Kernel Density Estimation and Non-Parametric Regression

Patrick Mellady

This explanation will explore kernels, kernel density estimation, and non-parametric regression. We start with the definition of a kernel.

Kernels

A kernel is a function k(x) such that $\int_{\mathbb{R}} k(x)dx = 1$, k(x) is symmetric, $k(x) \geq 0$, and $\int_{\mathbb{R}} x^2 k(x)dx < \infty$. Given a kernel and a bandidth, h, we can define

$$k_h(x) = \frac{1}{h}k(\frac{x}{h})$$

If $k: \mathbb{R}^d \to \mathbb{R}$ and we have a bandwidth matrix, H, we define

$$k_H(x) = \frac{1}{|H|} k(H^{-1}x)$$

Frequently, we will use H = hI and implement the following

$$k_H(x) = \frac{1}{h^d} \prod_{i=1}^n k(\frac{x_i}{h})$$

Kernel Density Estimation

Suppose we observe $Y_1, Y_2, \dots, Y_n \sim P$ with an unknown density. The kernel density estimate for the density of P is given by

$$\hat{p}(y) = \frac{1}{n} \sum_{i=1}^{n} k_h(Y_i - y)$$

Non-Parametric Regression

We will implement the estimator of the form

$$\hat{r}(x) = \sum_{i=1}^{n} w_i(x) Y_i$$

where the weights, $w_i(x)$ are given by

$$w_i(x) = \frac{k_h(X_i - x)}{\sum_{j=1}^n k_h(X_j - x)}$$

Implementation

We now implement the above methods to find kernel density estimates and non-paramteric regression methods in a variety of examples. First, in the single dimension case, we implement general functions for calculating the functions above.

```
k<-function(x, type="gaussian"){</pre>
  if(type=="gaussian"){
    temp<-dnorm(x)
  if(type=="logistic"){
    temp < -(2/pi) * exp(x) / (1 + exp(2 * x))
  if(type=="epanechnikov"){
    temp<-.75*(1-x^2)
  return(temp)
}
# Non-parametric regression
w<-function(x, h, X, type){</pre>
  num < -k((X-x)/h, type)/h
  denom < -sum(k((X-x)/h, type)/h)
  temp<-num/denom
  return(temp)
}
r_x<-function(x, h, X, Y, type){</pre>
  weight<-w(x, h, X, type)</pre>
  temp<-sum(weight*Y)</pre>
  return(temp)
}
r<-function(X, Y, n=100, h=1/10, type="gaussian"){
  n<-length(X)
  x<-seq(min(X), max(X), length.out=n)</pre>
  y_hat<-c()</pre>
  for(point in x){
    y_hat<-c(y_hat, r_x(point, h, X, Y, type))</pre>
  return(list(x=x, y_hat=y_hat))
# Density estimation
p_x<-function(x, h, X, type){</pre>
  n<-length(X)
  temp < -sum(k((x-X)/h, type)/h)/n
}
p<-function(X, n=1000, h=1/10, type="gaussian"){
  x \leftarrow seq(-10*max(abs(X)), 10*max(abs(X)), length.out=n)
  p_hat<-c()</pre>
  for(point in x){
    p_hat<-c(p_hat, p_x(point, h, X, type))</pre>
  return(list(x=x, p_hat=p_hat))
```

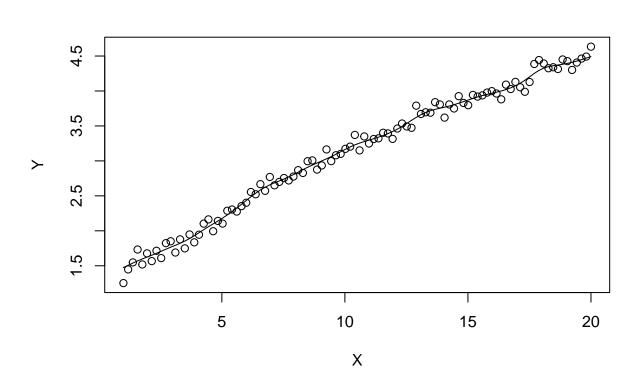
First Example

With the above functions in place, we examine some examples. The first example comes from simple normal data.

```
# Normal Example
## Non-parametric regression
n<-100
X<-seq(1, 20, length.out=n)
Y<-sqrt(X)+X*exp(-X)*sin(X)+rnorm(n, 0, .1)</pre>
```

The non-parametric regression is

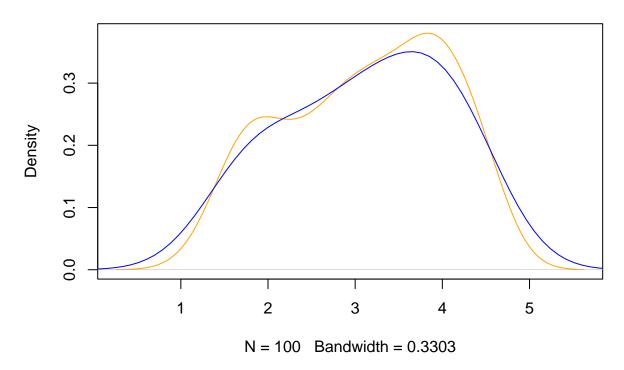
```
Y_hat<-r(X, Y, h=1/2)
plot(X, Y)
points(Y_hat$x, Y_hat$y_hat, type="1")</pre>
```



