

Optimal Boundary Kernels and Weightings for Local Polynomial Regression

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Abstract

Kernel smoothers are considered near the boundary of the interval. Kernels which minimize the expected mean square error are derived. These kernels are equivalent to using a linear weighting function in the local polynomial regression. It is shown that any kernel estimator that satisfies the moment conditions up to order m is equivalent to a local polynomial regression of order m with some non-negative weight function if and only if the kernel has at most m sign changes. A fast algorithm is proposed for computing the kernel estimate in the boundary region for an arbitrary placement of data points.

1 Introduction

We consider a traditional nonparametric curve estimation problem. Noisy measurements of an unknown function f are given: $y_i = f(x_i) + \varepsilon_i$, $i = 1, 2, \dots, N$, where the errors, ε_i , are independent random variables with zero mean and variance equal to σ^2 . The function, f , is assumed to have p continuous derivatives. Our goal is to estimate its q th derivative ($0 \leq q < p$) in the interval of measurements.

Presently, three methods are widely used: kernel smoothers, local polynomial regression, and smoothing splines. Excellent reviews of kernel smoothing can be found in the monographs by Hardle (1990) and Müller (1988). In this method, the estimator of $f^{(q)}$ has the form $\widehat{f^{(q)}}(t) = \sum_{i=1}^N K(t, x_i)y_i$. To ensure consistency, the kernel must satisfy certain moment conditions. The local polynomial regression method is described in works by Cleveland (1979), Lejeune (1985), Fan and Gijbels (1992), Fan (1993), Hastie and Loader (1993, including comments by Fan and by Marron, and by Müller), Jones (1994). For a given estimation point t , a fitting polynomial $\sum_{j=0}^{p-1} a_j x^j$ is sought to minimize $\sum_{i=1}^N w_i(t) \left(\sum_{j=0}^{p-1} a_j (x_i - t)^j - y_i \right)^2$. Then $q!a_q$ is taken as the estimate of $f^{(q)}(t)$. Parameters of the method are the non-negative weights, w_i , and the order of polynomial fitting, $p - 1$. The weights are usually scaled as $w_i(t) = W\left(\frac{x_i - t}{h}\right)$ where W is a non-negative function on $[-1, 1]$.

Silverman (1984) showed that smoothing splines are equivalent to a special case of kernel smoothers. Similarly, the local polynomial regression is equivalent to a kernel smoother $K(t, x_i) = w_i(t)P(x_i - t)$ where $P(x)$ is a polynomial of order $p - 1$ in x whose coefficients may depend on t (see Müller (1987), Jones (1994)). We show that *any kernel estimator that satisfies the moment conditions up to order $p - 1$ is equivalent to a local polynomial regression of order $p - 1$ if and only if the kernel has at most $p - 1$ sign changes.*

The optimal kernel support to minimize the mean square error (MSE) for a prescribed kernel shape dates back to Grenander and Rosenblatt (1957). Away from the beginning and end of the data, the optimal kernel shape (which minimizes the

MSE) was determined by Gasser and Müller (1979), Müller (1984, 1988), Gasser, Müller and Mammitzsch (1985). The bias of a nonparametric smoothing estimator typically is much higher in the boundary region than in the interior (see Rice and Rosenblatt (1981)). Thus, minimization of MSE in the boundary region is important and is a central focus of this article. We also notice that estimation near the boundary includes forecasting as a special case when $t < 0$ or $t > 1$.

Near the boundary of the observation interval, the kernel shape has to be smoothly transformed to allow nonsymmetrical support. Subject to the moment conditions and the smooth boundary transformation, we choose the kernel shape to minimize MSE. Various boundary transformation techniques are discussed in literature (Jones (1994)). In the generalized jackknifing boundary correction, Aitken extrapolation is used to reduce the order of the bias (Rice (1984)). Müller (1994) and Jones (1994) propose general methods which provide boundary transformation of the prescribed smoothness for any interior kernel. All these transformations satisfy the moment conditions and provide smooth estimates. They do not, however, minimize MSE near the boundary.

The boundary problem is solved automatically in the local polynomial regression method: the boundary region points are treated similarly to the interior points. In terms of equivalent kernels, the factor polynomial P depends on the estimation point and changes smoothly near the boundary. This produces a smooth boundary transformation of the equivalent kernel. The weighting function, however, which minimizes MSE in the interior, does not necessarily minimize MSE in the boundary region.

