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Local Polynomial Kernel Regression for Generalized Linear Models and Quasi-Likelihood Functions

Jianqing FAN, Nancy E. HECKMAN, and M. P. WAND*

We investigate the extension of the nonparametric regression technique of local polynomial fitting with a kernel weight to generalized linear models and quasi-likelihood contexts. In the ordinary regression case, local polynomial fitting has been seen to have several appealing features in terms of intuitive and mathematical simplicity. One noteworthy feature is the better performance near the boundaries compared to the traditional kernel regression estimators. These properties are shown to carry over to generalized linear model and quasi-likelihood settings. We also derive the asymptotic distributions of the proposed class of estimators that allow for straightforward interpretation and extensions of state-of-the-art bandwidth selection methods.

KEY WORDS: Bandwidth; Boundary effects; Local likelihood; Logistic regression; Nonparametric regression; Poisson regression.

1. INTRODUCTION

Generalized linear models were introduced by Nelder and Wedderburn (1972) as a means of applying techniques used in ordinary linear regression to more general settings. In an important further extension, first considered by Wedderburn (1974), the log-likelihood is replaced by a quasi-likelihood function, which requires only specification of a relationship between the mean and variance of the response. There are, however, many examples where ordinary least squares fails to produce a consistent procedure when the variance function depends on the regression function itself, so that a likelihood criterion is more appropriate. Variance functions that depend on the mean function occur in logit regression, log-linear models, and constant coefficient of variation models, for example.

McCullagh and Nelder (1988) gave an extensive account of the analysis of parametric generalized linear models. A typical parametric assumption is that some transformation of the mean of the response variable, usually called the link function, is linear in the covariates. In ordinary regression with a single covariate, this assumption corresponds to the scatterplot of the data being adequately fit by a straight line. But many scatterplots that arise in practice are not adequately fit by straight lines and other simple parametric curves. This has led to the proposal and analysis of several nonparametric regression techniques, sometimes called *scatterplot smoothers* (see, for example, Eubank 1988, Härdle 1990, and Wahba 1990). The same deficiencies of parametric modeling in ordinary regression apply to generalized linear models.

In this article we investigate the generalization of local polynomial fitting with kernel weights. We are motivated by the fact that local polynomial kernel estimators are both intuitively and mathematically simple, which allows for a

deeper understanding of their performance. Figure 1 shows how one version of the local polynomial kernel estimator works for a particular example. The scatterplot in Figure 1b corresponds to the proportions of surviving babies for 21 different birthweights, rounded to the nearest half kilogram. The data were taken from Karn and Penrose (1951). A local linear kernel estimator of the probability of survival for a given birthweight x is given by the solid curve. Figure 1a shows how this estimate was constructed. In this figure the scatterplot points correspond to the logit transforms of the proportions. The dashed curves show how the estimate was obtained at two particular values of x . At $x = 6$ a straight line was fitted to the log counts using a weighted version of the binomial log-likelihood where the weights correspond to the relative heights of the kernel function, which in this case is a scaled normal density function centered about $x = 6$ and is shown at the base of the plot. The estimate at this point is the height of the line above $x = 6$. For estimation at the second point, $x = 10$, the same principle is applied with the kernel function centered about $x = 10$. This process is repeated at all points x at which an estimate is required. The estimate of the probability itself is obtained by applying the inverse link function, in this case the standard logistic distribution function, to the kernel smooth in Figure 1a.

There have been several other proposals for extending nonparametric regression estimators to the generalized case. Extensions of smoothing spline methodology have been studied by Green and Yandell (1985), O'Sullivan, Yandell and Raynor (1986), and Cox and O'Sullivan (1990). Tibshirani and Hastie (1987) based their generalization on the "running lines" smoother. Staniswalis (1989) carried out a similar generalization of the Nadaraya-Watson kernel estimator (Nadaraya 1964; Watson 1964), which is equivalent to local constant fitting with a kernel weight.

In an important further extension of the generalized linear model, one needs only to model the conditional variance of the response variable as an arbitrary but known function of the conditional mean. This has led to the proposal of quasi-likelihood methods (McCullagh and Nelder 1988, chap. 9; Wedderburn 1974). Optimal properties of the quasi-likelihood methods have received considerable attention in

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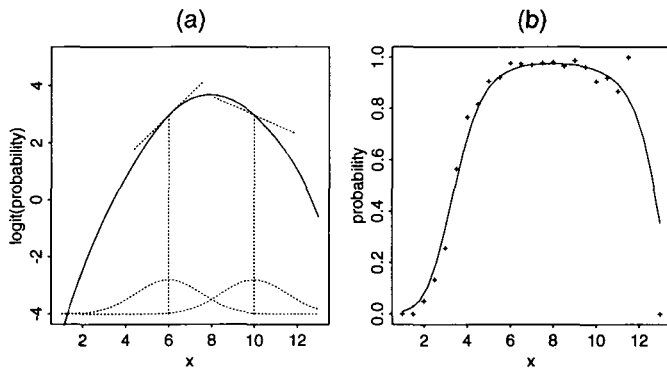


Figure 1. Estimates for Birthweight Data. (a) Illustration of how the kernel smoothing is done to estimate the logit of the probability of survival at points $x = 6$ and 10 . In each case the estimate is obtained by fitting a line to the data by maximum weighted conditional log-likelihood. The weights are with respect to the kernel function centered about x , shown at the base of the figure for these two values of x (dotted curves). (b) Local linear kernel estimate of the conditional probability of survival for a given birthweight, found by applying the inverse logit transformation to the estimate shown in (a). The plus signs show the proportion of surviving babies for a given birthweight.

the literature (see, for example, Cox 1983 and Godambe and Heyde 1987 and references therein).

The aforementioned kernel smoothing ideas can be easily extended to the case where a quasi-likelihood function is used, so we present our results at this level of generality. If the distribution of the responses is from an exponential family, then quasi-likelihood estimation with a correctly specified variance function is equivalent to maximum likelihood estimation. Thus results for exponential family models follow directly from those for quasi-likelihood estimation. Severini and Staniswalis (1992) considered quasi-likelihood estimation using locally constant fits, and Hunsberger (1993) studied semiparametric extensions of such estimators. Gu (1990) used adaptive smoothing splines for smooth quasi-likelihood estimation.

In the case of normal errors, quasi-likelihood and least squares techniques coincide. Thus the results presented here are a generalization of those for the local least squares kernel estimator for ordinary regression considered by Fan (1992, 1993) and by Ruppert and Wand (1994). These authors showed that in the ordinary regression context, local polynomial kernel regression has several attractive mathematical properties. This is particularly true when the polynomial is of odd degree, because the asymptotic bias near the boundary of the support of the covariates can be shown to be of the same order of magnitude as that of the interior. Because in applications the boundary region will often include 20% or more of the data, this is a very appealing feature. This is not the case for the Nadaraya–Watson kernel estimator, because it corresponds to degree-zero fitting. In addition, the asymptotic bias of odd-degree polynomial fits at a point x depends on x only through a higher-order derivative of the regression function itself, which allows for simple interpretation and expressions for the asymptotically optimal bandwidth. We are able to show that these properties carry over to generalized linear models.

When fitting local polynomials, an important choice is the degree of the polynomial. Boundary bias considerations indicate that one should, at the least, fit local lines. But for estimating regions of high curvature of the true function, such as at peaks and valleys, local line estimators can have a substantial amount of bias. This problem can be alleviated by fitting higher-degree polynomials such as quadratics and cubics, although there are costs in terms of increased variance and computational complexity that need to be considered. Nevertheless, in many examples that we have tried we have noticed that gains can often be made using higher-degree fits, and this is our main motivation for extending beyond linear fits.

A related approach to nonparametric regression in generalized linear models has been recently proposed by Weisberg and Welsh (1992). These authors considered kernel estimation of the link function.

In the related context of nonparametric robust regression, Tsybakov (1986) used local polynomial fitting as a device and established the asymptotic normality of such a procedure. Interesting minimax results found in this work support the wide applicability of the local polynomial approach.

In Section 2 we present some notation for the generalized linear model and quasi-likelihood functions. In Section 3 we deal with the locally weighted maximum quasi-likelihood approach to local polynomial fitting. We discuss the problem of choosing the bandwidth in Section 4. We present a real data example in Section 5, and a summary of our findings and further discussion in Section 6.

2. GENERALIZED LINEAR MODELS AND QUASI-LIKELIHOOD FUNCTIONS

In our definition of generalized linear models and quasi-likelihood functions, we will follow the notation of McCullagh and Nelder (1988). Let $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$ be a set of independent random pairs where, for each i , Y_i is a scalar response variable and \mathbf{X}_i is an \mathbb{R}^d -valued vector of covariates having density f with support $\text{supp}(f) \subseteq \mathbb{R}^d$. Let (\mathbf{X}, Y) denote a generic member of the sample. Then we will say that the conditional density of Y given $\mathbf{X} = \mathbf{x}$ belongs to a one-parameter exponential family if

$$f_{Y|\mathbf{X}}(y|\mathbf{x}) = \exp\{y\theta(\mathbf{x}) - b(\theta(\mathbf{x})) + c(y)\}$$

for known functions b and c . The function θ is usually called the canonical or natural parameter. In parametric generalized linear models it is usual to model a transformation of the regression function $\mu(\mathbf{x}) = E(Y|\mathbf{X} = \mathbf{x})$ as linear; that is,

$$\eta(\mathbf{x}) = \beta_0 + \sum_{i=1}^d \beta_i x_i, \quad \text{where } \eta(\mathbf{x}) = g(\mu(\mathbf{x}))$$

and g is the link function. If $g = (b')^{-1}$, then g is called the canonical link, because $b'(\theta(\mathbf{x})) = \mu(\mathbf{x})$. A further noteworthy result for the one-parameter exponential family is $\text{var}(Y|\mathbf{X} = \mathbf{x}) = b''(\theta(\mathbf{x}))$.

A simple example of this setup arises when the Y_i are binary variables, in which case it is easily shown that

$$f_{Y|\mathbf{X}}(y|\mathbf{x}) = \exp\{y \ln(\mu(\mathbf{x})/(1 - \mu(\mathbf{x}))) + \ln(1 - \mu(\mathbf{x}))\}.$$

The canonical parameter in this case is $\theta(\mathbf{x}) = \text{logit}(\mu(\mathbf{x}))$, and the logit function is the canonical link. But one can assume that $\eta(\mathbf{x}) = g(\mu(\mathbf{x}))$ is linear where g is any increasing function on $(0, 1)$. Common examples include $g(u) \doteq \Phi^{-1}(u)$, where Φ is the standard normal distribution function, and $g(u) = \ln\{-\ln(1-u)\}$. These are often referred to as the *probit* link and the *complementary log-log link*. The conditional density $f_{Y|\mathbf{X}}$ can be written in terms of η as

$$f_{Y|\mathbf{X}}(y|\mathbf{x}) = \exp[y(g \circ b')^{-1}(\eta(\mathbf{x})) - b\{(g \circ b')^{-1}(\eta(\mathbf{x}))\} + c(y)],$$

where \circ denotes function composition.

There are many practical circumstances in which even though the full likelihood is unknown, one can specify the relationship between the mean and variance. In this situation estimation of the mean can be achieved by replacing the conditional log-likelihood $\ln f_{Y|\mathbf{X}}(y|\mathbf{x})$ by a *quasi-likelihood function* $Q(\mu(\mathbf{x}), y)$. If the conditional variance is modeled as $\text{var}(Y|\mathbf{X} = \mathbf{x}) = V(\mu(\mathbf{x}))$ for some known positive function V , then the corresponding quasi-likelihood function $Q(w, y)$ satisfies

$$\frac{\partial}{\partial w} Q(w, y) = \frac{y - w}{V(w)} \quad (1)$$

(McCullagh and Nelder 1988, chap. 9; Wedderburn 1974). The quasi-score (1) possesses properties similar to those of the usual likelihood score function. That is, it satisfies the first two moment conditions of Bartlett's identities. Quasi-likelihood methods behave analogously to the usual likelihood methods and thus are reasonable substitutes when the likelihood function is not available. Note that the log-likelihood of the one-parameter exponential family is a special case of a quasi-likelihood function with $V = b'' \circ (b')^{-1}$.

3. LOCALLY WEIGHTED MAXIMUM QUASI-LIKELIHOOD

3.1 Single Covariate Case

Because of the quasi-likelihood's generality, we will present our results in this context. Results for the exponential family and generalized linear models follow as a special case. We will introduce the idea of local polynomial fitting for the case where $d = 1$. Multivariate extensions will be discussed in Section 3.2.

As we mentioned in the preceding section, the typical parametric approach to estimating $\mu(x)$ is to assume that $\eta(x) = g(\mu(x))$ is a linear function of x , say $\eta(x) = \beta_0 + \beta_1 x$. An obvious extension of this idea is to suppose that $\eta(x) = \beta_0 + \dots + \beta_p x^p$; that is, $\eta(x)$ is a p th degree polynomial in x . One would then estimate $\beta = (\beta_0, \dots, \beta_p)^T$ by maximizing the quasi-likelihood

$$\sum_{i=1}^n Q(g^{-1}(\beta_0 + \dots + \beta_p X_i^p), Y_i). \quad (2)$$

To enhance the flexibility of the fitted curve, the number of parameters $(p + 1)$ is typically large. But this means that the estimated coefficients are subject to large variability. Also,

there is a greater threat of numerical instability caused by an ill-conditioned design matrix.

A more appealing approach is to estimate $\eta(x)$ by *locally* fitting a low-degree polynomial at x , (e.g., $p = 1$ or 3). This involves centering the data about x and weighting the quasi-likelihood in such a way that it places more emphasis on those observations closest to x . The estimate of $\eta(x)$ is then the height of the local polynomial fit. There are many possible strategies for weighting the conditional quasi-likelihood (see Hastie and Tibshirani 1990, chap. 2 for several of these). Because of their mathematical simplicity, we will use kernel weights. Let K be a symmetric probability density having compact support, and let $K_h(z) = K(z/h)/h$ be a rescaling of K . The parameter $h > 0$ is usually called the *bandwidth* or *window width* and in the mathematical analysis will be taken to be a sequence that depends on n . Each observation in the quasi-likelihood is given the weight $K_h(X_i - x)$. The local polynomial kernel estimator of $\eta(x)$ is then given by

$$\hat{\eta}(x; p, h) = \hat{\beta}_0,$$

where $\hat{\beta} = (\hat{\beta}_0, \dots, \hat{\beta}_p)^T$ maximizes

$$\sum_{i=1}^n Q(g^{-1}(\beta_0 + \dots + \beta_p(X_i - x)^p), Y_i) K_h(X_i - x). \quad (3)$$

We will assume that the maximizer exists. This can be easily verified for standard choices of Q . The conditional mean $\mu(x)$ can then be estimated by applying the inverse of the link function to give

$$\hat{\mu}(x; p, h) = g^{-1}(\hat{\eta}(x; p, h)).$$

Note that in the case $p = 0$, the estimator for $\mu(x)$ is simply a weighted average,

$$\hat{\mu}(x; 0; h) = \sum_{i=1}^n K_h(X_i - x) Y_i / \sum_{i=1}^n K_h(X_i - x). \quad (4)$$

Although this estimator is simple and intuitive, it suffers serious drawbacks, including large boundary biases and low efficiency (Fan 1992).

The choice of the link function g is not as crucial as for parametric generalized linear models, because the fitting is localized. Indeed it is conceivable to dispense with the link function and just estimate $\mu(x)$ directly. But there are several drawbacks to having the link equal to the identity. An identity link may yield a quasi-likelihood that is not convex, allowing for the possibility of multiple maxima, inconsistency, and computational problems. Use of the canonical link guarantees convexity. Furthermore, the canonical link ensures that the final estimate has the correct range. For example, in the logistic regression context using the logit link leads to an estimate that is always a probability, whereas using the identity link does not. A final reason for preferring the canonical link is that the estimate of $\mu(x)$ approaches the usual parametric estimate as the bandwidth becomes large. This can be useful as a diagnostic tool.

Figure 1 and its accompanying discussion in Section 1 show how $\hat{\eta}(\cdot; p, h)$ and $\hat{\mu}(\cdot; p, h)$ are simple to understand intuitively. Notice that the bandwidth h governs the amount

of smoothing being performed. For h tending to zero, the estimate $\hat{\mu}(\cdot; p, h)$ will tend to interpolate the data, and its variance will increase. On the other hand, for increasing h , the estimate of η will tend towards the p th degree polynomial fit corresponding to (2), which in general corresponds to an increase in bias. This latter property is very appealing, because it means that the proposed estimators can be viewed as an extension of the traditional parametric approach.

Local polynomial fitting also provides consistent estimates of higher-order derivatives of η through the coefficients of the higher-order terms in the polynomial fit. Thus for $0 \leq r \leq p$, we can define the estimator of $\eta^{(r)}(x)$ to be

$$\hat{\eta}_r(x; p, h) = r! \hat{\beta}_r.$$

We will now investigate the asymptotic properties of $\hat{\eta}_r(x; p, h)$ and $\hat{\mu}(x; p, h)$. These are different for x lying in the interior of $\text{supp}(f)$ than for x lying near the boundary. Suppose that K is supported on $[-1, 1]$. Then the support of $K_h(x - \cdot)$ is $\mathcal{E}_{x,h} = \{z : |z - x| \leq h\}$. We will call x an interior point of $\text{supp}(f)$ if $\mathcal{E}_{x,h} \subseteq \text{supp}(f)$ and a boundary point otherwise. If $\text{supp}(f) = [a, b]$, then x is a boundary point if and only if $x = a + \alpha h$ or $x = b - \alpha h$ for some $0 \leq \alpha < 1$. Finally, let $\mathcal{D}_{x,h} = \{z : x - hz \in \text{supp}(f)\} \cap [-1, 1]$. Then x is an interior point if and only if $\mathcal{D}_{x,h} = [-1, 1]$.

For any measurable let $\mathcal{A} \in \mathbb{R}$, define $\nu_j(\mathcal{A}) = \int_{\mathcal{A}} z^j K(z) dz$. Let $\mathbf{N}_p(\mathcal{A})$ be the $(p + 1) \times (p + 1)$ matrix having (i, j) entry equal to $\nu_{i+j-2}(\mathcal{A})$ and let $\mathbf{M}_{r,p}(z; \mathcal{A})$ be the same as $\mathbf{N}_p(\mathcal{A})$, but with the $(r + 1)$ st column replaced by $(1, z, \dots, z^p)^T$. Then for $|\mathbf{N}_p(\mathcal{A})| \neq 0$, define

$$K_{r,p}(z; \mathcal{A}) = r! \{ |\mathbf{M}_{r,p}(z; \mathcal{A})| / |\mathbf{N}_p(\mathcal{A})| \} K(z). \quad (5)$$

In the case where $\mathcal{A} \supseteq [-1, 1]$, we will suppress the \mathcal{A} and simply write $\nu_l, \tau_l, \mathbf{N}_p, \mathbf{M}_{r,p}$, and $K_{r,p}$. One can show that $(-1)^r K_{r,p}$ is an order (r, s) kernel as defined by Gasser, Müller, and Mammitzsch (1985), where $s = p + 1$ if $p - r$ is odd and $s = p + 2$ if $p - r$ is even. This family of kernels

is useful for giving concise expressions for the asymptotic distribution of $\hat{\eta}_r(x; p, h)$ for x lying both in the interior of $\text{supp}(f)$ and near its boundaries. Also, let

$$\rho(x) = \{g'(\mu(x))^2 V(\mu(x))\}^{-1}.$$

Note that when the model belongs to a one-parameter exponential family and the canonical link is used, then $g'(\mu(x)) = 1/\text{var}(Y|X = x)$ and $\rho(x) = \text{var}(Y|X = x)$, if the variance V is correctly specified. The asymptotic variance of $\hat{\eta}_r(x; p, h)$ will depend on quantities of the form

$$\sigma_{r,p}^2(x; K, \mathcal{A}) = \text{var}(Y|X = x) g'(\mu(x))^2 f(x)^{-1} \times \int_{\mathcal{A}} K_{r,p}(z; \mathcal{A})^2 dz.$$

Again, this will be abbreviated to $\sigma_{r,p}^2(x; K)$ when $\mathcal{A} \supseteq [-1, 1]$. The following theorems are proved in the Appendix.

Theorem 1a. Let $p - r > 0$ be odd and suppose that Conditions 1-5 stated in the Appendix are satisfied. Assume that $h = h_n \rightarrow 0$ and $nh^3 \rightarrow \infty$ as $n \rightarrow \infty$. If x is a fixed point in the interior of $\text{supp}(f)$, then

$$\sqrt{nh^{2r+1}} \sigma_{r,p}(x; K)^{-1} \times \left[\hat{\eta}_r(x; p, h) - \eta^{(r)}(x) - \left\{ \int z^{p+1} k_{r,p}(z) dz \right\} \left\{ \frac{\eta^{(p+1)}(x)}{(p+1)!} \right\} h^{p-r+1} \{1 + O(h)\} \right] \rightarrow_D N(0, 1). \quad (6)$$

If $x = x_n$ is of the form $x = x_\delta + ch$, where x_δ is a point on the boundary of $\text{supp}(f)$ and $c \in [-1, 1]$, then (6) holds with $\sigma_{r,p}^2(x; K)$ and $\int z^{p+1} K_{r,p}(z) dz$ replaced by $\sigma_{r,p}^2(x; K, \mathcal{D}_{x,h})$ and $\int_{\mathcal{D}_{x,h}} z^{p+1} K_{r,p}(z; \mathcal{D}_{x,h}) dz$.

Theorem 1b. Let $p - r \geq 0$ be even and $p > 0$ and suppose that Conditions 1-5 stated in the Appendix are satisfied. Assume that $h = h_n \rightarrow 0$ and $nh^3 \rightarrow \infty$ as $n \rightarrow \infty$. If x is a fixed point in the interior of $\text{supp}(f)$, then

$$\sqrt{nh^{2r+1}} \sigma_{r,p}(x; K)^{-1} \left(\hat{\eta}_r(x; p, h) - \eta^{(r)}(x) - \left[\left\{ \int z^{p+2} K_{r,p}(z) dz \right\} \left\{ \frac{\eta^{(p+2)}(x)}{(p+2)!} \right\} + \left\{ \int z^{p+2} K_{r,p}(z) dz - r \int z^{p+1} K_{r-1,p}(z) dz \right\} \left\{ \frac{\eta^{(p+1)}(x)(\rho f)'(x)}{(\rho f)(x)(p+1)!} \right\} \right] h^{p-r+2} \{1 + O(h)\} \right) \rightarrow_D N(0, 1). \quad (7)$$

If $x = x_n$ is of the form $x = x_\delta + ch$, where x_δ is a point on the boundary of $\text{supp}(f)$ for some $c \in [-1, 1]$, then

$$\sqrt{nh^{2r+1}} \sigma_{r,p}(x; K, \mathcal{D}_{x,h})^{-1} \times \left[\hat{\eta}_r(x; p, h) - \eta^{(r)}(x) - \left\{ \int_{\mathcal{D}_{x,h}} z^{p+1} K_{r,p}(z) dz \right\} \times \left\{ \frac{\eta^{(p+1)}(x)}{(p+1)!} \right\} h^{p-r+1} \{1 + O(h)\} \right] \rightarrow_D N(0, 1). \quad (8)$$

For $p = 0$, (8) remains valid and the following modification of (7) holds:

$$\sqrt{nh} \sigma_{0,0}(x; K)^{-1} \times \left(\hat{\eta}_0(x; 0, h) - \eta(x) - h^2 \int z^2 K(z) dz \times \left[\frac{\mu''(x)}{2} + \frac{\mu'(x)f'(x)}{f(x)} \right] g'(\mu(x)) + o(h^2) \right) \rightarrow_D N(0, 1).$$

Remark 1. Although Theorem 1 describes the asymptotic behavior of $\hat{\eta}_r(x; p, h)$ for general r , it is the case $r = 0$, which corresponds to the estimation of η itself, that is of primary interest. The expressions involving $\int z^{j+1} K_{r,p}(z) dz$ and $\sigma_{r,p}^2(x; K)$ can be interpreted as the asymptotic bias and asymptotic variance of $\hat{\eta}(x; p, h)$. Notice that for odd p , the

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asymptotic bias is of the same order of magnitude near the boundary as in the interior. Indeed, the asymptotic mean squared error (AMSE) of $\hat{\eta}(x; p, h)$ is a continuous function of c . These mathematical quantifications of boundary bias are not a serious problem for odd-degree polynomial fits. The asymptotic bias and variance can be combined to give the AMSE of $\hat{\eta}(x; p, h)$ for interior points as

$$\begin{aligned} \text{AMSE} \{ \hat{\eta}(x; p, h) \} &= \left\{ \int z^{p+1} K_{0,p}(z) dz \right\}^2 \left\{ \frac{\eta^{(p+1)}(x)}{(p+1)!} \right\}^2 h^{2p+2} \\ &\quad + \sigma_{0,p}^2(x; K) n^{-1} h^{-1} \end{aligned}$$

for p odd and

$$\begin{aligned} \text{AMSE} \{ \hat{\eta}(x; p, h) \} &= \left\{ \int z^{p+2} K_{0,p}(z) dz \right\}^2 \\ &\quad \times \left\{ \frac{(\rho f)'(x) \eta^{(p+1)}(x)}{(\rho f)(x)(p+1)!} + \frac{\eta^{(p+2)}(x)}{(p+2)!} \right\}^2 h^{2p+4} \\ &\quad + \sigma_{0,p}^2(x; K) n^{-1} h^{-1} \end{aligned}$$

for p even and nonzero. Note that the bandwidth that minimizes $\text{AMSE} \{ \hat{\eta}(x; p, h) \}$ is of order $n^{-1/(2p+3)}$ for p odd and of order $n^{-1/(2p+5)}$ for p even. For a given sequence of bandwidths, the asymptotic variance is always $O(n^{-1}h^{-1})$, whereas the order of the bias tends to decrease as the degree of the polynomial increases. For instance, a linear fit gives bias of order h^2 , a quadratic fit gives bias of order h^4 , and a cubic gives bias of order h^4 . Therefore, there is a significant reduction in bias for quadratic or cubic fits compared to linear fits, particularly when estimating η at peaks and valleys, where typically $\eta''(x) \neq 0$. But it should also be realized that if globally optimal bandwidths are used, then it is possible for local linear fits to outperform higher-degree fits, even at peaks and valleys. This point was made visually by Marron (1992) in a closely related context.

With even-degree polynomial fits, the boundary bias dominates the interior bias and boundary kernels are required to make their asymptotic orders the same. This is not the case for odd-degree polynomial fits. Furthermore, the expression for the interior bias for even-degree fits is complicated, involving three derivatives of η instead of just one derivative. Therefore, we do not recommend using even-degree fitting. (For further discussion of this matter, see Fan and Gijbels 1992.)

Remark 2. Staniswalis (1989) and Severini and Staniswalis (1992) have considered the case for the local constant fit ($p = 0$) by using the explicit formula (4). But significant gains can be made by using local linear or higher-order fits, especially near the boundaries.

Remark 3. In the Appendix we actually derive the asymptotic joint distribution of the $\hat{\eta}_r(x; p, h)$ for all $r \leq p$. In addition, we are able to give expressions for the second-order bias terms in (6) and (8).

Remark 4. Because of the localness of the fitting, Theorems 1a and 1b hold regardless of whether or not V correctly

models the conditional variance. When estimating $\eta(x)$ with an odd-degree polynomial, as we recommend, the cost due to misspecification of the conditional variance is only of a second-order nature. That is, the asymptotic bias and variance in Theorem 1a do not depend on V .

Because $\hat{\mu}(x; p, h) = g^{-1}(\hat{\eta}(x; p, h))$, it is straightforward to derive the following.

Theorem 2. Under the conditions of Theorem 1, the error $\hat{\mu}(x; p, h) - \mu(x)$ has the same asymptotic behavior as $\hat{\eta}_0(x; p, h) - \eta(x)$ given in Theorem 1 with $r = 0$, except that the asymptotic bias is divided by $g'(\mu(x))$ and the asymptotic variance is divided by $g'(\mu(x))^2$.

Remark 5. Notice that the interior variance is asymptotic to

$$n^{-1} h^{-1} \text{var}(Y|X=x) f(x)^{-1} \int K_{0,p}(z)^2 dz.$$

The dependence of the asymptotic variance of $\hat{\mu}(x; p, h)$ on $\text{var}(Y|X=x) f(x)^{-1}$ reflects the intuitive notion that there is more variation in the estimate of the conditional mean for higher values of the conditional variance and regions of lower density of the covariate.

Example 1. Consider the case of a binary response variable with Bernoulli conditional likelihood. In this case $Q(w, y) = y \ln w + (1-y) \ln(1-w) = y \text{logit}(w) + \ln(1-w)$, and the canonical link is $g(u) = \text{logit}(u)$. For the canonical link with properly specified variance, we have $\rho(x) = \text{var}(Y|X=x) = \mu(x)\{1-\mu(x)\}$ and $\sigma_{r,p}^2(x; K, \mathcal{A}) = [\mu(x)\{1-\mu(x)\}f(x)]^{-1} \int_{\mathcal{A}} K_{r,p}(z; \mathcal{A})^2 dz$.

If the probit link $g(u) = \Phi^{-1}(u)$ is used instead, then we obtain $\rho(x) = [\mu(x)\{1-\mu(x)\}]^{-1} \phi(\Phi^{-1}(\mu(x)))^2$ and $\sigma_{r,p}^2(x; K, \mathcal{A}) = \mu(x)\{1-\mu(x)\} \phi(\Phi^{-1}(\mu(x)))^{-2} \int_{\mathcal{A}} K_{r,p}(z; \mathcal{A})^2 dz$, where ϕ is the standard normal density function.

Example 2. Consider the case of nonnegative integer response with Poisson conditional likelihood. In this case $Q(w, y) = y \ln w - w$, and the canonical link is $g(u) = \ln(u)$. For the canonical link with properly specified variance, we have $\rho(x) = \mu(x)$ and $\sigma_{r,p}^2(x; K, \mathcal{A}) = \{\mu(x)f(x)\}^{-1} \int_{\mathcal{A}} K_{r,p}(z; \mathcal{A})^2 dz$.

If instead the conditional variance is modeled as being proportional to the square of the conditional mean (i.e., $V(\mu(x)) = \gamma^2 \mu(x)^2$, where γ^2 is the coefficient of variation), then we have $Q(w, y) = (-y/w - \ln w)/\gamma^2$. If the logarithmic link is used, then we have $\rho(x) = 1/\gamma^2$ and $\sigma_{r,p}^2(x; K, \mathcal{A}) = \gamma^2 f(x)^{-1} \int_{\mathcal{A}} K_{r,p}(z; \mathcal{A})^2 dz$, provided that $V(\mu(x)) = \text{var}(Y|X=x)$.

3.2 Multiple Covariate Case

The extension of the local kernel estimator to the case of multiple covariates is straightforward for the important case of local linear fitting. The treatment of higher-degree polynomial fits in the multivariate case requires careful notation to keep the expressions simple. Higher-degree polynomial fits for multiple covariates can also be very computationally daunting, so we will concentrate on the local linear case in this section. For a flavor of asymptotic analyses of multivariate higher-order polynomial fits, see the work of Ruppert

and Wand (1994), which considers multivariate quadratic and cubic fits for the ordinary local least squares regression estimator.

A problem that must be faced when confronted with multiple covariates is the well-known “curse of dimensionality”—the fact that the performance of nonparametric smoothing techniques deteriorates as the dimensionality increases. One way of overcoming this problem is to assume that the model is additive in the sense that

$$\eta(\mathbf{x}) = \eta_1(x_1) + \dots + \eta_d(x_d),$$

where each η_i is a univariate function corresponding to the i th coordinate direction. This is the *generalized additive model* as described by Hastie and Tibshirani (1990), and it is recommended that each η_i be estimated by an appropriate scatterplot smoother. There are, however, many situations where the additivity assumption is not valid, in which case multivariate smoothing of the type presented in this section is appropriate.

Throughout this section we will take K to be a d -variate kernel with the properties that $\int K(\mathbf{z}) d\mathbf{z} = 1$, $\int \mathbf{z}\mathbf{z}^T K(\mathbf{z}) d\mathbf{z} = \nu_2 \mathbf{I}$, where $\nu_2 = \int_{\mathbb{R}^d} z_i^2 K(\mathbf{z}) d\mathbf{z}$ is nonzero and independent of i . In the multivariate case we define $K_{\mathbf{H}}(\mathbf{z}) = |\mathbf{H}|^{-1/2} K(\mathbf{H}^{-1/2}\mathbf{z})$, where \mathbf{H} is a positive definite matrix of bandwidths. The d -variate local linear kernel estimator of $\eta(\mathbf{x})$ is $\hat{\eta}(\mathbf{x}; \mathbf{H}) = \hat{\beta}_0$, where

$$\begin{aligned} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} &= \arg \max_{(\beta_0, \beta_1)^T} \\ &\times \sum_{i=1}^n Q(g^{-1}(\beta_0 + \beta_1^T(\mathbf{X}_i - \mathbf{x})), Y_i) K_{\mathbf{H}}(\mathbf{X}_i - \mathbf{x}). \end{aligned}$$

The corresponding estimator for $\mu(\mathbf{x})$ is $\hat{\mu}(\mathbf{x}; \mathbf{H}) = g^{-1}(\hat{\eta}(\mathbf{x}; \mathbf{H}))$.

Before giving the asymptotic distributions of these estimators, we need to extend some definitions to the multivariate setting. A point $x \in \mathbb{R}^d$ will be called an interior point of $\text{supp}(f)$ if and only if $\{\mathbf{z} : \mathbf{H}^{-1/2}(\mathbf{x} - \mathbf{z}) \in \text{supp}(K)\} \subseteq \text{supp}(f)$. The Hessian matrix of a η at a point \mathbf{x} will be denoted by $\mathcal{H}_{\eta}(\mathbf{x})$.