The kernel density estimate of the Y_i s is

```
## KDE
p_hat<-p(Y, h=1/2)
plot(density(Y), col="orange")
points(p_hat$x, p_hat$p_hat, type="l", col="blue")</pre>
```

density(x = Y)



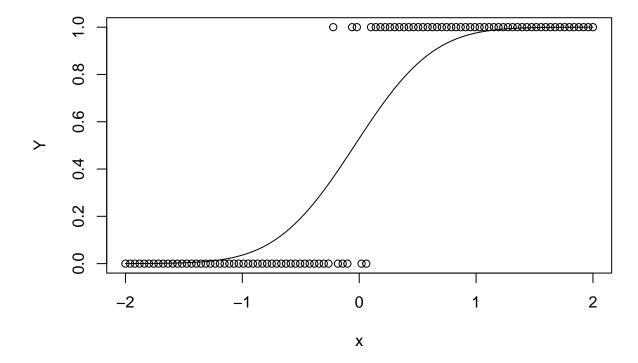
Second Example

We now try an example of logistically distributed data.

```
# Logistic Example
## Non-parametric regression
n<-100
h<-1/10
b<-5.01
x<-seq(-2, 2, length.out=n)
pi<-exp(x*b)/(1+exp(x*b))
Y<-c()
for(i in 1:n){
    Y<-c(Y, rbinom(1,1,pi[i]))
}</pre>
```

The non-parametric regression is

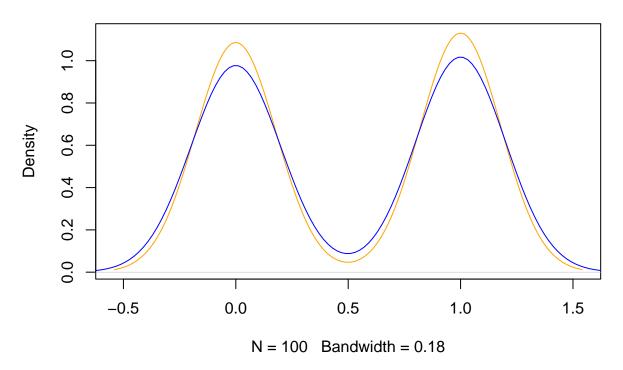
```
Y_hat<-r(x, Y, h=1/2)
plot(x, Y)
points(Y_hat$x, Y_hat$y_hat, type="1")</pre>
```



and the corresponding density estimate of the Y_i s is

```
## KDE
p_hat<-p(Y, h=1/5)
plot(density(Y), col="orange")
points(p_hat$x, p_hat$p_hat, type="l", col="blue")</pre>
```

density(x = Y)



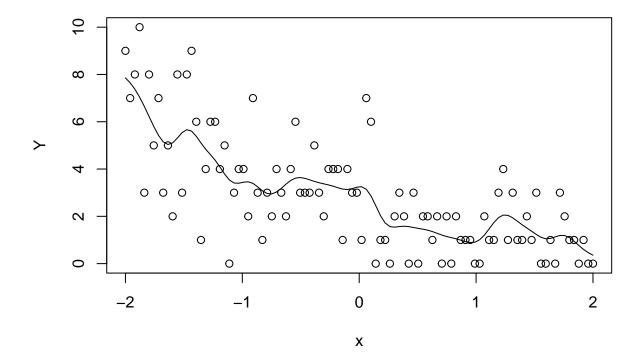
Example 3

In this example, we look at Poisson distributed data.

```
# Poisson Example
## Non-parametric regression
n<-100
x<-seq(-2,2,length.out=n)
X<-matrix(c(rep(1,n), x),ncol=2)
b<-c(.922,-.501)
lam<-exp(X%*%b)
Y<-c()
for(i in 1:n){
    Y<-c(Y, rpois(1, lam[i]))
}</pre>
```

The regression is

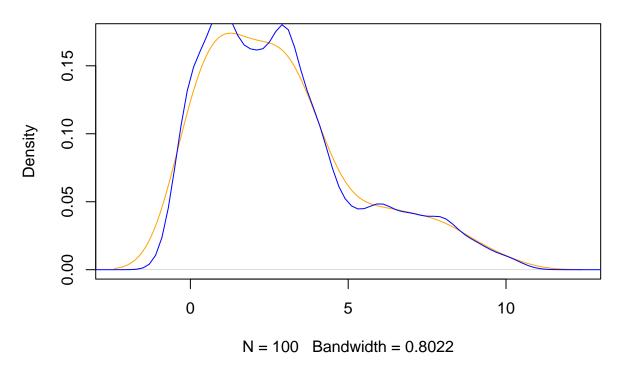
```
# Non-Parametric regression
Y_hat<-r(x, Y)
plot(x, Y)
points(Y_hat$x, Y_hat$y_hat, type="1")</pre>
```



and the density of the Y_i s is

```
# KDE
p_hat<-p(Y, h=1/2)
plot(density(Y), col="orange")
points(p_hat$x, p_hat$p_hat, type="l", col="blue")</pre>
```

density(x = Y)