In the present work, we investigate the problem of choosing a boundary kernel (or equivalently, selecting a weight function for the local polynomial regression) which minimizes MSE while providing continuity (smoothness) of the estimate. For a given kernel halfwidth in the boundary region, we derive the optimal boundary kernel and its approximation for large N , the asymptotically optimal kernel. Our boundary kernels have a simple form and are polynomials of the same order as the optimal

interior kernels. We show that in the case when the kernel halfwidth is constant in the boundary region, the estimate can be computed in $\mathcal{O}(N_T + N_E)$ operations, where N_T is the number of data points within the support, and N_E is the number of boundary region points where $f^{(q)}$ is to be estimated. The placement of data points can be arbitrary.

In Section 2, we review MSE of kernel smoothers. In Sections 3 and 4, we derive the optimal boundary kernel which minimizes the leading order MSE. In Section 5, we concentrate on the limiting case where the data points are spaced approximately regularly as $N \rightarrow \infty$. We derive simple analytical expressions for the optimal boundary kernels. In Section 6, we investigate the equivalence of the kernel smoother estimators and the local polynomial regression. In Section 7, we show that the optimal weighting in the boundary region is a linear function. In Section 8, we discuss estimation for non-equispaced data. In Section 9, we compare MSE of various estimators and show that the asymptotically optimal kernel is robust against the misspecification of the kernel halfwidth.

2 Expected Mean Square Error of Kernel Smoothers

Let $f(t)$ have p continuous derivatives and assume that $f^{(p)} \neq 0$ in the domain. We consider kernel estimators of $f^{(q)}(t)$ ($q < p$) of the form:

$$\widehat{f^{(q)}}(t) = \sum_{i=N_L}^{N_R} K(t, x_i) y_i . \tag{2.1}$$

The left and right endpoints of the summation are free parameters which we optimize. We denote x_{N_L} by x_L , x_{N_R} by x_R , and define $h_L \equiv t - x_L$ and $h_R \equiv x_R - t$. We define the kernel halfwidth, $h \equiv \frac{h_L + h_R}{2}$ and $N_T = N_R - N_L + 1$. For equispaced data, away from the data boundary, the most common kernel smoothers are *scale parameter kernels*: $K(t, x_i) = \frac{1}{Nh^{q+1}} G\left(\frac{x_i - t}{h}\right)$.

For given values of t , N_L , and N_R , we say a kernel, $K(t, x_i)$, with halfwidth, h , is

of type (q, p) if it satisfies the *moment conditions*:

$$\frac{1}{Nh} \sum_{i=N_L}^{N_R} \frac{1}{m!} \left(\frac{x_i - t}{h} \right)^m \mu_i = \delta_{m,q}, \quad m = 0, \dots, p-1, \quad (2.2)$$

$$B_p = \frac{1}{Nh} \sum_{i=N_L}^{N_R} \frac{1}{p!} \left(\frac{x_i - t}{h} \right)^p \mu_i \neq 0,$$

where $\mu_i = Nh^{q+1}K(t, x_i)$. Kernels of type (q, p) estimate the q th derivative of the function with a bias error of order $O(h^{p-q})$. The bias term can not be eliminated by setting $B_p = 0$: in such a case, the kernel would be of a higher order.

We assume that h_L and h_R are small ($N_L \ll N$ and $N_R \ll N$), and expand $f(x_i)$ in a Taylor series about $f(t)$. For a kernel smoother of type (q, p) , the bias of the estimator is

$$E[\widehat{f^{(q)}}(t)] - f^{(q)}(t) = B_p f^{(p)}(t) h^{p-q} + O(h^{p-q+1}). \quad (2.3)$$

The variance of the kernel estimator is

$$\text{Var}[\widehat{f^{(q)}}(t)] = \frac{\sigma^2}{N^2 h^{2q+2}} \sum_{i=N_L}^{N_R} \mu_i^2.$$

We define $m_2(\mu) = \frac{1}{Nh} \sum_{i=N_L}^{N_R} \mu_i^2$. In the case of scale parameter kernels, $m_2(\mu)$ converges to $\int_{-1}^1 G(y)^2 dy$. Correspondingly, B_p converges to $\int_{-1}^1 G(y) \frac{y^p}{p!} dy$. Thus the leading order MSE is

$$R(t) = B_p^2 |f^{(p)}(t)|^2 h^{2(p-q)} + \frac{\sigma^2 m_2(\mu)}{N h^{2q+1}}, \quad (2.4)$$

where the corrections are $O(h^{2(p-q)+1})$.

Solving (2.4) for the optimal value of the kernel scale size, h_0 , yields

$$h_0 = \left(\frac{2q+1}{2(p-q)} \frac{\sigma^2 m_2(\mu)}{B_p^2 N |f^{(p)}(t)|^2} \right)^{\frac{1}{2p+1}}. \quad (2.5)$$

The ratio $N|f^{(p)}|^2/\sigma^2$ is the expansion parameter for choosing the kernel's halfwidth. This ratio can be normalized to one by changing variables to $\tilde{t} = \alpha t$ where $\alpha = \left| \frac{N|f^{(p)}|^2}{\sigma^2} \right|^{\frac{1}{2p+1}}$. This transformation maps the interval $[0, 1]$ to $[0, \alpha]$. Then for each

specific point $t \in [0, \alpha]$, we consider a subinterval of length 1 (which contains about N/α measurements) around this point.

For the choice of kernel halfwidth given by (2.5), the leading order MSE equals to

$$R(t) = K_{q,p} \left| B_p f^{(p)}(t) \right|^{\frac{4q+2}{2p+1}} \left| \frac{\sigma^2 m_2(\mu)}{N} \right|^{\frac{2(p-q)}{2p+1}}, \quad (2.6)$$

where $K_{q,p} \equiv \left| \frac{2q+1}{2(p-q)} \right|^{\frac{2(p-q)}{2p+1}} + \left| \frac{2(p-q)}{2q+1} \right|^{\frac{2q+1}{2p+1}}$. The optimal h is proportional to $N^{-\frac{1}{2p+1}}$, and MSE is proportional to $N^{-\frac{2(p-q)}{2p+1}}$. If $f(t)$ has \tilde{p} continuous derivatives, where $q \leq \tilde{p} \leq p$, the optimal halfwidth scales as $N^{-\frac{1}{2\tilde{p}+1}}$, and the total square error is proportional to $N^{-\frac{2(\tilde{p}-q)}{2\tilde{p}+1}}$. The convergence rate given by (2.6) is theoretically optimal for functions with precisely p continuous derivatives (Stone (1982)). The leading constant depends on the kernel shape, however.

The estimate, $\widehat{f^{(q)}}(t)$ in (2.1), is C_l if and only if $K(t, x_i)$ is C_l over $[0, 1]$ for every x_i . To impose smoothness of order l on $\widehat{f^{(q)}}$, some researchers require that the kernel and its first l derivatives vanishes at the boundaries of the support. *This is not necessary when the boundary does not change as t varies: in particular, when the support borders one of the ends of the interval $[0, 1]$.* In the present paper, we consider the case $l = 0$, so we seek an estimate, $\widehat{f^{(q)}}(t)$, that is continuous in t .

3 Orthogonal Polynomial Representation of the Optimal Kernels

In view of moment conditions (2.2), we expand the kernel in orthogonal polynomials. Let P_k be a polynomial of order k ($k = 0, 1, \dots$) such that $\frac{1}{Nh} \sum_{i=N_L}^{N_R} P_k \left(\frac{x_i - \bar{x}}{h} \right) P_j \left(\frac{x_i - \bar{x}}{h} \right) = g_k \delta_{kj}$ where $\bar{x} = \frac{1}{2}(x_L + x_R)$ and g_k is a normalization. We expand $K(t, x) = \frac{2}{Nh^{q+1}} \sum_k b_k P_k \left(\frac{x - \bar{x}}{h} \right)$. The moment conditions are rewritten as $\sum_k C_{kj} b_k = \delta_{qj}$ for $j = 0, \dots, p-1$, where $C_{kj} = \sum_{i=N_L}^{N_R} P_k \left(\frac{x_i - \bar{x}}{h} \right) \frac{1}{j!} \left(\frac{x_i - t}{h} \right)^j$. The matrix C_{kj} is upper triangular, and its diagonal entries are not zero. We solve for $b_0, b_1 \dots b_{p-1}$:

$$b_j = 0 \quad \text{with } j = 0, \dots, q-1,$$

$$b_q = \frac{1}{C_{qq}}, \quad (3.1)$$

$$b_j = -\frac{1}{C_{jj}} \sum_{i=q}^{j-1} C_{ij} b_i \quad \text{with } j = q+1, \dots, p-1.$$

Any kernel satisfying the moment conditions has the coefficients $b_0, b_1 \dots b_{p-1}$ prescribed by (3.1) while coefficients b_p, b_{p+1}, \dots are free parameters. The leading order bias equals $f^{(p)}(t)h^{p-q} \sum_{k=q}^p C_{kp} b_k$. The summation stops at $k = p$ because $C_{kp} = 0$ for $k > p$. In the absence of boundary conditions, MSE attains the minimum when $b_k = 0$ for $k > p$. Then MSE is a quadratic function of b_p , and the optimal value b_p can be easily found:

$$R(t) = \frac{\sigma^2}{Nh^{2q+1}} \sum_{k \geq q} g_k b_k^2 + \left(f^{(p)}(t) h^{p-q} \sum_{k=q}^p C_{kp} b_k \right)^2. \quad (3.2)$$

If there are no boundary conditions, the minimum is attained when $b_k = 0$ for $k > p$ and

$$b_p = - \left(\sum_{k=q}^{p-1} C_{kp} b_k \right) / \left(C_{pp} + \frac{g_p \sigma^2}{C_{pp} N h^{2p+1} (f^{(p)}(t))^2} \right). \quad (3.3)$$

We name the kernel, $K(t, x) = \frac{2}{Nh^{q+1}} \sum_{k=q}^p b_k P_k \left(\frac{x-\bar{x}}{h} \right)$ with coefficients b_k given by (3.1) and (3.3), the *optimal kernel*. When $t < 0$ or $t > 1$, this optimal kernel can be used for forecasting.

If we optimize the kernel shape over the whole interval, $[0,1]$, the optimal kernel still minimizes the leading order MSE. However, the bias estimate in (2.3) is based on the Taylor series expansion of $f(x_i)$ about $f(t)$. When the kernel support is not small with respect to the characteristic scale of the $f(t)$, the actual bias error may be unrelated to the leading order MSE in (3.2).

4 Optimal Boundary Kernels

Away from the ends of the data, we center the support of the kernel about the estimation point. As the estimation point, t , approaches the left endpoint of the

interval $[0, 1]$, the kernel halfwidth, $h(t)$, eventually becomes equal to t , and the support touches the left end, 0. We name the point where it happens the *touch point* and denote by t_0 . At this point, $h(t_0) = t_0$. We refer to the subinterval $[0, t_0]$ as the *left boundary region*. When the estimation point belongs to this region, we place the left end of the support at the left end of the interval: $t - h_L(t) = 0$. The right end of the support equals $2h(t)$, where $h(t) = (h_L(t) + h_R(t)) / 2$.

In the boundary region, we may consider two options: fixed or variable kernel halfwidth. Variable halfwidth choice, $h = h(t)$, allows to reduce MSE by taking into account changes in $f^{(p)}$ (see Müller and Stadtmüller (1987)). We show in Section 5 that using a fixed halfwidth in the boundary region results in the minimum MSE as $N \rightarrow \infty$. Moreover, using a fixed halfwidth in the boundary region has three important advantages: (i) prior estimation of $f^{(p)}(t)$ in the boundary region is not required, (ii) the continuity of the estimate can be ensured while using kernels which do not vanish at the ends of the kernel support (and thus MSE decreases), and (iii) computational costs can be reduced drastically as we show below.

Indeed, if the support, $[0, 2h]$, is the same for all estimation points $t \in [0, h]$, then the same system of orthogonal polynomials P_k can be used for all t . The only dependence of formulae (3.1) on t is due to the fact that $C_{kj} = C_{kj}(t)$ is a polynomial of order j in t . The orthogonal polynomials $P_0\left(\frac{x}{h} - 1\right), P_1\left(\frac{x}{h} - 1\right), \dots, P_p\left(\frac{x}{h} - 1\right)$ and the coefficients of the polynomials $C_{kj}(t)$ can be calculated in $\mathcal{O}(N_T)$ operations where N_T is the number of data points in the boundary region. We also need $\mathcal{O}(N_T)$ operations to compute the inner products $s_j = \sum_{i=1}^{N_T} P_j\left(\frac{x_i}{h} - 1\right) y_i$ for $j = q, q + 1, \dots, p$. After that, for each t , we need only $\mathcal{O}(1)$ operations to compute $b_q(t), b_{q+1}(t), \dots, b_p(t)$ and the estimate, $\widehat{f^{(q)}}(t) = \sum_{j=q}^p b_j(t) s_j$.

In general, the same computational scheme also can be applied when the kernel has a fixed support, is a polynomial of a given order, and the coefficients of its orthogonal polynomial expansion are rational functions in t .

5 Optimal Boundary Kernels in Continuum Limit

for $p = q + 2$

Equispaced data arise increasingly often with the widespread use of digital signal processing. In the limiting case, when the data points are regularly spaced and their number is large, analytic expressions for optimal interior kernels were obtained by Gasser, Müller and Mammitzsch (1985). In this section, we consider even more broadly defined limit where every subinterval of length $\frac{1}{\alpha}$ with $\alpha = \mathcal{O}\left(N^{\frac{1}{2p+1}}\right)$ contains $\left(\frac{1}{\alpha} + o(1)\right)N$ data points as $N \rightarrow \infty$.

In the continuum limit, the discrete kernel function, $K_N(t, x_i)$, $i = 1, 2, \dots, N$, is replaced with a function $K(t, x)$, $x \in [0, 1]$. Namely, if $x_i \rightarrow x$ then $N \cdot K_N(t, x_i) \rightarrow K(t, x)$. Summation over x_i is replaced with integration over x , and the discrete orthogonal polynomials are replaced with their continuous analog, Legendre polynomials (see Appendix A).

The *optimal interior kernel* of type (q, p) (see Granovsky and Müller (1989)) is the kernel which minimizes the leading order MSE subject to the constraint that the number of sign changes in the open interval of the kernel support is at most $p - 2$. The prescribed value of sign changes is the minimal possible, see Müller (1985). As we show in Section 6, the number of sign changes of the kernel is related to the existence of an equivalent estimator in the local polynomial regression.

From now to the end of this section, we restrict ourselves to the case of $p = q + 2$. In this case, the optimal interior kernel, in the continuum limit, can be represented as $K(t, x) = \frac{1}{h^{q+1}}G\left(\frac{x-t}{h}\right)$, where

$$G(y) = \gamma_q \cdot (P_q(y) - P_{q+2}(y)), \quad (5.1)$$

P_q, P_{q+2} are the Legendre polynomials, and $\gamma_q = \frac{1}{2} \prod_{k=1}^q (2k + 1)$. The leading order MSE is minimal for the halfwidth

$$h_0(t) = \left(\frac{4(2q+3)(2q+5)\sigma^2\gamma_q^2}{Nf^{(p)}(t)^2} \right)^{\frac{1}{2p+1}}. \quad (5.2)$$

With this halfwidth, the leading order MSE equals $\frac{2q+3}{2q+1} \frac{\sigma^2 \gamma_q^2}{Nh_0(t)^{2q+1}}$. The optimal interior kernel vanishes at the ends of the support and thus ensures the continuity of the estimate.

We seek a boundary kernel in the form: $K(t, x) = \frac{1}{h^{q+1}} G\left(\frac{t}{h} - 1, \frac{x}{h} - 1\right)$. The function $G(z, y)$ is the *normalized boundary kernel*, and its domain is $y \in [-1, 1]$, $z \in [-1, 0]$ (we notice that $z \leq 0$ because $h_L < h_R$ in the left boundary region). We may use the same normalized kernel, G , to represent a boundary kernel in the *right boundary region* (where t is close to 1) : $K(t, x) = \frac{(-1)^q}{h^{q+1}} G\left(\frac{1-t}{h} - 1, \frac{1-x}{h} - 1\right)$ with $x \in [1 - 2h, 1]$.

Using the Legendre polynomials, P_j , we expand the normalized boundary kernel: $G(z, y) = \gamma_q \sum_j b_j(z) P_j(y)$. From Appendix A, equation (3.1) reduces in the continuous limit to

$$b_j = 0 \quad \text{with } j = 0, \dots, q-1; \quad b_q = 1; \quad b_{q+1} = (2q+3)z. \quad (5.3)$$

These are an equivalent of the *moment conditions* for the kernel. Correspondingly, the leading order MSE of the kernel estimator in Eq. (3.2) reduces to

$$R(t) = \frac{\sigma^2 \gamma_q^2}{Nh_0(t)^{2q+1}} \bar{R}\left(\frac{t}{h} - 1\right),$$

where \bar{R} is the *normalized risk*:

$$\begin{aligned} \bar{R}(z) &= \frac{2}{\beta^{2q+1}} \left(\frac{1}{2q+1} + (2q+3)z^2 + \sum_{j \geq q+2} \frac{b_j^2}{2j+1} \right) \\ &+ (2q+3)(2q+5)\beta^4 \left(\frac{1}{2q+3} - z^2 + \frac{2b_{q+2}}{(2q+3)(2q+5)} \right)^2, \end{aligned} \quad (5.4)$$

$\beta = h/h_0(t)$ is the *normalized halfwidth*, which depends on t , and h_0 is given by (5.2).

In the continuum limit, Eq. (3.3) reduces to $b_{q+2} = ((2q+3)z^2 - 1) / \left(\frac{2q+3}{(2q+5)\beta^{2q+5}} + \frac{2}{2q+5} \right)$.

Thus we have

Theorem 1. *Among all boundary kernels with support $[0, 2h]$, the minimum leading order MSE is provided by the kernel $K(t, x) = \frac{1}{h^{q+1}} G\left(\frac{t}{h} - 1, \frac{x}{h} - 1\right)$ where*

$$G(z, y) = \gamma_q \cdot \left[P_q(y) + (2q+3)z P_{q+1}(y) + \frac{(2q+3)z^2 - 1}{\frac{2q+3}{(2q+5)\beta^{2q+5}} + \frac{2}{2q+5}} P_{q+2}(y) \right], \quad (5.5)$$

P_q, P_{q+1}, P_{q+2} are the Legendre polynomials, and $\beta = h/h_0(t)$.

We use $\beta = \frac{h}{h_0(t)}$ in Eq. (5.5) in place of $f^{(p)}(t)$ because we are interested in kernels which have a fixed halfwidth in the boundary region: $h(t) = h_0(t_0)$ and $\beta = \frac{h_0(t_0)}{h_0(t)}$ where t_0 is the touch point.

Let us examine the two special cases: $t = h$ (when the estimation point is the touch point) and $t = 0$ (when the estimation point is the left edge of $[0,1]$).

When $t = h = h_0(t)$, the optimal boundary kernel is identical to the optimal interior kernel (see (5.1)). Thus using the optimal boundary kernel *guarantees the continuity of the estimate* if at the touch point we apply the optimal interior kernel of the optimal halfwidth.

In the edge case, $t = 0$, the halfwidth, $h_0(t)$ as given by Eq. (5.2), is a singular point of the MSE functional for the optimal boundary kernel. In Appendix B, we show that the optimal boundary kernel with this halfwidth has the minimum value of the leading order MSE among all boundary kernels which have at most $p - 1$ sign changes in the open interval of their support (and thus are equivalent to a local polynomial regression estimator with non-negative weighting; see Section 6). We name this kernel (with $t = 0$, $h = h_0(0)$) the *edge optimal kernel*. The kernel has a simple expression: $K(0, x) = \frac{1}{h^{q+1}} G\left(\frac{x}{h} - 1\right)$ where $h = h_0(0)$ and

$$G(y) = \gamma_q \cdot [P_q(y) - (2q + 3)P_{q+1}(y) + (2q + 2)P_{q+2}(y)] .$$

The leading order MSE equals $4(q + 1)^2 \frac{2q+3}{2q+1} \frac{\sigma^2 \gamma_q^2}{N h_0(t)^{2q+1}}$, which is *exactly* $4(q + 1)^2$ times larger than for the optimal interior kernel.

The expressions for the optimal halfwidths are identical for both interior and edge estimation cases. This fact supports our suggestion to use a constant halfwidth in the boundary region.

We assume that in the interior, $t \geq t_0$, the optimal halfwidth, $h_0(t)$, is used. Then the natural choice for the constant halfwidth in the boundary region is $h = h_0(t_0)$: this ensures the continuity of the estimate at the touch point. When $N \rightarrow \infty$, the optimal halfwidth, $h_0(t_0) = t_0$ scales as $N^{-\frac{1}{2p+1}}$ and tends to zero. Thus $\frac{f^{(p)}(\theta t_0)}{f^{(p)}(t_0)} \rightarrow 1$

and $\frac{h_0(\theta t_0)}{h_0(t_0)} \rightarrow 1$ uniformly for $\theta \in [0, 1]$.

For $h(t) = h_0(t)$, the optimal boundary kernel of Eq. (5.5) is simplified to

$$G(z, y) = \gamma_q \cdot \left[P_q(y) + (2q + 3)zP_{q+1}(y) + ((2q + 3)z^2 - 1)P_{q+2}(y) \right]. \quad (5.6)$$

Therefore, we have

Corollary 2. *If $h(t) \equiv h_0(t_0)$ in the boundary region, the normalized optimal boundary kernel of Eq. (5.5) tends to the kernel of Eq. (5.6) as $N \rightarrow \infty$.*

We name this limit the *asymptotically optimal kernel*. Its analytic expression is simpler and does not depend on $f^{(p)}(t)$, but its leading order MSE might be larger than the optimal. In contrast, the coefficient for P_{q+2} in (5.5) depends on β which involves $f^{(p)}(t)$. Section 9 shows that the asymptotically optimal kernel achieves nearly the same MSE as the optimal kernel when the kernel halfwidth is close to its optimal value. As N tends to infinity, the optimal halfwidth can be estimated with increasing accuracy, and little performance degradation results from using the asymptotically optimal kernel instead of the optimal kernel.