Theorem 3. Suppose that Conditions 1 and 3 in the Appendix are satisfied and that f and all entries of \mathcal{H}_{η} are continuous at \mathbf{x} . Also suppose that the $n^{-1}|\mathbf{H}|^{-3/2}$ and all entries of \mathbf{H} tend to zero in such a way that \mathbf{H} remains positive definite and the ratio of the largest to smallest eigenvalues of \mathbf{H} remains bounded. If x is an interior point of $\text{supp}(f)$, then

$$\begin{aligned} \sqrt{n|\mathbf{H}|^{-1/2}} \left\{ \text{var}(Y|\mathbf{X} = \mathbf{x}) g'(\mu(\mathbf{x}))^2 f(\mathbf{x})^{-1} \int K(\mathbf{z})^2 d\mathbf{z} \right\}^{-1/2} \\ \times [\hat{\eta}(\mathbf{x}; \mathbf{H}) - \eta(\mathbf{x}) - \frac{1}{2} \nu_2 \text{tr}\{\mathbf{H}\mathcal{H}_{\eta}(\mathbf{x})\} \{1 + o(1)\}] \rightarrow_D \\ N(0, 1). \end{aligned}$$

Theorem 4. Under the conditions of Theorem 3 and g^{-1} being differentiable, if \mathbf{x} is an interior point of $\text{supp}(f)$, then the error $\hat{\mu}(\mathbf{x}; \mathbf{H}) - \mu(\mathbf{x})$ has the same asymptotic normal distribution as $\hat{\eta}(\mathbf{x}; \mathbf{H}) - \eta(\mathbf{x})$ given in Theorem 3, except

that the bias is divided by $g'(\mu(\mathbf{x}))$ and the variance is divided by $g'(\mu(\mathbf{x}))^2$.

4. BANDWIDTH SELECTION

As is the case for all nonparametric curve estimators, the smoothing parameter (in this case the bandwidth) plays a very important role in the trade-off between reducing bias and variance. Often the user will be able to satisfactorily choose the bandwidth by eye; however, it is also desirable to have a reliable data-driven rule for selecting the value of h .

In simpler curve estimation settings, such as kernel density estimation, there has been considerable recent progress in the objective choice of the bandwidth. (See Park and Marron 1990 for a discussion and comparison of several of these developments.)

A straightforward bandwidth selection idea is that of cross-validation. The extension of this idea to the generalized linear model setting is trivial. But cross-validation performs poorly in simpler settings, exhibiting a large amount of sample variation, and this behavior carries over to this setting. Therefore, we do not view cross-validation as a sensible bandwidth selection rule for practice.

An alternative bandwidth selection idea that makes use of the results derived in Sections 2 and 3 is that based on “plugging in” estimates of unknown quantities to a formula for the asymptotically optimal bandwidth. This has been shown to be more stable in both theoretical and practical performance (see, for example, Park and Marron 1990 and Sheather and Jones 1991). Indeed, Fan and Marron (1992) showed that in the density estimation case, the plug-in selector is an asymptotically efficient method from a semi-parametric point of view. For odd-degree polynomial fits, the simplicity of the bias and variance expressions indicates that it would be reasonably straightforward to extend the plug-in ideas used in kernel density estimation to estimation of η and hence of μ . In the following suppose that p is odd. A convenient approximate error criterion for $\hat{\eta}(\cdot; p, h)$ is

$$\begin{aligned} \text{AMISE} \{ \hat{\eta}(\cdot; p, h) \} \\ &= h^{2p+2} \left\{ \int z^{p+1} K_{0,p}(z) dz \right\}^2 \\ &\times \int \left\{ \frac{\eta^{(p+1)}(x)}{(p+1)!} \right\}^2 f(x) w(x) dx + n^{-1} h^{-1} \\ &\times \int \sigma_{0,p}^2(x; K) f(x) w(x) dx. \end{aligned}$$

We will call this the asymptotic mean integrated squared error (AMISE), because it is obtained from the foregoing AMSE expression by integrating over $\text{supp}(f)$. The design density f and weight function w are included for stability purposes. With respect to this criterion, the optimal bandwidth is

$$h_{\text{AMISE}} = \left[\frac{\{(p+1)!\}^2 \int \sigma_{0,p}^2(x, K) f(x) w(x) dx}{(2p+2) \left\{ \int z^{p+1} K_{0,p}(z) dz \right\}^2 \left\{ \int \eta^{(p+1)}(x)^2 f(x) w(x) dx \right\} n} \right]^{1/(2p+3)} \quad (9)$$

A plug-in bandwidth selection rule that replaces the unknown quantities by other local polynomial kernel estimators would be a worthwhile future project. But it is also possible to use (9) to motivate “rough-and-ready” bandwidth selectors. For example, one could define \hat{h}_q to be the bandwidth obtained by replacing η in (9) by a q th-degree polynomial parametric fit, where $q \geq p + 1$. Although such a selector would not have any asymptotic optimality properties, it should return a bandwidth that is reasonable for a wide range of functions that arise in practice.

5. APPLICATION TO BURNS DATA

We applied the local linear estimate to a data set consisting of dispositions of burn victims and several covariates. The data were collected at the University of Southern California General Hospital Burn Center. The binary response variable Y is 1 for those victims who survive their burns and 0 otherwise. As a predictor, we used

$$X = \ln(\text{area of third-degree burn} + 1).$$

Because children have significantly smaller body areas, only the 435 adults (older than age 17 years) who suffered third-degree burns were considered in our study.

We applied the local linear kernel estimator with the Bernoulli likelihood and logit link function to these data. The kernel was the standard normal density. The maximization was performed using Newton–Raphson iteration. We used the data-driven bandwidth $\hat{h}_2 = 1.242$ as defined in the previous section. Figure 2 shows (a) the kernel estimate of $\eta(x) = \text{logit}\{P(Y = 1 | X = x)\}$ and (b) $\mu(x) = P(Y = 1 | X = x)$, the survival probability for a given third-degree burn area (measured in square centimeters). The plus signs represent the (jittered) data. As expected, the survival probability de-

creases, although Figure 2a suggests that this decrease is slightly nonlinear in the logit space.

6. DISCUSSION

We have shown that, besides simplicity, the class of polynomial kernel estimators has many attractive mathematical properties. This is especially true for low odd-degree polynomial fits, such as lines and cubics. Although we have shown the applicability of these estimators through real data examples, there is still room for further study of their practical implementation and performance. Two important issues that deserve further attention are fast computation of the estimator and automatic selection of the bandwidth. Fast computation could be achieved through adaptation of the binned kernel estimators that have been developed for fast computation of ordinary regression estimators (see, for example, Fan and Marron 1994 and Härdle and Scott 1992). The main idea involves discretization of the data on a fine, equally spaced mesh of grid points. This process, usually referred to as “binning,” involves replacing the original data by “grid counts.” The usual kernel estimators are then replaced by appropriate approximations based on the grid counts. The main gain is that the number of distinct kernel evaluations is typically much less than the number of grid points, which represents a substantial saving over direct computational methods. Bandwidth selection rules of the type considered by Park and Marron (1990) and Sheather and Jones (1991) could also be developed. The theory for estimating higher-order derivatives of η derived in this article would be important for this problem.

APPENDIX: PROOFS OF THEOREMS

For brevity, we derive the theorems for $p > 0$. The case $p = 0$ requires separate treatment and can be easily handled using the explicit formula for $\hat{\eta}(x; 0, h)$. From here on, assume that $p > 0$.

Because $\hat{\beta}$ is calculated using X_i near x , we would expect that $\hat{\beta}_0 + \hat{\beta}_1(X_i - x) + \dots + \hat{\beta}_p(X_i - x)^p \sim \eta(x) + \eta'(x)(X_i - x) + \dots + \eta^{(p)}(x)(X_i - x)^p/p!$.

