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How sensitive are average derivatives?*

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Average derivatives are the mean slopes of regression functions. In practice they are estimated via a nonparametric smoothing technique. Every smoothing method needs a calibration parameter that determines the finite sample performance. In this paper we use the kernel estimation method and develop a formula for the bandwidth that describes the sensitivity of the average derivative estimator. One can determine an optimal smoothing parameter from this formula which tries out to undersmooth the density of the regression variable.

1. Average derivatives in discrete choice analysis

The average derivative is the mean of the slope of a regression function. In a regression setting $Y = m(X) + \varepsilon$ with regression curve $m: \boldsymbol{R}^d \to \boldsymbol{R}$, the average derivative is the mean gradient $\mathrm{E}_X(m'(X))$, or, more generally, the weighted mean gradient

$$\delta = \mathrm{E}_X(m'(X)\,w(X)), \tag{1.1}$$

where $m'(x)$ is the gradient

$$m'(x) = \left(\frac{\partial m}{\partial x_1}, \ldots, \frac{\partial m}{\partial x_d}\right) \in R^d,$$

$x_1, \ldots, x_d$ are components of the vector x, $w(x)$ is some weight function, and E_X is the expectation with respect to the (marginal) X-distribution.

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The average derivative δ is interesting in the context of discrete choice analysis, where in the case of binary choice we want to infer on the function

$$P(Y = 1 \mid X = x) = m(x),$$

from observations $\{(X_i, Y_i)\}_{i=1}^n$, $X_i \in \boldsymbol{R}^d$, $Y_i \in \{0, 1\}$. A pure nonparametric approach to estimation of $m(x)$ is possible [see, for example, the recent monographs by Müller (1988), Eubank (1988), Wahba (1990), and Härdle (1990)]. It is well-known though that this approach is not costless: the precision of the estimator is exponentially decreasing as the dimension d increases. In order to avoid this difficulty one could of course fall back into pure parametric models for $m(x)$.

One such model would be

$$m(x) = G(x^T \beta), \tag{1.2}$$

where G, the link function, is of known form, e.g., $G = \Phi$ would postulate a Probit model.

A model comprising the advantages and simplicity of (1.2) and the flexibility of a nonparametric smoothing approach is a single-index model,

$$m(x) = g(x^T \beta), \tag{1.3}$$

with an unknown link function g and index $x^T \beta$.

It is well-known that β in (1.3) can only be identified up to scale [see Härdle and Stoker (1989)]: the (weighted) average derivative (ADE) for this model is

$$\delta = \mathrm{E}_X \left[\frac{\mathrm{d}g}{\mathrm{d}(X^T \beta)} w(X) \right] \beta = \gamma_\beta \cdot \beta, \tag{1.4}$$

so we see that we can estimate β (up to scale) if we know how to estimate δ and if γ_β is different from zero. A simple example for (1.4) is a linear link function $g(\cdot)$; then the coefficients β are multiplied by the slope of $g(\cdot)$ times $\mathrm{E}_X(w(X))$. For general, nonlinear $g(\cdot)$, as in binary choice models, the β coefficients are multiplied by the average slope

$$\gamma_\beta = \mathrm{E}_X \left[\frac{\mathrm{d}g}{\mathrm{d}(X^T \beta)} w(X) \right].$$

We use kernel estimators for the average derivative δ since they are straightforward to implement and easy to understand on an intuitive level. Other possibilities include splines and orthogonal series, but to our knowledge these techniques have not been employed to estimate average derivatives. The main point in this paper is about the selection of the bandwidth, the kernel smoothing parameter, for the d-dimensional case. The one-dimensional case with a focus on estimation of income effects is treated in Härdle, Hart, Marron, and Tsybakov (1991). From an asymptotical viewpoint the choice of bandwidth does not affect the behavior of ADE estimators. It influences only the higher-order terms of asymptotic expansions for mean squared error, not the main term which is of order $O(1/n)$, where n is the number of observations. In practice though, the choice of the smoothing parameter is an important issue as has been pointed out by Hsieh and Manski (1987, p. 551).

In this paper we consider the special choice of weight function: $w(x) = f(x)$, where $f(x)$ is the marginal density of X [cf. Powell, Stock, and Stoker (1989)]. This is motivated by several reasons. First, under such choice of w we avoid the random denominator appearing if $w(x) \equiv 1$ [in fact, for $w(x) \equiv 1$ the ADE estimators contain the density estimator in denominator; see Härdle and Stoker (1989) for details]. Because of the random denominator the necessary asymptotic expansions hold under somewhat restrictive assumptions on the underlying density f [Härdle and Stoker (1989), Härdle, Hart, Marron, and Tsybakov (1991)]. Next, for the multi-dimensional case the $O(1/n)$ rate of the mean-squared error is not attained unless the oscillating higher-order kernels are implemented. This causes a difficulty in treating the case of $w(x) \equiv 1$: the ADE estimator is not well-defined and it requires some truncation [Härdle and Stoker (1989)]. The choice of truncation threshold appears to be crucial in this context. This creates an additional problem which could be easily eliminated if $w(x) = f(x)$.