Both the optimal and asymptotically optimal boundary kernels are linear combinations of the low order Legendre polynomials. In these linear combinations, only the coefficients b_j depend on t . When the interval of the support, $[0, 2h]$, is the same for all $t \in [0, h]$, the kernel estimate is just a linear combination of these $b_j(t)$ functions:

$$\widehat{f^{(q)}}(t) = \frac{\gamma_q}{h^{q+1}} \sum_j b_j \left(\frac{t-h}{h} \right) \left[\int_0^{2h} P_j \left(\frac{x-h}{h} \right) Y(x) dx \right],$$

where $Y(x)$ is the data. In particular, the asymptotically optimal boundary kernel produces an estimate, $\widehat{f^{(q)}}(t)$, which is a quadratic function of t .

6 Equivalence of Local Polynomial Regression and Kernel Estimators

In the local polynomial regression, we minimize

$$F(a_0, a_1, \dots, a_{p-1}) = \sum_{i=1}^N w_i(t) \cdot \left(\sum_{j=0}^{p-1} a_j (x_i - t)^j - y_i \right)^2$$

and take $q!a_q$ as the estimate of $f^{(q)}(t)$. The weights, $w_i(t)$, are non-negative and considered as given. Since the functional is quadratic and non-negative, the minimum exists and satisfies

$$0 = \frac{\partial F}{\partial a_k} = \sum_{j=0}^{p-1} \left[\sum_{i=1}^N (x_i - t)^{k+j} w_i(t) \right] a_j - \sum_{i=1}^N (x_i - t)^k w_i(t) y_i$$

for $k = 0, 1, \dots, p-1$. This system of linear equations can be rewritten as

$$\sum_{j=0}^{p-1} d_{kj}(t) (a_j h^j) = m_k(t), \quad k = 0, 1, \dots, p-1, \quad (6.1)$$

where

$$d_{kj}(t) = \frac{1}{Nh} \sum_{i=1}^N \left(\frac{x_i - t}{h} \right)^{k+j} w_i(t), \quad m_k(t) = \frac{1}{Nh} \sum_{i=1}^N \left(\frac{x_i - t}{h} \right)^k w_i(t) y_i.$$

If the number of data points with non-zero weights is at least p , the matrix $[d_{kj}(t)]$ is non-singular. Let $[\tilde{d}_{jk}(t)]$ be the inverse matrix. Then $a_q h^q = \sum_{k=0}^{p-1} \tilde{d}_{qk}(t) m_k(t)$ and $q!a_q = \sum_{i=1}^N K(t, x_i) y_i$, where

$$K(t, x_i) = w_i(t) \left[\frac{q!}{Nh^{q+1}} \sum_{k=0}^{p-1} \tilde{d}_{qk}(t) \left(\frac{x_i - t}{h} \right)^k \right]. \quad (6.2)$$

Thus for a given estimation point t and weights w_i , the local polynomial regression estimator is equivalent to a kernel estimator whose kernel is the product of the weights with a polynomial in $\frac{x_i - t}{h}$ of order $p-1$. The equivalent kernel automatically satisfies the moment conditions and thus is a kernel of type (q, p) .

We name the polynomial in x_i inside the brackets on the right hand side of (6.2) the *factor polynomial*. We say that a discrete function $Q(x_i)$ has a sign change

between x_j and x_{j+k} if $Q(x_j)Q(x_{j+k}) < 0$ and $Q(x_{j+1}) = \dots = Q(x_{j+k-1}) = 0$. The weights, $w_i(t)$, are non-negative, and the factor polynomial has at most $p - 1$ roots. Therefore, for the given t , the equivalent kernel $K(t, x_i)$ has at most $p - 1$ sign changes. Answering the question: “which kernel estimators can be represented as a local polynomial regression?” we show that the necessary condition is also sufficient.

Theorem 3. *A kernel of type (q, p) is the equivalent kernel of local polynomial regression of order $p - 1$ with non-negative weights if and only if the kernel has no more than $p - 1$ sign changes.*

It is known (see Müller (1985)) that any kernel of type (q, p) has at least $p - 2$ sign changes. This implies

Corollary 4. *The actual order of the factor polynomial is at least $p - 2$.*

To solve system (6.1), we can expand $w_i(t) \left(\frac{x_i - t}{h}\right)^{k+j}$ in orthogonal polynomials. The representation of the equivalent kernel in terms of these polynomials was described in Section 3 and corresponds to a QR-decomposition of the matrix $[d_{kj}]$. Furthermore, when the regression support in the boundary region is fixed, one of the parts of this decomposition (namely, the matrix of coefficients of the orthogonal polynomials) is independent of the estimation point, t . Thus the equivalent orthogonal polynomial representation is a computationally convenient implementation of the local polynomial regression in the boundary region.

