STAT 824 hw 02

Multivariate Taylor expansion, closeness of points in high-dimensional space, Nadaraya-Watson and local polynomial estimators, CV for bandwidth selection

1. For a function $f : \mathbb{R}^d \to \mathbb{R}$, let

$$\nabla f(x_0) = \left.\begin{bmatrix} \frac{\partial}{\partial x_1} f(x) \\ \vdots \\ \frac{\partial}{\partial x_d} f(x) \end{bmatrix}\right|_{x=x_0} \quad \text{and} \quad \nabla^2 f(x_0) = \left.\begin{bmatrix} \frac{\partial^2}{\partial x_1^2} f(x) & \dots & \frac{\partial^2}{\partial x_1 \partial x_d} f(x) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial x_d \partial x_1} f(x) & \dots & \frac{\partial^2}{\partial x_d} f(x) \end{bmatrix}\right|_{x=x_0}.$$

For $x, x_0 \in \mathbb{R}^d$, show that

$$\sum_{|\alpha| \leq 2} \frac{D^\alpha f(x_0)}{\alpha!}(x - x_0)^\alpha = f(x_0) + [\nabla f(x_0)]^T (x - x_0) + \frac{1}{2}(x - x_0)^T [\nabla^2 f(x_0)](x - x_0),$$

which is the second-order Taylor expansion of f around x_0 evaluated at x.

Interpreting the multi-index notation carefully gives

$$\sum_{|\alpha|=0} \frac{D^\alpha f(x_0)}{|\alpha|}(x - x_0)^\alpha = f(x_0)$$

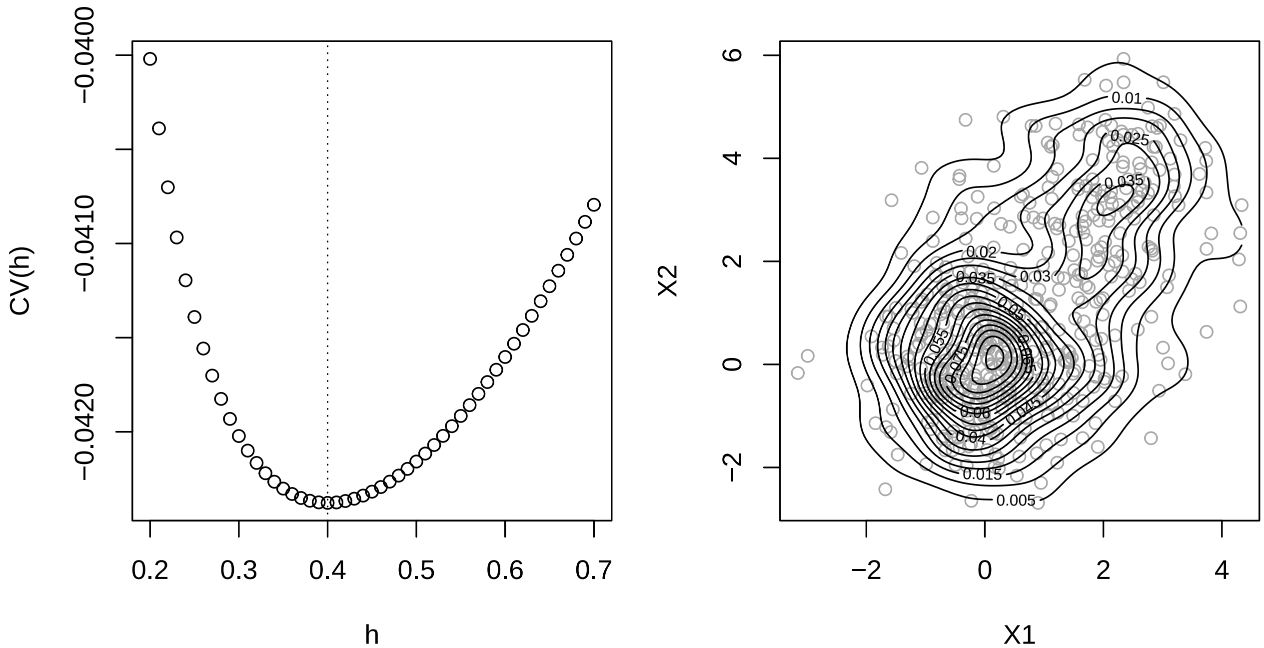
$$\begin{aligned} \sum_{|\alpha|=1} \frac{D^\alpha f(x_0)}{|\alpha|}(x - x_0)^\alpha &= \sum_{j=1}^{d} \left[\frac{\partial}{\partial x_j} f(x) \Big|_{x=x_0} \right] (x_j - x_{0j}) \\ &= [\nabla f(x_0)]^T (x - x_0) \end{aligned}$$