In section 2 we quantify the sensitivity of ADE via a second-order expansion of mean squared error of a kernel estimator for δ. Section 3 is devoted to the proof of our main theorem. In the appendix we prove some lemmas.

2. The sensitivity of ADE

Assume that independent pairs (X_i, Y_i), $i = 1, \dots, n$, of random variables, $X_i \in R^d$, $Y_i \in R^1$, are observed and that they have the same distribution as (X, Y), $X \in R^d$, $Y \in R^1$.

Let the regression function $m(x) = \mathrm{E}(Y|X = x)$ exist and let X have the density $f(x)$ with respect to Lebesgue measure in R^d. Suppose, moreover, that the regression function m and the density f are continuously differentiable and that $f(x)$ *vanishes outside a compact set*, the support of X.

Using partial integration (over the support of X) we get

$$\begin{aligned}\delta &= \int m'(x) f^2(x)\,\mathrm{d}x \\ &= -2\int m(x) f'(x) f(x)\,\mathrm{d}x \\ &= -2\mathrm{E}(Yf'(X)),\end{aligned} \tag{2.1}$$

where $f'(x) = (\partial f/\partial x_1, \ldots, \partial f/\partial x_d)$ and the expectation is now taken over the joint distribution of (X, Y).

If we knew the marginal density f we could estimate δ by means of the sum $-(2/n)\sum_{i=1}^{n} Y_i f'(X_i)$ which is obtained if one substitutes the expectation in (2.1) by the empirical average.

In our approach we do not know the density function. We shall estimate it from the data via the kernel method. The marginal density $f(\cdot)$ is estimated by

$$\hat{f}_h(x) = n^{-1} \sum_{i=1}^{n} \mathscr{K}_h(x - X_i), \tag{2.2}$$

where $\mathscr{K}_h(u) = h^{-d}\mathscr{K}(u_1/h, \ldots, u_d/h)$ for a multivariate kernel function,

$$\mathscr{K}(u_1, \ldots, u_d) = \prod_{j=1}^{d} K(u_j), \quad u = (u_1, \ldots, u_d) \in R^d, \tag{2.3}$$

based on a one-dimensional kernel K. The scaling of $\mathscr{K}$ is through $h > 0$, the bandwidth, or smoothing parameter.

The gradient $f'(x)$ is estimated by

$$\hat{f}'_h(x) = \frac{1}{n}\sum_{i=1}^{n} \mathscr{K}'_h(x - X_i), \tag{2.4}$$

where

$$\mathscr{K}'_h(u) = h^{-d-1} K'\left(\frac{u_j}{h}\right) \prod_{k \neq j} K\left(\frac{u_j}{h}\right),$$

and K' denotes the derivative of one-dimensional kernel K.

Using (2.4) we can construct an estimate of the average derivative

$$\hat{\delta}_n = -\frac{2}{n}\sum_{i=1}^{n} Y_i \hat{f}'_h(X_i). \tag{2.5}$$

We study the asymptotic mean squared error of $\hat{\delta}_n$ under the following assumptions:

(A1) The kernel K is bounded, continuously differentiable, symmetric with support $[-1, 1]$; $K'(0) = 0$.

(A2) $\int K(u)\,\mathrm{d}u = 1$, and there exists a positive integer $k \geq 2$ such that $\int u^j K(u) \times \mathrm{d}u = 0$, $j = 1, \ldots, k-1$, $\int u^k K(u)\,\mathrm{d}u = \mathrm{d}_K \neq 0$.

(A3) The marginal density $f(x)$ of X is compactly supported and has continuous partial derivatives up to the order $k+1$ on R^d.

(A4) The regression function $m(x)$ has continuous partial derivatives up to the order $k+1$ on R^d.

(A5) The conditional variance $\sigma^2(x) = \operatorname{var}(Y \mid X = x)$ is bounded on the support of f.

(A6) $h = h_n \to 0$, and $n^2 h_n^{d+2} \to \infty$ as $n \to \infty$.

Later $|\cdot|$ denotes Euclidean norm when applied to vectors.

Theorem. Under the assumptions (A1)–(A6),

$$\mathrm{E}(|\hat{\delta}_n - \delta|^2) = Q_1 n^{-1} + Q_2 n^{-2} h_n^{-d-2} + Q_3 h_n^{2k} + \mathrm{O}\left(\frac{h_n^k}{n} + \frac{1}{n^2}\right) + \mathrm{o}\left(\frac{1}{n^2 h_n^{d+2}} + h_n^{2k}\right), \qquad n \to \infty,$$

where

$$Q_1 = 4[\mathrm{E}(|f(X)m'(X)|^2) - |\mathrm{E}(f(X)m'(X))|^2 + \mathrm{E}(\sigma^2(X)|f'(X)|^2)],$$

$$Q_2 = 4C_K \int \sigma^2(x) f^2(x)\,\mathrm{d}x,$$

$$Q_3 = 4\left|\int S_K(x) f(x) m(x)\,\mathrm{d}x\right|^2,$$

and

$$C_K = \int |\mathscr{K}'(u)|^2\,\mathrm{d}u = d \int (K'(u))^2\,\mathrm{d}u \left(\int K^2(u)\,\mathrm{d}u\right)^{d-1},$$

$$S_K(x) = d_K \frac{(-1)^k}{k!} \sum_{j=1}^{d} \begin{pmatrix} \partial^{k+1} f(x)/\partial x_1 \partial x_j^k \\ \vdots \\ \partial^{k+1} f(x)/\partial x_d \partial x_j^k \end{pmatrix}.$$

From the Theorem we see that the bandwidth h_n minimizing $\mathrm{E}(|\hat{\delta}_n - \delta|^2)$ is given by

$$h_n^* = h_0 n^{-2/(2k+d+2)},$$

where

$$h_0 = \left(\frac{Q_2(d+2)}{2kQ_3}\right)^{1/(2k+d+2)}.$$

For $h_n = h_n^*$, we have

$$\mathrm{E}(|\hat{\delta}_n - \delta|^2) = Q_1 n^{-1} + Cn^{-4k/(2k+d+2)} + \mathrm{o}(n^{-4k/(2k+d+2)}) + \mathrm{O}\left(\frac{1}{n^2}\right), \qquad n \to \infty, \tag{2.6}$$

where

$$C = \left[\left(\frac{2k}{d+2}\right)^{(d+2)/(2k+d+2)} + \left(\frac{d+2}{2k}\right)^{2k/(2k+d+2)}\right] \times Q_2^{2k/(2k+d+2)} Q_3^{(d+2)/(2k+d+2)}.$$

Optimization of k. This in fact is reasonable if one believes that f and m are infinitely many times continuously differentiable. It follows from (2.6) that the best rate for mean squared error equals n^{-1} and it is attained if $k > (d+2)/2$. For example, in one-dimensional case ($d = 1$) it suffices to take $k = 2$. Then the second term in (2.6) equals $Cn^{-8/7}$, and h_n^* is proportional to $n^{-2/7}$ [cf. Härdle, Hart, Marron, and Tsybakov (1991)].

Assumptions (A1) and (A2) entail that the order k of the kernel should be necessarily even. Thus, the condition for choosing k that guarantees the best rate of convergence becomes:

k is the minimal even number such that $k > (d+2)/2$.

Optimization of K. The factor C depends on the kernel K. Optimizing this factor in K leads to the minimization problem (in view of the definition of Q_2 and Q_3):

$$\min_{K \in \mathscr{K}_k} \left(\int u^k K(u)\,\mathrm{d}u\right)^{d+2} \left(\int (K'(u))^2\,\mathrm{d}u\right)^{2k} \left(\int K^2(u)\,\mathrm{d}u\right)^{2(d-1)},$$

where $\mathscr{U}_k$ is the class of kernels satisfying (A1) and (A2). For $d = 1$, this problem was solved by Mammitzsch (1990) who showed that the optimal K is the quartic kernel

$$K(u) = \tfrac{15}{16}(1 - u^2)^2 \, I(|u| \le 1),$$

where $I(\cdot)$ denotes the indicator function. If $d \ge 2$, then $k \ge 4$, and the optimal K is, clearly, an oscillating kernel taking positive and negative values.

3. Proof of the Theorem

Denote

$$\delta_n^* = \frac{\hat{\delta}_n}{2} = -\frac{1}{n}\sum_{i=1}^{n} Y_i \hat{f}'_h(X_i), \qquad \delta^* = \frac{\delta}{2} = -\int m(x) f'(x) f(x)\,\mathrm{d}x.$$

Clearly,

$$\mathrm{E}(|\hat{\delta}_n - \delta|^2) = 4\mathrm{E}(|\delta_n^* - \delta^*|^2). \tag{3.1}$$

Write the estimator δ_n^* as

$$\delta_n^* = \frac{1}{n}\sum_{i=1}^{n} (m(X_i) + \varepsilon_i)\hat{f}'_h(X_i),$$

where $\varepsilon_i = Y_i - m(X_i)$. Since $\mathrm{E}(\varepsilon_i | X_i) = 0$, we have

$$\begin{aligned}
&\mathrm{E}(|\delta_n^* - \delta^*|^2) \\
&= \mathrm{E}\left(\left|\frac{1}{n}\sum_{i=1}^{n} \varepsilon_i \hat{f}'_h(X_i)\right|^2\right) + \mathrm{E}\left(\left|\frac{1}{n}\sum_{i=1}^{n} m(X_i)\hat{f}'_h(X_i) - \delta^*\right|^2\right) \\
&= \mathrm{E}\left(\left|\frac{1}{n}\sum_{i=1}^{n} \varepsilon_i \hat{f}'_h(X_i)\right|^2\right) + \mathrm{E}\left(\left|\frac{1}{n}\sum_{i=1}^{n} [\zeta_i - \mathrm{E}(\zeta_i)]\right|^2\right) \\
&\quad + \left|\frac{1}{n}\sum_{i=1}^{n} \mathrm{E}(\zeta_i) - \delta^*\right|^2,
\end{aligned} \tag{3.2}$$

where $\zeta_i = m(X_i)\hat{f}'_h(X_i)$.

