuitively, small distance values mean points are close and large values mean points are far away.

0.2.1 Euclidean distance

The Euclidean distance between two vectors x and y equals

$$d(x, y) = \left[\sum_i (x_i - y_i)^2\right]^{1/2}$$

or in vector notation

$$d(x, y) = \left[(x - y)'(x - y)\right]^{1/2}$$

For example,

[147]:
```
x = 1

euclideanDistance = function(x,y){
    return( sqrt(t(x-y)%*%(x-y)) )
}

print("Single Numbers")
distance = euclideanDistance(c(1),c(4))
print(distance)

print("Vectors")
distance = euclideanDistance(c(1,2,3),c(4,5,6))
print(distance)
```

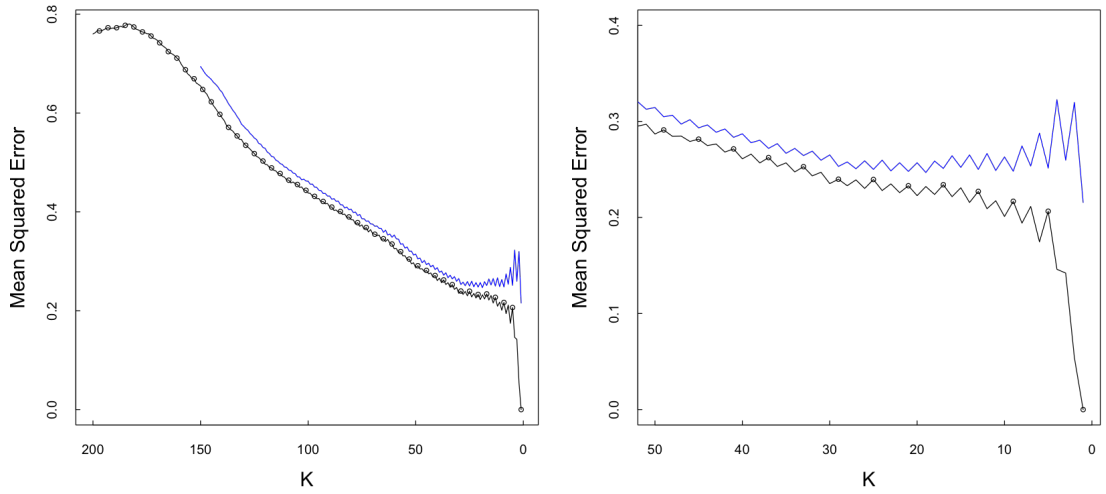
```
[1] "Single Numbers"
     [,1]
[1,]    3
[1] "Vectors"
         [,1]
[1,] 5.196152
```

The above KNN regression uses Euclidean distance to define neighborhoods.

0.3 Bias - variance tradeoff

[146]:
```
d = read.csv('./dataSet1.csv')
N = nrow(d)

#KNN regression
library(FNN)

#two plots
options(repr.plot.width=7*2.0,repr.plot.height=7)
par(mfrow=c(1,2))

#TRAINING MSE
MSEs = rep(0,200)
for (k in 1:200){
    KNN = knn.reg(train = d, test=d, y = d$y, k = k)
    MSE = t(KNN$pred - d$y)%*%(KNN$pred - d$y)/N
    MSEs[k] = MSE
}
results = data.frame("k"=1:200,"MSE"=MSEs)

plot(results$k[seq(1,200,4)],results$MSE[seq(1,200,4)]
     ,xlim=c(200,1)
     ,tck=0.01
     ,xlab='K'
     ,ylab='Mean Squared Error'
     ,cex=0.75
     ,cex.lab=1.5)
lines(results$k,results$MSE,xlim=c(200,1))

#TESTING MSE
Folds = 20
dataFolds = split(d,1:Folds)


cvErrors = rep(0,150)
for(k in 1:150){

    MSEs = rep(0,Folds)
    for(i in 1:Folds){
        testSet = dataFolds[[i]]
        N = nrow(testSet)

        exceptI = setdiff(1:Folds,i)
        trainingSet = do.call(rbind,dataFolds[exceptI])

        KNN = knn.reg(train = trainingSet
```

```
                        ,test=testSet
                        ,y = trainingSet$y
                        ,k = k)
        MSE = t(KNN$pred - testSet$y)%*%(KNN$pred - testSet$y)/N
        MSEs[i] = MSE
    }
    cvErrorForSingleK = mean(MSEs)
    cvErrors[k] = cvErrorForSingleK
}
lines(1:150,cvErrors,col='blue')


#SECOND PLOT
plot(results$k[seq(1,200,4)],results$MSE[seq(1,200,4)]
     ,xlim=c(50,1)
     ,ylim =c(0,0.4)
     ,tck=0.01
     ,xlab='K'
     ,ylab='Mean Squared Error'
     ,cex=0.75
     ,cex.lab=1.5)
lines(results$k,results$MSE,xlim=c(200,1))
lines(1:150,cvErrors,col='blue')
```



The training MSE decreases as we make our neighborhood size smaller. The model considers fewer points to create an average and is able to fit more complicated models. When K is small our model will have lower bias.

We pay a penalty for small neighborhoods and lower bias. If we reduce K to values smaller than

20, our test MSE begins to increase. Our model is beginning to overfit our training data.

[ ]: