Chapter 1. Nonparametric Curve Estimation Part 4

January 31, 2007

1 Other bandwidth selection methods

Since the bandwidth plays an essential role, some other methods have also been proposed

1.1 Generalized Cross-validation methods

Recall that

$$\hat{m}(x) = \sum_{i=1}^{n} K_h(X_i - x)Y_i / \sum_{i=1}^{n} K_h(X_i - x) = \ell_n(x)^{\top} Y$$

where $Y = (Y_1, \dots, Y_n)^{\top}$ and

$$\ell_n(x) = \{ \sum_{i=1}^n K_h(X_i - x) \}^{-1} (K_h(X_1 - x), \dots, K_h(X_n - x))^{\top}$$

Let

$$S_n = \begin{pmatrix} \ell_n(X_1) \\ \ell_n(X_2) \\ \vdots \\ \ell_n(X_n) \end{pmatrix}$$

we have

$$\begin{pmatrix} \hat{m}(X_1) \\ \hat{m}(X_2) \\ \dots \\ \hat{m}(X_n) \end{pmatrix} = S_n Y$$

Then, one can prove that

$$CV(h) = n^{-1} \sum_{i=1}^{n} \frac{(Y_i - \hat{m}(X_i))^2}{(1 - S_n(i, i))^2}$$

Based on this, Craven and Wahba (1979) proposed to consider the so called generalized cross-validation

$$GCV(h) = \frac{n^{-1} \sum_{i=1}^{n} (Y_i - \hat{m}(X_i))^2}{\{1 - tr(S_n)/n\}^2}$$

The bandwidth selected by GCV is

$$\hat{h} = \arg\min_{h} GCV(h)$$

Example 1.1 (simulation) 100 observations from

$$Y = cos(2\pi X) + 0.2\varepsilon$$

where $X \sim uniform(0,1)$ and $\varepsilon \sim N(0,1)$

the estimated regression function is shown in Fig. 1

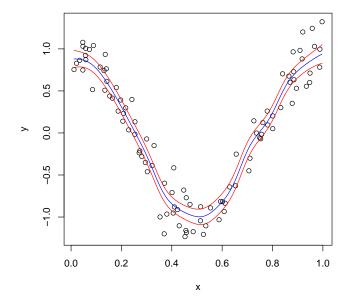


Figure 1: calculation results for Example 1.1 (Gcvh), (ks), (code)

Example 1.2 (motorcycle) (data) the bandwidth is chosen to be 1.38 by GCV as well as CV. the estimated regression function is shown in Fig. 2

1.2 plug-in method

Recall the optimal bandwidth is

$$h_{opt}(x) = \left\{ \frac{d_0 \sigma^2}{4f(x)c_2^2 \left\{ \frac{1}{2}m''(x) + f^{-1}(x)m'(x)f'(x) \right\}^2} \right\}^{1/5} n^{-1/5}.$$

Select an initial bandwidth h, say the one below. The estimator of m(x) is

$$\hat{m}(x) = \sum_{i=1}^{n} K_h(X_i - x)Y_i / \sum_{i=1}^{n} K_h(X_i - x)$$

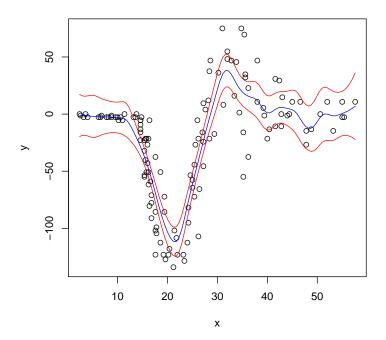


Figure 2: calculation results for Example 1.2 (code)

Therefore, we have

$$\hat{m}'(x) = d\left[\sum_{i=1}^{n} K_h(X_i - x)Y_i / \sum_{i=1}^{n} K_h(X_i - x)\right] / dx$$

and

$$\hat{m}''(x) = d^2 \left[\sum_{i=1}^n K_h(X_i - x) Y_i / \sum_{i=1}^n K_h(X_i - x) \right] / dx^2$$

For the density

$$\hat{f}(x) = n^{-1} \sum_{i=1}^{n} K_h(X_i - x).$$

and

$$\hat{f}'(x) = n^{-1} \sum_{i=1}^{n} \frac{dK_h(X_i - x)}{dx}.$$

We can then estimate the bandwidth $h_{opt}(x)$ based on these functions.

1.3 The bandwidth for density estimation

Consider the estimation of density function of X. Suppose X_1, \dots, X_n are samples. Bickel and Doksum (1977) and Silverman (1986) proved that if the true density of X is normal,

then the optimal bandwidth is

Gaussian kernel: $h = 1.06s_x n^{-1/5}$

Epanechnikov: $h = 2.34s_x n^{-1/5}$.

where
$$s_x = (n^{-1} \sum_{i=1}^n (X_i - \bar{X})^2)^{1/2}$$
.

For the estimation regression function, we can also use it after we standardize Y.