$$\begin{aligned} \sum_{|\alpha|=2} \frac{D^\alpha f(x_0)}{|\alpha|}(x - x_0)^\alpha &= \frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{d} \left[\frac{\partial^2}{\partial x_j x_j} f(x) \Big|_{x=x_0} \right] (x_j - x_{0j})(x_k - x_{0k}) \\ &= \frac{1}{2}(x - x_0)^2 [\nabla^2 f(x_0)](x - x_0) \end{aligned}$$

2. Obtain $n = 500$ realizations of (X_1, X_2) by running the code

```
n <- 500; alpha <- 1/3; Z <- runif(n) < alpha; X <- matrix(NA,n,2)
X[,1] <- rnorm(n,2*Z,1);X[,2] <- rnorm(n,3*Z,1)
```

Use leave-one-out crossvalidation to select the bandwidth for a bivariate kernel density estimator (write your own code for this). Then make a plot showing the CV criterion as a function of h and a scatterplot of your (X_1, X_2) values with contours of your estimate (at the CV choic of bandwidth) overlaid. Report your chosen bandwidth. My selected bandwidth was $\hat{h} = 0.4$. These are my plots:



We can perform leave-one-out crossvalidation just as in the univariate case; the only complication is how we compute the integral $\int_{\mathbb{R}^2} \hat{f}_n(x)dx$. We can get a numerical approximation to this integral by computing the height of $\hat{f}_n(x)$ over a grid. See the below code:

```
n <- 500
alpha <- 1/3
Z <- runif(n) < alpha
X <- matrix(NA,n,2)
X[,1] <- rnorm(n,2*Z,1)
X[,2] <- rnorm(n,3*Z,1)

biv_kde <- function(x,Y,h){

  val <- mean(dnorm(Y[,1] - x[1],0,h) * dnorm(Y[,2]-x[2],0,h))
  return(val)

}

hh <- seq(.2,.7,by=.01)
gridsize <- 120
x1.seq <- seq(min(X[,1]),max(X[,1]),length = gridsize)
x2.seq <- seq(min(X[,2]),max(X[,2]),length = gridsize)
zz <- matrix(0,gridsize,gridsize)

CV <- numeric(length(hh))
for(k in 1:length(hh)){
```

```
  h <- hh[k]

  for( i in 1:gridsize)
    for( j in 1:gridsize){

      zz[i,j] <- biv_kde(x = c(x1.seq[i],x2.seq[j]),Y = X, h = h)

    }

  Ahat <- sum(zz^2*diff(x1.seq)[1] * diff(x2.seq)[2])
  # sum(zz*diff(x1.seq)[1] * diff(x2.seq)[2]) # should be close to 1

  Bhat <- 0
  for(i in 1:n){
    fnii <- biv_kde(x = X[i,],Y = X[-i,], h = h)
    Bhat <- Bhat + 2 * fnii / n
  }

  CV[k] <- Ahat - Bhat
  print(k)

}

h_cv <- hh[which.min(CV)]

for( i in 1:gridsize)
  for( j in 1:gridsize){

    zz[i,j] <- biv_kde(x = c(x1.seq[i],x2.seq[j]),Y = X, h = h_cv)

  }

par(mfrow = c(1,2), mar = c(4.1,4.1,1.1,1.1))

plot(CV ~ hh,
     xlab = "h",
     ylab = "CV(h)")
abline(v = h_cv, lty = 3)

plot(X[,2]~X[,1],
     col = "dark gray",
     xlab = "X1",
     ylab = "X2",
     )

contour(x1.seq, x2.seq, zz, add = TRUE, nlevels = 20)
```

3. Let $X, X_1, \ldots, X_n \in [0,1]^d$ be independent random vectors with the elements of each being independent and uniformly distributed on the interval $[0,1]$. For a vector $x \in \mathbb{R}^d$, let $\|x\|_\infty = \max_{1\leq k\leq d} |x_k|$.