It follows from (A1) that $\mathscr{K}'_h(0) = 0$, and thus

$$\hat{f}'_h(X_i) = \frac{1}{n} \sum_{\substack{j=1 \\ i \neq j}}^{n} \mathscr{K}'_h(X_i - X_j). \tag{3.3}$$

Thus,

$$\mathrm{E}(\zeta_i) = \mathrm{E}(\zeta_1) = \mathrm{E}(m(X_1)\hat{f}'_h(X_1)) = \frac{n-1}{n}\,\tilde{q}, \tag{3.4}$$

where $\tilde{q} = \mathrm{E}(m(X_1)\mathscr{K}'_h(X_1 - X_2))$. Here we used (2.4) and the fact that $\mathscr{K}'_h(0) = 0$ which follows from (A1). Now, (3.2) and (3.4) entail

$$\mathrm{E}(|\delta^*_n - \delta^*|^2) = V_1 + V_2 + V_3, \tag{3.5}$$

where

$$V_1 = \mathrm{E}\left(\left|\frac{1}{n}\sum_{i=1}^{n} \varepsilon_i \hat{f}'_h(X_i)\right|^2\right),$$

$$V_2 = \mathrm{E}\left(\left|\frac{1}{n}\sum_{i=1}^{n} (\zeta_i - \mathrm{E}(\zeta_1))\right|^2\right),$$

$$V_3 = |\mathrm{E}(\zeta_1) - \delta^*|^2.$$

Let us evaluate the terms V_1, V_2, and V_3.

Clearly,

$$\mathrm{E}(\varepsilon_i\varepsilon_l | X_1, \ldots, X_n) = \begin{cases} \sigma^2(X_i), & i = l, \\ 0, & i \neq l. \end{cases} \tag{3.6}$$

From (3.3) and (3.6) we get

$$V_1 = \mathrm{E}\left(\frac{1}{n^2}\sum_{i,l=1}^{n} \varepsilon_i\varepsilon_l(\hat{f}'_h(X_i), \hat{f}'_h(X_l))\right)$$

$$= \frac{1}{n^2}\sum_{i=1}^{n} \mathrm{E}\left(\sigma^2(X_i)\left|\frac{1}{n}\sum_{\substack{j=1 \\ i\neq j}}^{n} \mathscr{K}'_h(X_i - X_j)\right|^2\right) \tag{3.7}$$

$$= \frac{1}{n^3} \int \sigma^2(X_1)\,\mathrm{E}\left(\left|\sum_{j=2}^{n} \mathscr{K}'_h(X_1 - X_j)\right|^2\right) f(X_1)\,\mathrm{d}X_1$$

$$= \frac{1}{n^3} \int \sigma^2(x)\,\mathrm{E}\left(\sum_{j,s=2}^{n} (\mathscr{K}'_h(x - X_j), \mathscr{K}'_h(x - X_s))\right) f(x)\,\mathrm{d}x.$$

Here and later $(\cdot,\cdot)$ denotes the scalar product. We have

$$\mathrm{E}\left(\sum_{j,s=2}^{n} (\mathscr{K}'_h(x - X_j), \mathscr{K}'_h(x - X_s))\right)$$

$$= \sum_{j=2}^{n} \mathrm{E}(|\mathscr{K}'_h(x - X_j)|^2) + \sum_{\substack{j,s=2 \\ j\neq s}}^{n} |\mathrm{E}(\mathscr{K}'_h(x - X_j))|^2 \tag{3.8}$$

$$= (n-1)\,\mathrm{E}(|\mathscr{K}'_h(x - X_1)|^2)$$

$$+ (n-1)(n-2)|\mathrm{E}(\mathscr{K}'_h(x - X_1))|^2.$$

It follows from Lemmas 1 and 2 and (3.8) that

$$\mathrm{E}\left(\sum_{j,s=2}^{n} (\mathscr{K}'_h(x - X_j), \mathscr{K}'_h(x - X_s))\right)$$

$$= (n-1)(C_K f(x) h^{-d-2} + \beta_3(h, x))$$

$$+ (n-1)(n-2)|f'(x) + h^k S_K(x) + \beta_1(h, x)|^2.$$

Hence

$$V_1 = \frac{1}{n} \int \sigma^2(x)|f'(x)|^2 f(x)\,\mathrm{d}x + \frac{1}{n^2 h^{d+2}} C_K \int \sigma^2(x) f^2(x)\,\mathrm{d}x$$

$$+ \mathrm{o}\left(\frac{1}{n^2 h^{d+2}}\right) + \mathrm{O}\left(\frac{h^k}{n} + \frac{1}{n^2}\right), \qquad n \to \infty, \tag{3.9}$$

where we used the properties of β_1, β_3 and the fact that by (A3) the function $|S_K(x)|$ is uniformly bounded on the support of f.