2 Local linear kernel smoothing

Again, consider the conditional expectation of Y given X = x. Suppose that $(X_i, Y_i), i = 1, \dots, n$ are samples.

$$Y_i = m(X_i) + \varepsilon_i$$

For any given point x and any X_i , if X_i is close to x we consider a local linear approximation

$$m(X_i) \approx m(x) + m'(x)(X_i - x).$$

Thus the model is

$$Y_i \approx m(x) + m'(X_i - x) + \varepsilon_i$$

or

$$Y_1 \approx m(x) + m'(x)(X_i - x) + \varepsilon_1$$

$$Y_2 \approx m(x) + m'(x)(X_i - x) + \varepsilon_2$$

:

$$Y_n \approx m(x) + m'(x)(X_i - x) + \varepsilon_n$$

This is a linear regression model with parameters m(x) and m'(x). It is easy to see that we care the approximation at x. Therefore, we give higher weight to those points close to x. The weight can be defined as

$$K_h(X_i - x) = h^{-1}K\left(\frac{X_i - x}{h}\right)$$

We use the following weighted least squares problem to estimate the value m(x) and m'(x).

$$\sum_{i=1}^{n} \{Y_i - m(x) - m'(x)(X_i - x)\}^2 K_h(X_i - x).$$

The minimizer to the above value is

$$\begin{pmatrix} \hat{m}(x) \\ \hat{m}'(x) \end{pmatrix} = \left\{ \sum_{i=1}^{n} K_h(X_i - x) \begin{pmatrix} 1 \\ X_i - x \end{pmatrix} \begin{pmatrix} 1 \\ X_i - x \end{pmatrix}^{\top} \right\}^{-1} \times \sum_{i=1}^{n} K_h(X_i - x) \begin{pmatrix} 1 \\ X_i - x \end{pmatrix} Y_i$$

We can write it as

$$\hat{m}(x) = \frac{n^{-1} \sum_{i=1}^{n} \{s_{n,2}(x) K_h(X_i - x) - s_{n,1}(x) K_h(X_i - x)\} Y_i}{s_{n,2}(x) s_{n,0}(x) - s_{n,1}^2(x)}$$

where

$$s_{n,k}(x) = n^{-1} \sum_{i=1}^{n} K_h(X_i - x) \left(\frac{X_i - x}{h}\right)^k, \quad k = 0, 1, 2$$

Let

$$\mathbf{X} = \begin{pmatrix} 1 & X_1 - x \\ 1 & X_2 - x \\ \dots & \\ 1 & X_n - x \end{pmatrix}$$

and W be the diagonal matrix of weights

$$W = diag\{K_h(X_i - x)\}.$$

and $\beta = (m(x), m'(x))^{\top}$. Then the least squares problem can be written as

$$(Y - \mathbf{X}\beta)^{\top} \mathbf{W} (\mathbf{Y} - \mathbf{X}\beta)$$

The minimizer to the above problem is

$$\hat{\beta} = \begin{pmatrix} \hat{m}(x) \\ \hat{m}'(x) \end{pmatrix} = \{ \mathbf{X}^{\top} \mathbf{W} \mathbf{X} \}^{-1} \mathbf{X}^{\top} \mathbf{W} \mathbf{Y}$$

Example 2.1 (simulation) 100 observations from

$$Y = cos(2\pi X) + 0.2\varepsilon$$

where $X \sim uniform(0,1)$ and $\varepsilon \sim N(0,1)$. with h = 0.05, we have the following simulations; see Fig 3

From this simulation, we can see that local linear kernel smoothing estimator has better performance at the boundary points than NW local constant estimator.

Example 2.2 (air pollution in Hong Kong) (data); Ozone is a second pollutant, i.e. it is generated by chemical reaction of other pollutants such as SO_2 and NO_2 with sunlight.

Apply local linear kernel smoothing method, we find the relation as shown Fig 4

From this simulation, we can see that local linear kernel smoothing estimator has better performance at the boundary points than NW local constant estimator.

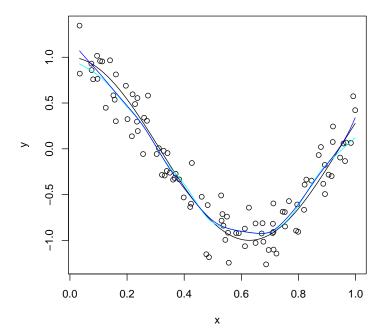


Figure 3: calculation results for Example 2.1. black: true function; cyan: NW estimator; blue: LL kernel estimator. (ksLL) (code)

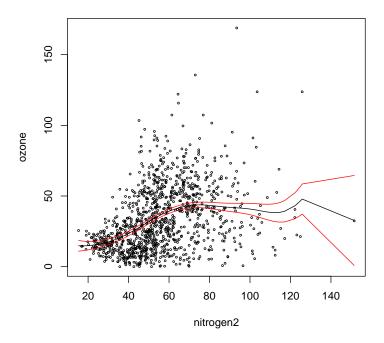


Figure 4: calculation results for Example 2.2. black: true function; cyan: NW estimator; blue: LL kernel estimator. (ksLL) (code)