   (a) Show that

$$\mathbb{E} \min_{1\leq i\leq n} \|X - X_i\|_\infty \geq \frac{d}{2(d+1)} \cdot \frac{1}{n^{1/d}}.$$

We have

$$\begin{aligned}
P\left(\min_{1\leq i\leq n} \|X - X_i\|_\infty \leq t\right) &\leq nP(\|X - X_1\|_\infty \leq t) \\
&= P(\max_{1\leq k\leq d} |X_k - X_{1k}| \leq t) \\
&= nP(|U_1 - U_2| \leq t)^d, \quad U_1, U_2 \overset{\text{ind}}{\sim} \text{Uniform}(0,1) \\
&= n(2t - t^2)^d \\
&\leq n(2t)^d.
\end{aligned}$$

We could also get this bound by noting that the volume of a d-dimensional unit cube width $2t$ in each dimension is $(2t)^d$; that is the set of points $\{x : \max_{1\leq j\leq d} |x_j| \leq t\}$ has volume $(2t)^d$, which gives the bound $P(\|X - X_1\|_\infty \leq t) \leq (2t)^d$.

We then get the result by integrating over the corresponding lower bound for the survival function (where this is nonnegative). We have

$$\mathbb{E} \min_{1\leq i\leq n} \|X - X_i\|_\infty \geq \int_0^{1/(2n^{1/d})} (1 - n \cdot (2t)^d) dt,$$

which gives the bound.

   (b) Give an interpretation of the claim.

As the dimension of the space in which the data lie grows, the far-between-ness of the points grows, such that to maintain a dense "cloud" of points in a higher and higher dimensional space, one must increase the number of points *extremely* fast.

4. For a set of points $(X_1, Y_1), \ldots, (X_n, Y_n)$, the Nadaraya-Watson estimator of $m(x) = \mathbb{E}[Y|X = x]$ is

$$\hat{m}_n^{\text{NW}}(x) = \sum_{i=1}^n W_{ni}(x) Y_i, \quad \text{with} \quad W_{ni}(x) = \frac{K(h^{-1}(X_i - x))}{\sum_{j=1}^n K(h^{-1}(X_j - x))}.$$

(a) Show that if $K \geq 0$ we have $\hat{m}_n^{\mathrm{NW}}(x) = \underset{\theta \in \mathbb{R}}{\operatorname{argmin}} \ \sum_{i=1}^n (Y_i - \theta)^2 K(h^{-1}(X_i - x)$.

(b) Suppose $\int K(u)du = 1$ and $\int uK(u)du = 0$ and consider the kernel density estimators

$$\hat{f}_n(x, y) = \frac{1}{nh^2} \sum_{i=1}^n K\left(\frac{Y_i - y}{h}\right) K\left(\frac{X_i - x}{h}\right) \quad \text{and} \quad \hat{f}_n(x) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right)$$

of $f(x, y)$ and $f(x)$ and let $\hat{f}_n(y|x) = \hat{f}_n(x, y)/\hat{f}_n(x)$. Show that $\hat{m}_n^{\mathrm{NW}}(x) = \int y\hat{f}_n(y|x)dy$, so it is $\mathbb{E}[Y|X = x]$ taken with respect to the estimated conditional density $\hat{f}_n(y|x)$.