Therefore, we would expect that $r! \hat{\beta}_r \rightarrow \eta^{(r)}(x)$. We thus study the asymptotics of

$$\hat{\beta}^* = (nh)^{1/2} \begin{bmatrix} \hat{\beta}_0 - \eta(x) \\ h \{ \hat{\beta}_1 - \eta'(x) \} \\ \vdots \\ h^p \{ p! \hat{\beta}_p - \eta^{(p)}(x) \} \end{bmatrix}$$

so that each component has the same rate of convergence. Let $\mathbf{Q}_p(\mathcal{A})$ and $\mathbf{T}_p(\mathcal{A})$ be the $(p+1) \times (p+1)$ matrices having (i, j) th entry equal to $v_{i+j-1}(\mathcal{A})$ and $\int_{\mathcal{A}} z^{i+j-2} K(z)^2 dz$. Also, define $\mathbf{D} = \text{diag}(1, 1/1!, \dots, 1/p!)$, $\Sigma_x(\mathcal{A}) = \rho(x) f(x) \mathbf{D} \mathbf{N}_p(\mathcal{A}) \mathbf{D}$,

$$\Gamma_x(\mathcal{A}) = \frac{f(x) \text{var}(Y | X = x)}{\{V(\mu(x))g'(\mu(x))\}^2} \mathbf{D} \mathbf{T}_p(\mathcal{A}) \mathbf{D},$$

$$\Lambda_x(\mathcal{A}) = (\rho f)'(x) \mathbf{D} \mathbf{Q}_p(\mathcal{A}) \mathbf{D},$$

$$a_{1,i}(\mathcal{A}) = \frac{\eta^{(p+1)}(x)}{(p+1)!} \int_{\mathcal{A}} z^{p+1} K_{i-1,p}(z; \mathcal{A}) dz,$$

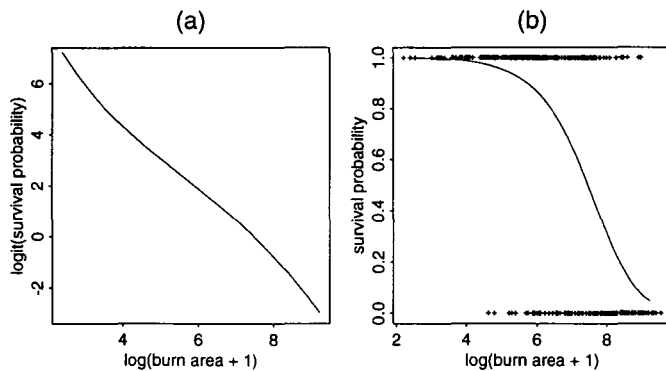


Figure 2. Estimates for Burns Data. (a) Local linear kernel estimate of logit $P(Y = 1 | X = x)$ for the burns data as described in the text. The number of observations is $n = 435$, and the bandwidth is $\hat{h}_2 = 1.24$. (b) Estimate of $P(Y = 1 | X = x)$ obtained from the estimate in (a) by application of the inverse logit transformation. The plus signs indicate the observed data and have been randomly jittered by $N(0, .2)$ variates for graphical display.

and

$$a_{2,i} = \frac{\partial^{(p+2)}(x)}{(p+2)!} \int_{\mathcal{A}} z^{p+2} K_{i-1,p}(z; \mathcal{A}) dz + \frac{\eta^{p+1}(x) (\rho f)'(x)}{(p+1)! (\rho f)(x)} \times \left\{ \int_{\mathcal{A}} z^{p+2} K_{i-1,p}(z; \mathcal{A}) dz - (i-1) \times \int_{\mathcal{A}} z^{p+1} K_{i-2,p}(z; \mathcal{A}) dz - \frac{1}{p!} \times \int_{\mathcal{A}} z^{p+1} K_{i-1,p}(z; \mathcal{A}) dz \int_{\mathcal{A}} z^{p+1} K_{p,p}(z; \mathcal{A}) dz \right\}.$$

Let $\mathbf{b}_x(\mathcal{A})$ be the $(p+1) \times 1$ vector having i th entry equal to $nh^{2p+3}a_{1,i} + nh^{2p+5}a_{2,i}$. Finally, let $q_i(x, y) = (\partial^i/\partial x^i)Q(g^{-1}(x), y)$. Note that q_i is linear in y for fixed x and that

$$q_1(\eta(x), \mu(x)) = 0 \quad \text{and} \quad q_2(\eta(x), \mu(x)) = -\rho(x). \quad (\text{A.1})$$

Conditions

1. The function $q_2(x, y) < 0$ for $x \in \mathbb{R}$ and y in the range of the response variable.
2. The functions $f', \eta^{(p+2)}, \text{var}(Y|X = \cdot), V'',$ and g''' are continuous.
3. For each $x \in \text{supp}(f), \rho(x), \text{var}(Y|X = x),$ and $g'(\mu(x))$ are nonzero.
4. The kernel K is a symmetric probability density with support $[-1, 1]$.
5. For each point x_∂ on the boundary of $\text{supp}(f)$, there exists an interval \mathcal{C} containing x_∂ having nonnull interior such that $\inf_{x \in \mathcal{C}} f(x) > 0$.

Condition 1 guarantees that $\{\hat{\beta}_n\}$, the sequence of maximizers of (3), lies in a compact set. Note that Condition 2 implies that $q_1, q_2, q_3, \rho',$ and μ' are continuous and that Conditions 1 and 3 imply that ρ is strictly positive over $\text{supp}(f)$. If the canonical link is used and if the variance is correctly specified, then Condition 1 holds. In this case Condition 1 is equivalent to $b'' > 0$, which holds because of $\text{var}(Y|X = x) = b''(\theta(x))$. If the variance is misspecified, then Condition 1 need not hold.

Theorems 1a and 1b are simple consequences of the following main theorem.

Main Theorem

Suppose that the foregoing conditions hold and that $h = h_n \rightarrow 0, nh^3 \rightarrow \infty$ as $n \rightarrow \infty$. If x is an interior point of $\text{supp}(f)$ and $p > 0$, then

$$\{\Sigma_x([-1, 1])^{-1} \Gamma_x([-1, 1]) \Sigma_x([-1, 1])^{-1}\}^{-1/2} \times \{\hat{\beta}^* - \mathbf{b}_x([-1, 1]) + o\{(nh^{2p+5})^{1/2}\}\} \rightarrow_D N(\mathbf{0}, \mathbf{I}_{p+1}).$$

If $x = x_n$, is of the form $x = x_\partial + hc$, where $c \in [-1, 1]$ is fixed and x_∂ is a fixed point on the boundary of $\text{supp}(f)$, then

$$\{\Sigma_x(\mathcal{D}_{x,h})^{-1} \Gamma_x(\mathcal{D}_{x,h}) \Sigma_x(\mathcal{D}_{x,h})^{-1}\}^{-1/2} \times \{\hat{\beta}^* - \mathbf{b}_x(\mathcal{D}_{x,h}) + o\{(nh^{2p+5})^{1/2}\}\} \rightarrow_D N(\mathbf{0}, \mathbf{I}_{p+1}).$$

The proof of the main theorem follows directly from Lemmas 1 and 2. The following lemma outlines the key idea of our proof.

Quadratic Approximation Lemma

Let $\{c_n(\theta): \theta \in \Theta\}$ be a sequence of random concave functions defined on a convex open subset Θ of \mathbb{R}^k . Let \mathbf{F} and \mathbf{G} be nonrandom matrices, with \mathbf{F} positive definite and \mathbf{U}_n a sequence of random

vectors that is stochastically bounded. Finally, let α_n be a sequence of constants tending to zero. Write $c_n(\theta) = U_n^T \theta - \frac{1}{2} \theta^T (\mathbf{F} + \alpha_n \mathbf{G}) \theta + f_n(\theta)$. If for each $\theta \in \Theta, f_n(\theta) = o_p(1)$, then $\hat{\theta}_n = \mathbf{F}^{-1} \mathbf{U}_n + o_p(1)$, where $\hat{\theta}_n$ (assumed to exist) maximizes c_n . If, in addition, $f'(\theta) = o_p(\alpha_n)$ uniformly in θ in a neighborhood of $\hat{\theta}$, then

$$\hat{\theta}_n = \mathbf{F}^{-1} \mathbf{U}_n - \alpha_n \mathbf{F}^{-1} \mathbf{G} \mathbf{F}^{-1} \mathbf{U}_n + o_p(\alpha_n).$$

Proof. The first statement follows from the convexity lemma (see, for example, Pollard 1991). Denote $\theta_0 = \mathbf{F}^{-1} \mathbf{U}_n$. Let $c'_n(\theta)$ and $c''_n(\theta)$ be the gradient and the Hessian matrix of $c_n(\theta)$. Taylor's expansion leads to

$$\mathbf{0} = c'_n(\hat{\theta}_n) = c'_n(\theta_0) + c''_n(\theta_0)(\hat{\theta}_n - \theta_0)\{1 + o_p(1)\},$$

so that

$$\begin{aligned} \hat{\theta}_n - \theta_0 &= -\{c''_n(\theta_0)\}^{-1} c'_n(\theta_0)\{1 + o_p(1)\} \\ &= (\mathbf{F} + \alpha_n \mathbf{G})^{-1} \{\mathbf{U}_n - (\mathbf{F} + \alpha_n \mathbf{G})\theta_0 + o_p(\alpha_n)\} \\ &\quad \times \{1 + o_p(1)\} \\ &= -\alpha_n \mathbf{F}^{-1} \mathbf{G} \mathbf{F}^{-1} \mathbf{U}_n + o_p(\alpha_n). \end{aligned}$$

The conclusion follows from the last display.