Next,

$$V_2 = \frac{1}{n^2} \sum_{i,j=1}^{n} \mathrm{E}((\zeta_i, \zeta_j)) - |\mathrm{E}(\zeta_1)|^2 = V_{21} + V_{22} - |\mathrm{E}(\dot{\zeta}_1)|^2, \tag{3.10}$$

where

$$V_{21} = \frac{1}{n^2} \sum_{i=1}^{n} \mathrm{E}(|\zeta_i|^2), \qquad V_{22} = \frac{1}{n^2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \mathrm{E}((\zeta_i, \zeta_j)).$$

We have

$$\mathrm{E}(|\zeta_i|^2) = \frac{1}{n^2} \mathrm{E}\left(m^2(X_i) \sum_{\substack{l,s=1 \\ l,s \neq i}}^{n} (\mathscr{K}'_h(X_i - X_l), \mathscr{K}'_h(X_i - X_s)) \right).$$

Hence

$$V_{21} = \frac{1}{n^3} \mathrm{E}\left(m^2(X_1) \sum_{l,s=2}^{n} (\mathscr{K}'_h(X_1 - X_l), \mathscr{K}'_h(X_1 - X_2)) \right).$$

Using the same argument as in (3.7)-(3.9), we find

$$V_{21} = \frac{1}{n} \int m^2(x) |f'(x)|^2 f(x) \, \mathrm{d}x + \frac{1}{n^2 h^{d+2}} C_K \int m^2(x) f^2(x) \, \mathrm{d}x$$

$$+ \mathrm{o}\left(\frac{1}{n^2 h^{d+2}} \right) + \mathrm{O}\left(\frac{h^k}{n} + \frac{1}{n^2} \right), \qquad n \to \infty. \tag{3.11}$$

Consider the term V_{22} now. Applying (3.3) we obtain

$$V_{22} = \frac{n-1}{n} \mathrm{E}((\zeta_1, \zeta_2)) = \frac{n-1}{n^3}$$

$$\times \left\{ \mathrm{E}\left[m(X_1) m(X_2) \times \sum_{\substack{l,s=1 \\ l \neq 1 \\ s \neq 2}}^{n} (\mathscr{K}'_h(X_1 - X_l), \mathscr{K}'_h(X_2 - X_s)) \right] \right\}$$

$$= \frac{n-1}{n^3} \sum_{\substack{l,s=1 \\ l \neq 1 \\ s \neq 2}}^{n} \Delta_{ls}, \tag{3.12}$$

where

$$\Delta_{ls} = \mathrm{E}[m(X_1)m(X_2)(\mathscr{K}'_h(X_1 - X_l), \mathscr{K}'_h(X_2 - X_s))].$$

Let us treat Δ_{ls} separately in the following four cases:

(i) $s = l$,

(ii) $s \neq l, l \neq 2, s \neq 1$,

(iii) $s \neq l$ and either $l = 2, s \neq 1$ or $l \neq 2, s = 1$,

(iv) $s \neq l, l = 2, s = 1$.

In case (i),

$$\begin{aligned} \Delta_{ls} = \Delta_{ll} &= \mathrm{E}[m(X_1)m(X_2)(\mathscr{K}'_h(X_1 - X_3), \mathscr{K}'_h(X_2 - X_3))] \\ &= \mathrm{E}_{X_3}[|\mathrm{E}_{X_1}(m(X_1)\mathscr{K}'_h(X_1 - X_3))|^2] \stackrel{\text{def}}{=} B_1. \end{aligned} \tag{3.13}$$

In case (ii),

$$\begin{aligned} \Delta_{ls} &= \mathrm{E}[m(X_1)m(X_2)(\mathscr{K}'_h(X_1 - X_l), \mathscr{K}'_h(X_1 - X_s))] \\ &= |\mathrm{E}(m(X_1)\mathscr{K}'_h(X_1 - X_l))|^2 = |\bar{q}|^2. \end{aligned} \tag{3.14}$$

In case (iii),

$$\begin{aligned} \Delta_{ls} &= \mathrm{E}[m(X_1)m(X_2)(\mathscr{K}'_h(X_1 - X_2), \mathscr{K}'_h(X_2 - X_s))] \\ &= \mathrm{E}[(m(X_1)m(X_2)(\mathscr{K}'_h(X_1 - X_2)), \mathscr{K}'_h(X_2 - X_3))] \stackrel{\text{def}}{=} B_2. \end{aligned} \tag{3.15}$$