We have

$$\begin{aligned}
\int y\hat{f}_n(y|x)dy &= \int y \frac{1}{nh^2} \sum_{i=1}^n K((Y_i - y)/h)K((X_i - x)/h)/\hat{f}_n(x)dy \\
&= \hat{f}_n(x)^{-1} \frac{1}{nh^2} \sum_{i=1}^n K((X_i - x)/h) \int yK((Y_i - y)/h)dy \\
&= \hat{f}_n(x)^{-1} \frac{1}{nh} \sum_{i=1}^n K((X_i - x)/h) \int (Y_i - hu)K(u)du \\
&= \hat{f}_n(x)^{-1} \frac{1}{nh} \sum_{i=1}^n K((X_i - x)/h)Y_i \\
&= \frac{\sum_{i=1}^n K((X_i - x)/h)Y_i}{\sum_{j=1}^n K((X_j - x)/h)},
\end{aligned}$$

which is the N-W estimator $\hat{m}_n^{\mathrm{NW}}(x)$.

(c) Show that

$$\frac{Y_i - \hat{m}_n^{\mathrm{NW}}(X_i)}{1 - W_{ni}(X_i)} = Y_i - \hat{m}_{n,-i}^{\mathrm{NW}}(X_i).$$

We have

$$\begin{aligned}
Y_i - \hat{m}_{n,-i}^{\mathrm{NW}}(X_i) &= Y_i - \frac{\sum_{j \neq i} Y_j K(h^{-1}(X_j - X_i))}{\sum_{k \neq i}^n K(h^{-1}(X_k - X_i))} \\
&= Y_i - \frac{\sum_{j=1}^n Y_j K(h^{-1}(X_j - X_i)) - Y_i K(h^{-1}(X_i - X_i))}{\sum_{k \neq i}^n K(h^{-1}(X_k - X_i))} \\
&= Y_i - \frac{\hat{m}_n^{\mathrm{NW}}(X_i) - Y_i \cdot W_{ni}(X_i)}{1 - W_{ni}(X_i)} \\
&= \frac{Y_i - \hat{m}_n^{\mathrm{NW}}(X_i)}{1 - W_{ni}(X_i)},
\end{aligned}$$

where we obtain the third equality by dividing the numerator and denominator of the fraction by $\sum_{k=1}^n K(h^{-1}(X_k - X_i))$.

(d) Explain why the fact in part (c) is useful.

This is useful because it allows us to write

$$\mathrm{CV}_n(h) = \frac{1}{n}\sum_{i=1}^n [Y_i - \hat{m}^{\mathrm{NW}}_{n,-i}(X_i)]^2 = \frac{1}{n}\sum_{i=1}^n \left[\frac{Y_i - \hat{m}^{\mathrm{NW}}_n(X_i)}{1 - W_{ni}(X_i)}\right]^2,$$

so that we may compute the crossvalidation prediction risk without actually doing crossvalidation computationally; this saves time.

5. For $n = 200$, generate data according to $Y_i = m(X_i) + \varepsilon_i$, $i = 1, \dots, n$, where $X_1, \dots, X_n \overset{\text{ind}}{\sim} \text{Beta}(1/2, 1/2)$, independent of $\varepsilon_1, \dots, \varepsilon_n \overset{\text{ind}}{\sim} \text{Normal}(0, 1)$, where

$$m(x) = -250 \cdot (x - 1/2) \cdot \phi\left(10(x - 1/2)\right), \quad \phi(z) = (1/\sqrt{2\pi})e^{-z^2/2}.$$

Choose via crossvalidation a value of the bandwidth h for the local linear estimator (local polynomial of order $\ell = 1$) using ϕ as the kernel function. *Note: You will have to specify a grid of candidate h values.*