In the proofs of Lemmas 1 and 2 we will suppress the region of integration \mathcal{A} . If x is in the interior of $\text{supp}(f)$, then \mathcal{A} can be taken to be $[-1, 1]$. If $x = x_n$ is a boundary point, then $\mathcal{A} = \mathcal{D}_{x,h}$. For example, for x an interior point, $\int K_{r,p}(z)^2 dz$ will be shorthand for $\int_{-1}^1 K_{r,p}(z)^2 dz$, whereas for x a boundary point it will be shorthand for $\int_{\mathcal{D}_{x,h}} K_{r,p}(z; \mathcal{D}_{x,h})^2 dz$.

Lemma 1

Let $\bar{\eta}(x, u) = \eta(x) + \eta'(x)(u-x) + \dots + \eta^{(p)}(x)(u-x)^p/p!$,

$$\mathbf{Y}_i^* = q_1(\bar{\eta}(x, X_i), Y_i) K\{(X_i - x)/h\} \begin{bmatrix} 1 \\ (X_i - x)/h \\ \vdots \\ (X_i - x)^p/(h^p p!) \end{bmatrix} \quad \text{and} \quad \mathbf{W}_n = (nh)^{-1/2} \sum_{i=1}^n \mathbf{Y}_i^*.$$

Then, under the foregoing conditions,

$$\hat{\beta}^* = \Sigma_x^{-1} \mathbf{W}_n - h \Sigma_x^{-1} \Lambda_x \Sigma_x^{-1} \mathbf{W}_n + o_p(h).$$

Proof. Recall that $\hat{\beta}$ maximizes (3). Let

$$\beta^* = (nh)^{1/2} \begin{bmatrix} \beta_0 - \eta(x) \\ h\{\beta_1 - \eta'(x)\} \\ \vdots \\ h^p\{p!\beta_p - \eta^{(p)}(x)\} \end{bmatrix} \quad \text{and} \quad \mathbf{Z}_i = \begin{bmatrix} 1 \\ (X_i - x)/h \\ \vdots \\ (X_i - x)^p/(h^p p!) \end{bmatrix}.$$

Then $\beta_0 + \beta_1(X_i - x) + \dots + \beta_p(X_i - x)^p = \bar{\eta}(x, X_i) + a_n \beta^{*T} \mathbf{Z}_i$ where $a_n = (nh)^{-1/2}$. If $\hat{\beta}$ maximizes (3), then $\hat{\beta}^*$ maximizes $\sum_{i=1}^n Q(g^{-1}(\bar{\eta}(x, X_i) + a_n \beta^{*T} \mathbf{Z}_i), Y_i) K\{(X_i - x)/h\}$ as a function of β^* . To study the asymptotic properties of $\hat{\beta}^*$, we use the quadratic approximation lemma applied to the maximization of the normalized function

$$l_n(\beta^*) = \sum_{i=1}^n \{Q(g^{-1}(\bar{\eta}(x, X_i) + a_n \beta^{*T} \mathbf{Z}_i), Y_i) - Q(g^{-1}(\bar{\eta}(x, X_i)), Y_i)\} K\{(X_i - x)/h\}.$$

Then $\hat{\beta}^*$ maximizes l_n . We remark that Condition 1 implies that

l_n is concave in β^* . Using a Taylor series expansion of $Q(g^{-1}(\cdot), Y_i)$,

$$l_n(\beta^*) = a_n \sum_{i=1}^n q_1(\bar{\eta}(x, X_i), Y_i) \beta^{*T} \mathbf{Z}_i K\{(X_i - x)/h\} + \frac{a_n^2}{2} \sum_{i=1}^n q_2(\bar{\eta}(x, X_i), Y_i) (\beta^{*T} \mathbf{Z}_i)^2 K\{(X_i - x)/h\} + \frac{a_n^3}{6} \sum_{i=1}^n q_3(\eta_i, Y_i) (\beta^{*T} \mathbf{Z}_i)^3 K\{(X_i - x)/h\}, \quad (\text{A.2})$$

where η_i is between $\bar{\eta}(x, X_i)$ and $\bar{\eta}(x, X_i) + a_n \beta^{*T} \mathbf{Z}_i$.

Let $\mathbf{A}_n = a_n^2 \sum_{i=1}^n q_2(\bar{\eta}(x, X_i), Y_i) K\{(X_i - x)/h\} \mathbf{Z}_i \mathbf{Z}_i^T$. Then the second term in (A.2) equals $\frac{1}{2} \beta^{*T} \mathbf{A}_n \beta^*$. Now $(\mathbf{A}_n)_{ij} = (E\mathbf{A}_n)_{ij} + O_p\{\{\text{var}(\mathbf{A}_n)_{ij}\}^{1/2}\}$ and $E\mathbf{A}_n = h^{-1} E\{q_2(\bar{\eta}(x, X_1), \mu(X_1)) K\{(X_1 - x)/h\} \mathbf{Z}_1 \mathbf{Z}_1^T\}$. We will use a Taylor expansion of q_2 about $(\eta(X_1), \mu(X_1))$. Because $\text{supp}(K) = [-1, 1]$, we need only consider $|X_1 - x| \leq h$, and thus

$$\bar{\eta}(x, X_1) - \eta(X_1) = -\frac{\eta^{(p+1)}(x)}{(p+1)!} (X_1 - x)^{p+1} - \frac{\eta^{(p+2)}(x)}{(p+2)!} (X_1 - x)^{p+2} + o(h^{p+2}). \quad (\text{A.3})$$

Using the second result of (A.1), we obtain

$$(i-1)!(j-1)!(E\mathbf{A}_n)_{ij} = -(\rho f)(x) \nu_{i+j-2} - h(\rho f)'(x) \nu_{i+j-1} + o(h).$$

Similar arguments show that $\text{var}\{(\mathbf{A}_n)_{ij}\} = O\{(nh)^{-1}\}$ and that the last term in (A.2) is $O_p\{(nh)^{-1/2}\}$. Therefore, $l_n(\beta^*) = \mathbf{W}_n^T \beta^* - \frac{1}{2} \beta^{*T} (\boldsymbol{\Sigma}_x + h\boldsymbol{\Lambda}_x) \beta^* + o_p(h)$, because $nh^3 \rightarrow \infty$ and $h \rightarrow 0$. Similar arguments show that $l'_n(\beta^*) = \mathbf{W}_n - (\boldsymbol{\Sigma}_x + h\boldsymbol{\Lambda}_x) \beta^* + o_p(h)$ and $l''_n(\beta^*) = -(\boldsymbol{\Sigma}_x + h\boldsymbol{\Lambda}_x) + o_p(h)$. The result follows directly from the quadratic approximation lemma.

Lemma 2

Suppose that the conditions of Theorem 1 hold. For \mathbf{W}_n as defined in Lemma 1,

$$\{\boldsymbol{\Sigma}_x^{-1} - h\boldsymbol{\Sigma}_x^{-1} \boldsymbol{\Lambda}_x \boldsymbol{\Sigma}_x^{-1}\} E(\mathbf{W}_n) = \mathbf{b}_x + o\{(nh^{2p+5})^{1/2}\},$$

$$\boldsymbol{\Gamma}_x^{-1/2} \text{cov}(\mathbf{W}_n) \rightarrow \mathbf{I}_{p+1}, \quad \text{and}$$

$$\boldsymbol{\Gamma}_x^{-1/2} (\mathbf{W}_n - E\mathbf{W}_n) \rightarrow_D N(\mathbf{0}, \mathbf{I}_{p+1}).$$

Proof. We compute the mean and covariance matrix of the random vector \mathbf{W}_n by studying \mathbf{Y}_1^* , as defined in Lemma 1. The mean of the i th component of \mathbf{Y}_1^* is easily shown to be

$$(E\mathbf{Y}_1^*)_i = \frac{h}{(i-1)!} \int q_1(\bar{\eta}(x, x+hz), \mu(x+hz)) z^{i-1} K(z) f(x+hz) dz.$$

Now by Taylor expansion, (A.1), and (A.3),

$$q_1(\bar{\eta}(x, x+hz), \mu(x+hz)) = \left\{ (hz)^{p+1} \frac{\eta^{(p+1)}(x)}{(p+1)!} + (hz)^{p+2} \frac{\eta^{(p+2)}(x)}{(p+2)!} \right\} \rho(x+hz) + o(h^{p+2}).$$