In case (iv),

$$\begin{aligned} \Delta_{ls} &= \mathrm{E}[m(X_1)m(X_2)(\mathscr{K}'_h(X_1 - X_2), \mathscr{K}'_h(X_2 - X_1))] \\ &= -\mathrm{E}[(m(X_1)m(X_2)|\mathscr{K}'_h(X_1 - X_2)|^2) \stackrel{\text{def}}{=} B_3. \end{aligned} \tag{3.16}$$

In (3.16) we used the fact that $\mathscr{K}'_h$ is antisymmetric:

$$\mathscr{K}'_h(-u) = -\mathscr{K}'_h(u).$$

It follows from (3.12)–(3.16) that

$$V_{22} = \frac{n-1}{n^3}\left[(n-2)B_1 + (n^2-5n+6)|\hat{q}|^2 + 2(n-2)B_2 + B_3\right]. \tag{3.17}$$

Now we use Lemma 4 in the appendix, which implies, together with (3.17), that

$$\begin{aligned} V_{22} = {} & \frac{1}{n}\left[\int f^3(x)|m'(x)|^2\,dx - \int m^2(x)|f'(x)|^2 f(x)\,dx\right] \\ & + |\hat{q}|^2 + \left(1-\frac{6}{n}\right) - \frac{C_K}{n^2h^{d+2}}\int m^2(x)f^2(x)\,dx \\ & + O\left(\frac{h^k}{n}+\frac{1}{n^2}\right) + o\left(\frac{1}{n^2h^{d+2}}\right), \qquad n\to\infty. \end{aligned} \tag{3.18}$$

From (3.4), (3.10), (3.11), and (3.18), we find

$$\begin{aligned} V_2 & = V_{21} + V_{22} - \left|\frac{n-1}{n}\hat{q}\right|^2 \\ & = V_{21} + V_{22} - |\hat{q}|^2\left(1-\frac{2}{n}+\frac{1}{n^2}\right) \\ & = \frac{1}{n}\left[\int f^3(x)|m'(x)|^2\,dx - 4|\hat{q}|^2\right] \\ & \quad + O\left(\frac{h^k}{n}+\frac{1}{n^2}\right) + o\left(\frac{1}{n^2h^{d+2}}\right), \qquad n\to\infty. \end{aligned} \tag{3.19}$$

By substitution on (A.2) into (3.19), we obtain

$$\begin{aligned} V_2 = {} & \frac{1}{n}\left[\int f^3(x)|m'(x)|^2\,dx - 4|\delta^*|^2\right] \\ & + O\left(\frac{h^k}{n}+\frac{1}{n^2}\right) + o\left(\frac{1}{n^2h^{d+2}}\right), \qquad n\to\infty. \end{aligned} \tag{3.20}$$

It remains to find the asymptotic expression for V_3.

By (A.2) we have

$$V_3 = \left|\frac{n-1}{n}\hat{q} - \delta^*\right|^2$$

$$= \left|\frac{q}{n} + h^k \int S_K(x) f(x)\, m(x)\,\mathrm{d}x + \beta_2(h)\right|^2 \tag{3.21}$$

$$= h^{2k}\left|\int S_K(x) f(x)\, m(x)\,\mathrm{d}x\right|^2$$

$$+ \mathrm{O}\left(\frac{h^k}{n} + \frac{1}{n^2}\right) + \mathrm{o}(h^{2k}), \qquad n \to \infty.$$

From (3.5), (3.9), (3.20), and (3.21) one gets

$$\mathrm{E}(|\delta_n^* - \delta^*|^2)$$

$$= \frac{1}{n}\left[\int f^{3\alpha}(x)|m'(x)|^2\,\mathrm{d}x - 4|\delta^*|^2 + \int \sigma^2(x)|f'(x)|^2 f(x)\,\mathrm{d}x\right]$$

$$+ \frac{1}{n^2 h^{d+2}} C_K \int \sigma^2(x) f^2(x)\,\mathrm{d}x + h^{2k}\left|\int S_K(x) f(x)\, m(x)\,\mathrm{d}x\right|^2$$

$$+ \mathrm{O}\left(\frac{h^k}{n} + \frac{1}{n^2}\right) + \mathrm{o}\left(\frac{1}{n^2 h^{d+2}}\right), \qquad n \to \infty.$$

This, in view of (3.1), proves the Theorem.

Appendix

Lemma 1. Let assumptions (A1)–(A4) be satisfied. Then

$$\mathrm{E}(\mathscr{K}_h'(x - X_1)) = -f'(x) - h^k S_K(x) - \beta_1(h, x), \qquad \forall x \in R^d, \tag{A.1}$$

where $\sup_x|\beta_1(h,x)| = o(h^k)$ *as* $h \to 0$, *and*

$$\hat{q} = \delta^* - h^k \int S_K(x) f(x) m(x)\,dx + \beta_2(h), \tag{A.2}$$

where $|\beta_2(h)| = o(h^k)$ *as* $h \to 0$.