(a) Make a plot of the function

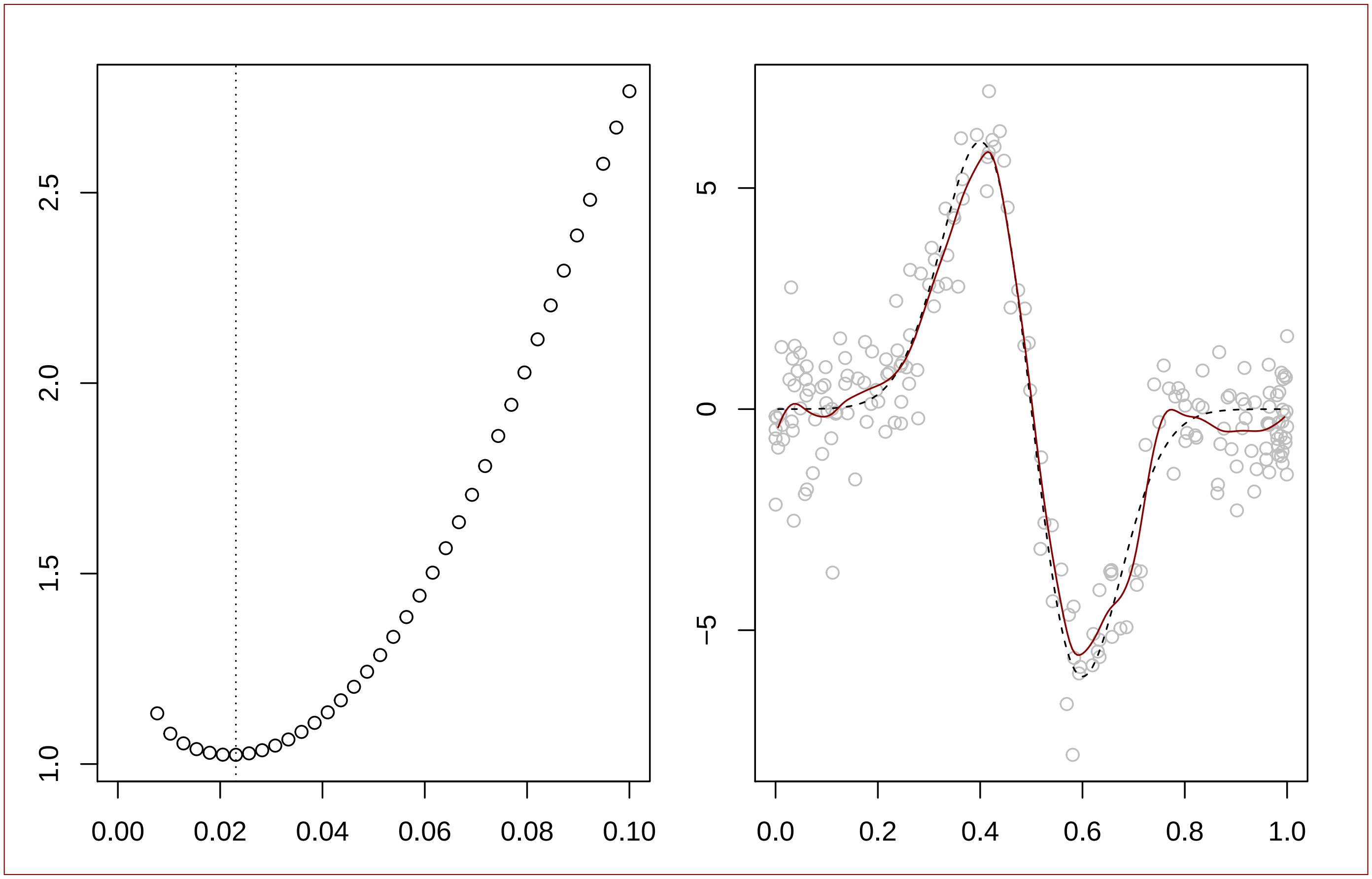
$$\mathrm{CV}_n(h) = \frac{1}{n}\sum_{i=1}^n \left[\frac{Y_i - \hat{m}^{\mathrm{LP}}_{n,1}(X_i)}{1 - W^*_{ni}(X_i)}\right]^2$$

over your grid of candidate bandwidths. It should dip down and rise back up. The weights $W^*_{ni}(X_i)$ are the values such that $\hat{m}^{\mathrm{LP}}_{n,1}(X_i) = \sum_{i=1}^n W^*_{ni}(X_i)Y_i$.

(b) Make a scatterplot of the data and overlay the true function; include in the scatterplot the estimated function at your chosen value of the bandwidth.

(c) Turn in your code.

My plot looks like


1.0
1.5
2.0
2.5
0.00
0.02
0.04
0.06
0.08
0.10
−5
0
5
0.0
0.2
0.4
0.6
0.8
1.0