Thus

$$(E\mathbf{Y}_1^*)_i = h^{p+2} \frac{\eta^{(p+1)}(x)}{(p+1)!} \frac{(\rho f)(x)}{(i-1)!} \nu_{p+i} + h^{p+3} \frac{\zeta_p(x)(\rho f)'(x)}{(i-1)!} \nu_{p+i+1} + o(h^{p+3}), \quad (\text{A.4})$$

where

$$\zeta_p(x) = \frac{\eta^{(p+2)}(x)}{(p+2)!} + \frac{\eta^{(p+1)}(x)}{(p+1)!} \frac{(\rho f)'(x)}{(\rho f)(x)}.$$

The i th component of $\boldsymbol{\Sigma}_x^{-1} E\mathbf{W}_n$ is

$$(\boldsymbol{\Sigma}_x^{-1} E\mathbf{W}_n)_i = (nh^{2p+3})^{1/2} \frac{\eta^{(p+1)}(x)}{(p+1)!} \int z^{p+1} K_{i-1,p}(z) dz + (nh^{2p+5})^{1/2} \zeta_p(x) \int z^{p+2} K_{i-1,p}(z) dz + o(nh^{2p+5})^{1/2}$$

by Lemma 3. Next, consider the second term in the expectation,

$$h(\boldsymbol{\Sigma}_x^{-1} \boldsymbol{\Lambda}_x \boldsymbol{\Sigma}_x^{-1} E\mathbf{W}_n)_i = (nh^{2p+5})^{1/2} \frac{\eta^{(p+1)}(x)}{(p+1)!} \frac{(\rho f)'(x)}{(\rho f)(x)} (i-1)! \times \sum_{j=1}^{p+1} (\mathbf{N}_p^{-1} \mathbf{Q}_p \mathbf{N}_p^{-1})_{ij} \nu_{p+j} + O\{(nh^{2p+7})^{1/2}\}.$$

Using the fact that $(\mathbf{Q}_p)_{kl} = (\mathbf{N}_p)_{k,l+1}$ for $l < p+1$, it can be shown that

$$(\mathbf{N}_p^{-1} \mathbf{Q}_p \mathbf{N}_p^{-1})_{ij} = (\mathbf{N}_p^{-1})_{i-1,j} + \left\{ \sum_{k=1}^{p+1} (\mathbf{N}_p^{-1})_{i,k} \nu_{p+k} \right\} (\mathbf{N}_p^{-1})_{p+1,j}$$

for $i = 2, \dots, p+1$ and that

$$(\mathbf{N}_p^{-1} \mathbf{Q}_p \mathbf{N}_p^{-1})_{1j} = \left\{ \sum_{k=1}^{p+1} (\mathbf{N}_p^{-1})_{1,k} \nu_{p+k} \right\} (\mathbf{N}_p^{-1})_{p+1,j}.$$

So by Lemma 3,

$$(i-1)! \sum_{j=1}^{p+1} (\mathbf{N}_p^{-1} \mathbf{Q}_p \mathbf{N}_p^{-1})_{ij} \nu_{p+j} = (i-1) \int z^{p+1} K_{i-2,p}(z) dz + \frac{1}{p!} \int z^{p+1} K_{p,p}(z) dz \int z^{p+1} K_{i-1,p}(z) dz.$$

The statement concerning the asymptotic mean follows immediately.

By (A.4), the covariance between the i th and j th component of \mathbf{Y}_1^* is $E((\mathbf{Y}_1^*)_i (\mathbf{Y}_1^*)_j) + O(h^{2p+4})$. By a Taylor series expansion,

$$E((\mathbf{Y}_1^*)_i (\mathbf{Y}_1^*)_j) = \frac{1}{(i-1)!(j-1)!} \times E[q_1^2(\eta(X_1), Y_1) K^2\{(X_1 - x)/h\} \times \{(X_1 - x)/h\}^{i+j-2}] + O(h^2),$$

and one easily calculates

$$\{\text{cov}(\mathbf{Y}_1^*)\}_{i,j} = \frac{h f(x) \text{var}(Y|X=x)}{[V(\mu(x)) g'(\mu(x))]^2} \int \frac{z^{i+j-2}}{(i-1)!(j-1)!} K(z)^2 dz + o(h).$$

Therefore, $\boldsymbol{\Gamma}_x^{-1/2} \text{cov}(\mathbf{W}_n) \rightarrow \mathbf{I}_{p+1}$.

We now use the Cramer-Wold device to derive the asymptotic normality of \mathbf{W}_n . For any unit vector $\mathbf{u} \in \mathbb{R}^{p+1}$, if

$$(na_n^2)^{-1/2} \mathbf{u}^T \text{cov}(\mathbf{Y}_1^*)^{-1/2} (\mathbf{W}_n - E\mathbf{W}_n) \rightarrow_D N(0, 1), \quad (\text{A.5})$$

then $h^{1/2} \text{cov}(\mathbf{Y}_1^*)^{-1/2} \mathbf{W}_n - E\mathbf{W}_n \rightarrow_D N(\mathbf{0}, \mathbf{I}_{p+1})$, and so $\boldsymbol{\Gamma}_x^{-1/2} (\mathbf{W}_n - E\mathbf{W}_n) \rightarrow_D N(\mathbf{0}, \mathbf{I}_{p+1})$. To prove (A.5), we need only

check Lyapounov's condition for that sequence, which can be easily verified.

Lemma 3

For $l = 0, 1, \dots$,

$$\int_{\mathcal{A}} z^{p+l+1} K_{r,p}(z; \mathcal{A}) dz = r! \sum_{i=1}^{p+1} \{N_p(\mathcal{A})^{-1}\}_{r+1,i} \nu_{p+i+l}(\mathcal{A}).$$

Proof. Let c_{ij} denote the cofactor of $\{N_p(\mathcal{A})\}_{ij}$. By expanding the determinant of $M_{r,p}(z; \mathcal{A})$ along the $(r + 1)$ st column, we see that

$$\begin{aligned} \int z^{p+l+1} K_{r,p}(z) dz &= \frac{r!}{|N_p|} \int \sum_{i=1}^{p+1} z^{p+i+l} c_{i,r+1} K(z) dz \\ &= r! \sum_{i=1}^{p+1} \frac{c_{i,r+1}}{|N_p|} \nu_{p+i+l}. \end{aligned}$$

The lemma follows, because $(N_p^{-1})_{ij} = c_{ij}/|N_p|$ from the symmetry of N_p and a standard result concerning cofactors.

Lemma 4

Let $K_{r,p}(z; \mathcal{A})$ be as defined by (5), where K satisfies Condition 4. Then for $p \geq r$, $p - r$ even, $\int_{-1}^1 z^{p+1} K_{r,p}(z) dz = 0$.

Proof. Suppose that both p and r are odd. The case when both p and r are even is handled similarly. Then by writing $\int_{-1}^1 z^{p+1} K_{r,p}(z) dz$ in terms of the defining determinants, interchanging integral and determinant signs, and interchanging rows and columns of the determinant, we can obtain a determinant of the form

$$\begin{vmatrix} \mathbf{M}_1 & \mathbf{0}_{(p+1)/2, (p-1)/2} \\ \mathbf{0}_{(p+1)/2, (p+3)/2} & \mathbf{M}_2 \end{vmatrix},$$

where $\mathbf{0}_{l,k}$ is an $l \times k$ matrix of zeros. Because \mathbf{M}_1 is $\frac{1}{2}(p + 1) \times \frac{1}{2}(p + 3)$, there exists a nonzero vector \mathbf{x} in $\mathbb{R}^{(p+3)/2}$ such that $\mathbf{M}_1 \mathbf{x} = \mathbf{0}$. Thus the determinant is zero.

Proof of Theorem 1

Theorem 1 follows from the main theorem by reading off the marginal distributions of the components of $\hat{\beta}^*$. To calculate the asymptotic variance, we calculate the $(r + 1, r + 1)$ entry of $(r!)^2 N_p(\mathcal{A})^{-1} T_p(\mathcal{A}) N_p(\mathcal{A})^{-1}$ as

$$(r!)^2 \sum_{k=1}^{p+1} \sum_{l=1}^{p+1} \frac{c_{r+1,k} c_{r+1,l}}{|N_p(\mathcal{A})|^2} \{T_p(\mathcal{A})\}_{kl} = \int_{\mathcal{A}} K_{r,p}(z; \mathcal{A})^2 dz,$$

where c_{ij} is the cofactor of $\{N_p(\mathcal{A})\}_{ij}$.

Proof of Theorem 3

The proof of this theorem can be accomplished using exactly the same arguments as for the univariate case with $p = 1$ and $r = 0$ and using multivariate approximations analogous to those used by Ruppert and Wand (1994).

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