Proof. By partial integration,

$$\begin{aligned} E(\mathscr{K}_h'(x - X_1)) &= \frac{1}{h^{d+1}} \int \mathscr{K}'\left(\frac{x-z}{h}\right) f(z)\,dz \\ &= -\frac{1}{h}\int \mathscr{K}'(u) f(x - uh)\,du \\ &= \frac{1}{h}\int (f(x-uh))' \mathscr{K}(u)\,du \\ &= -\int f'(x-uh)\mathscr{K}(u)\,du, \end{aligned} \tag{A.3}$$

where we used the fact that $\mathscr{K}$ and f are compactly supported. Assumption (A3) entails that the Taylor expansion is valid, and thus, uniformly in $u \in \mathrm{supp}\,\mathscr{K}$,

$$\left| f'(x-uh) - \sum_{\alpha:|\alpha|\le k} \frac{1}{\alpha!}(-1)^{|\alpha|} u^\alpha h^{|\alpha|} \begin{pmatrix} \partial^{|\alpha|+1} f(x)/\partial x_1 \partial x^\alpha \\ \vdots \\ \partial^{|\alpha|+1} f(x)/\partial x_d \partial x^\alpha \end{pmatrix} \right|$$

$$\le \beta_1(h,x), \tag{A.4}$$

where $\sup_x|\beta_1(h,x)| = o(h^k)$, $h \to 0$, and $\alpha = (\alpha, \ldots, \alpha_d)$ is multi-index, $\alpha_j \ge 0$, $|\alpha| = \alpha_1 + \cdots + \alpha_d$, $\alpha! = \alpha_1! \cdots \alpha_d!$, $u^\alpha = u_1^{\alpha_1} \cdot \cdots \cdot u_d^{\alpha_d}$ for $u = (u_1, \ldots, u_d) \in R^d$, and $\partial^{|\alpha|}/\partial x^\alpha = \partial^{|\alpha|}/\partial x_1^{\alpha_1} \cdot \cdots \cdot \partial x_d^{\alpha_d}$ for $x = (x_1, \ldots, x_d) \in R^d$.

It follows from (A2) that

$$\int u^\alpha \mathscr{K}(u)\,du = 0, \qquad 0 \le |\alpha| \le k-1, \tag{A.5}$$

$$\int u^\alpha \mathscr{K}(u)\,du = \begin{cases} 0, & |\alpha| = k,\ \mathrm{card}\{j:\ \alpha_j \ne 0\} > 1, \\ d_K, & |\alpha| = k,\ \mathrm{card}\{j:\ \alpha_j \ne 0\} = 1. \end{cases}$$

From (A.3)–(A.5) we get

$$\begin{aligned}
&\mathrm{E}(\mathscr{K}'h(x - X_1)) \\
&= -f'(x) - \frac{1}{k!} h^k (-1)^k \sum_{\alpha:|\alpha|=k} \begin{pmatrix} \partial^{|\alpha|+1} f(x)/\partial x_1 \partial x^\alpha \\ \vdots \\ \partial^{|\alpha|+1} f(x)/\partial x_d \partial x^\alpha \end{pmatrix} \\
&\quad \times \int u^\alpha \mathscr{K}(u)\,\mathrm{d}u - \beta_1(h, x) \qquad \text{(A.6)} \\
&= -f'(x) - h^k S_K(x) - \beta_1(h, x),
\end{aligned}$$

which proves (A.1). To get (A.2) note that by (A.1)

$$\begin{aligned}
\dot{q} &= \mathrm{E}(m(X_1)\mathscr{K}'_h(X_1 - X_2)) \\
&= \mathrm{E}(m(X_1)\,\mathrm{E}_{X_2}(\mathscr{K}'_h(X_1 - X_2)) \\
&= \mathrm{E}(m(X_1)\,(-f'(X_1) - h^k S_K(X_1) - \beta_1(h, X_1))) \\
&= \delta^* - h^k \int S_K(x) f(x)\, m(x)\,\mathrm{d}x - \int m(x) f(x)\, \beta_1(h, x)\,\mathrm{d}x.
\end{aligned}$$

Now, $\sup_x |\beta_1(h, x)| = \mathrm{o}(h^k)$, and $\int m(x) f(x)\,\mathrm{d}x < \infty$ since m and f are bounded on the compact support of f. This proves (A.2).

Lemma 2. Let assumptions (A1)–(A4) be satisfied. Then

$$\mathrm{E}(|\mathscr{K}'_h(x - X_1)|^2) = C_K f(x) h^{-d-2} + \beta_3(h, x),$$

where $\sup_x |\beta_3(h, x)| = \mathrm{o}(h^{-d-2})$, $h \to 0$.