Multivariate Example

We implement the non-parametric regression method below

```
r<-function(X, Y, intercept, n=100, h=1/10, type="gaussian"){
  if(is.matrix(X)==FALSE){
    x<-seq(min(X), max(X), length.out=n)</pre>
    y_hat<-c()
    for(point in x){
       y_hat<-c(y_hat, r_x(point, h, X, Y, type))</pre>
    }
  }
  if(is.matrix(X)==TRUE){
    if(intercept==TRUE){
      d \le -ncol(X) - 1
      x<-matrix(rep(0,n*d), ncol=d)</pre>
      for(j in 1:d){
         x[,j] \leftarrow seq(min(X[,j+1]), max(X[,j+1]), length.out=n)
      X < -X[,-1]
    if(intercept==FALSE){
      d<-ncol(X)</pre>
      x<-matrix(rep(0,n*d), ncol=d)</pre>
      for(j in 1:d){
         x[,j] \leftarrow seq(min(X[,j]), max(X[,j]), length.out=n)
```

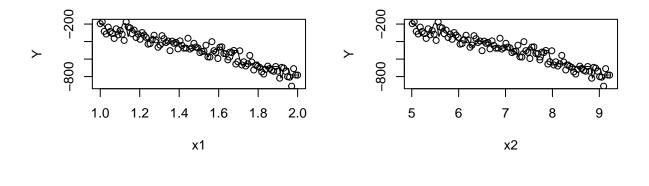
```
}
}
y_hat<-c()
for(i in 1:n){
    point<-x[i,]
    num<-c()
    for(l in 1:nrow(X)){
        num<-c(num, prod(k((X[1,]-point)/h, type)/h))
}
denom<-sum(num)
    W<-num/denom
    y_hat<-c(y_hat,sum(W*Y))
}
return(list(x=x, y_hat=y_hat))
}</pre>
```

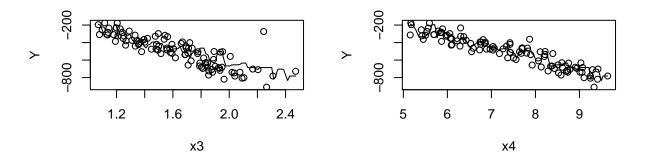
Using this, we generate some normal data and show and examine the non-parametric fit

```
# Normal Example
## Non-parametric regression
n<-100
b<-matrix(c(5.01, 9.22, -12.22, 1, 2), ncol=1)
x1<-seq(1, 2, length.out=n)
x2<-seq(5.01,9.22,length.out=n)
x3<-x1+rgamma(n,1,8)
x4<-x2+rgamma(n,1,4)
X<-matrix(c(rep(1,n),x1^2, x2^2, x3, x4^2), ncol=5)
Y<-X%*%b+rnorm(n, 0, 50)</pre>
Y_hat<-r(X, Y, intercept=TRUE, h=c(.75, .5), n=100)
```

To examine the fit, we plot the profile of the non-parametric regression

```
par(mfrow=c(2,2))
plot(x1, Y)
points(sqrt(Y_hat$x[,1]), Y_hat$y_hat, type="1")
plot(x2,Y)
points(sqrt(Y_hat$x[,2]), Y_hat$y_hat, type="1")
plot(x3, Y)
points(Y_hat$x[,3], Y_hat$y_hat, type="1")
plot(x4,Y)
points(sqrt(Y_hat$x[,4]), Y_hat$y_hat, type="1")
```





Further, we can examine how Poisson distributed data is fit by a non-parametric regression

```
# Poisson Example
## Non-parametric regression
n<-100
b<-matrix(c(5.01, 9.22, 12.22), ncol=1)
x1<-seq(1, 2, length.out=n)
x2<-seq(5.01,9.22,length.out=n)
X<-matrix(c(rep(1,n),x1^2, x2), ncol=3)
lam<-exp(X%*%b)
Y<-c()
for(i in 1:n){
    Y<-c(Y, rpois(1, lam[i]))
}</pre>
Y_hat<-r(X, Y, intercept=TRUE, h=c(.75, .5), n=100)</p>
```

We now plot the profile of the non-parametric regression

```
par(mfrow=c(1,2))
plot(x1, Y)
points(sqrt(Y_hat$x[,1]), Y_hat$y_hat, type="1")
plot(x2,Y)
points(Y_hat$x[,2], Y_hat$y_hat, type="1")
```