Proof.

$$\begin{aligned}
\mathrm{E}(|\mathscr{K}'_h(x - X_1)|^2) &= \frac{1}{h^{2d+2}} \int \left| \mathscr{K}'\left(\frac{x - z}{h}\right) \right|^2 f(z)\,\mathrm{d}z \\
&= \frac{1}{h^{d+2}} \int |\mathscr{K}'(u)|^2 f(x - uh)\,\mathrm{d}u.
\end{aligned}$$

It follows from (A3) that f is Lipschitz continuous on its support with some Lipschitz constant L_f. Thus,

$$\left|\frac{1}{h^{d+2}}\int|\mathscr{K}'(u)|^2 f(x-uh)\,\mathrm{d}u-\frac{1}{h^{d+2}}f(x)\,C_K\right|\le\frac{L_f}{h^{d+1}}\int|\mathscr{K}'(u)|^2\,|u|\,\mathrm{d}u.$$

This proves the lemma.

Lemma 3. Let assumptions (A1)–(A4) be satisfied. Then

$$\mathrm{E}(m(X_1)\mathscr{K}_h'(x-X_1))=-(m(x)f(x))'-h^k S_{1K}(x)-\beta_4(h,x),$$

where

$$S_{1K}(x)=d_K\frac{(-1)^k}{k!}\sum_{j=1}^{d}\begin{pmatrix}\partial^{k+1}(f(x)m(x))/\partial x_1\partial x_j^k\\ \vdots\\ \partial^{k+1}(f(x)m(x))/\partial x_d\partial x_j^k\end{pmatrix}$$

and $\sup_x|\beta_4(h,x)=\mathrm{o}(h^k)$, $h\to 0$.

Proof. The proof is similar to the proof of (A.1). In fact, instead of (A.3) we now have

$$\begin{aligned}\mathrm{E}(m(X_1)\mathscr{K}_h'(x-X_1))&=\int(f(x-uh)m(x-uh))'\mathscr{K}(u)\,\mathrm{d}u\\&=-\int[f'(x-uh)\,m(x-uh)\\&\qquad+f(x-uh)m'(x-uh)]\,\mathscr{K}(u)\,\mathrm{d}u.\end{aligned}$$

Lemma 4. Let assumptions (A1)–(A4) be satisfied. Then, as $h\to 0$,

$$\begin{aligned}B_1=&\int|m'(x)|^2 f(x)\,\mathrm{d}x+\int m^2(x)|f'(x)|^2 f(x)\,\mathrm{d}x\\&+2\int m(x)\,(m'(x),f'(x))\,f^2(x)\,\mathrm{d}x+\mathrm{O}(h^k),\end{aligned}\tag{A.7}$$

$$\begin{aligned}B_2=&-\int m^2(x)|f'(x)|^2 f(x)\,\mathrm{d}x\\&-\int m(x)\,(m'(x),f'(x))\,f^2(x)\,\mathrm{d}x+\mathrm{O}(h^k),\end{aligned}\tag{A.8}$$

$$B_3=\frac{1}{h^{d+2}}\left(C_K\int m^2(x)f^2(x)\,\mathrm{d}x+\mathrm{o}(1)\right).\tag{A.9}$$

Proof. By Lemma 3,

$$B_1 = \int f(x)|\mathrm{E}(m(X_1)\mathscr{K}_h'(X_1 - x))|^2 \,\mathrm{d}x$$

$$= \int f(x)|(m(x)f(x))' + h^k S_{1K}(x) + \beta_4(x, h)|^2 \,\mathrm{d}x$$

$$= \int f(x)|(m(x)f(x))'|^2 \,\mathrm{d}x + \mathrm{O}(h^k),$$

which gives (A.7).

Using Lemmas 1 and 3 and the antisymmetric property of $\mathscr{K}_h'$, we get

$$B_2 = \int m(x)m(y)(\mathscr{K}_h'(x-y), \mathscr{K}_h'(y-z))f(x)f(y)f(z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$= \int f(y)m(y)\left(\int \mathscr{K}_h'(x-y)f(x)\,m(x)\,\mathrm{d}x, \int f(z)\mathscr{K}_h'(y-z)\,\mathrm{d}z\right)\mathrm{d}y$$

$$= \int f(y)m(y)\,((m(y)f(y))' + h^k S_{1K}(y) + \beta_4(h, y),$$

$$-f'(y) - h^k S_K(y) - \beta_1(h, y))\,\mathrm{d}y$$

$$= -\int f(y)m(y)\,((m(y)f(y))', f'(y))\,\mathrm{d}y.$$

This proves (A.8). To prove (A.9) note that with $w = (x-y)/h$ we have

$$B_3 = \int m(x)m(y)f(x)f(y)|\mathscr{K}_h'(x-y)|^2\,\mathrm{d}x\,\mathrm{d}y$$

$$= -\frac{1}{h^{d+2}}\int m(y)f(y)m(y+wh)f(y+wh)|\mathscr{K}_h'(w)|^2\,\mathrm{d}y\,\mathrm{d}w.$$

It follows from assumptions (A3) and (A4) that f and m are Lipschitz continuous on the support of f. Hence

$$B_3 = -\frac{1}{h^{d+2}}\left[\int m^2(y)f^2(y)\,\mathrm{d}y \int |\mathscr{K}_h'(w)|^2\,\mathrm{d}w(1 + \mathrm{O}(h))\right],$$

and (A.9) follows.

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