7 Optimal Weighting in Local Polynomial Regression

It is known (Müller (1987), Fan(1993)) that the optimal interior kernel of type (q, p) , $p - q \equiv 0 \pmod{2}$, in the continuum limit, is produced by the scaling weight function $W(y) = 1 - y^2$. We show that this choice is not unique.

Theorem 5. *Let $p - q$ be even. If data points, x_i , in the interval of support, $[t - h, t + h]$, are symmetric around the estimation point, t , and their weights are chosen*

as $w_i = W\left(\frac{x_i - t}{h}\right)$, then each of the functions $W_1(y) = 1 - y$, $W_2(y) = 1 + y$, $W_3(y) = 1 - y^2$ produces the same estimator.

Because of the optimality in the interior, the Bartlett-Priestley weighting, $W(y) = 1 - y^2$, is used often in the boundary region as well (Hastie and Loader (1993)). Since the kernel support is not symmetric around the estimation point, choosing the Bartlett-Priestley weighting is somewhat arbitrary. Even in the limiting case, this weighting does not provide the minimum MSE.

As we showed in Section 3, the leading order MSE is minimal when we use the optimal kernel given by Eq. (3.1) and (3.3). In the interval of its support, this is a polynomial of order p . If the optimal kernel has no more than $p - 1$ sign changes, there exists an equivalent weighting in the local polynomial regression. The true order of the factor polynomial is either $p - 1$ or $p - 2$. Then the optimal weighting, which provides the minimum value of the leading order MSE, must be a linear or quadratic function.

The optimal boundary kernel depends on the derivative $f^{(p)}(t)$ whose value might be unknown. This dependence is eliminated in the asymptotically optimal kernel which approximates the optimal kernel as $N \rightarrow \infty$. For the case $p = q + 2$, the asymptotically optimal kernel was determined in Section V, Eq. (5.6).

The following result shows that the asymptotically optimal kernel is representable as a local polynomial regression estimator with a non-negative weight function.

Theorem 6. *The asymptotically optimal kernel has no more than $p - 1$ roots in the open interval of its support, $[0, 2h]$. Its equivalent weighting is a linear function which is non-negative on $[0, 2h]$. In the case of edge estimation ($t = 0$), the equivalent weighting equals $2h - x$. For the touch point ($t = t_0$), the equivalent weighting can be chosen as either $2h - x$ or x and produces the same estimate as the Bartlett-Priestley weighting.*

For the intermediate estimation points, $0 < t < t_0$, the slope of the weighting line varies as t changes. For example, if $q = 0$, the equivalent weighting can be

represented as $(1 - z^2)h + (z + \sqrt{1 - 3z^2 + 3z^4})(x - h)$ where $z = \frac{t-h}{h}$.

In the case when we allow variable halfwidth in the boundary region, we have to optimize simultaneously the kernel shape (or weighting) and halfwidth. We carry out this optimization in Appendix B. The optimal weighting in this case is the linear function $2h(t) - x$ which vanishes at the right end of the support. (The vanishing guarantees the continuity of the estimate as a function of t .) The optimal halfwidth, $h = h(t)$, is a root of a polynomial equation. The equivalent kernel does not transform into the optimal interior kernel, however. Thus this estimator is useful only if we estimate $f^{(q)}(t)$ in the boundary region and not in the interior.

8 Estimation Near the Boundary for Discrete Data

For discrete data, we propose two slightly different methods for estimation near the boundary. Both of them reduce MSE relative to the local polynomial regression with Bartlett-Priestley weighting. First, the kernel of Section 3 is optimal for an arbitrary placement of points in the boundary region. The kernel estimate can be computed in $\mathcal{O}(N_T + N_E)$ operations, where N_E is the number of estimation points t in the boundary region (see Section 4).

The second method is to use the local polynomial regression with the asymptotically optimal weighting (the linear weighting function given in Theorem 6).

In the interior, when the data points are not equispaced, the requirement that the kernel vanishes at the ends of its support (in order to ensure the continuity of the estimate) is in conflict with the kernel shape optimization. The equivalent kernel of the local polynomial regression with Bartlett-Priestley weighting vanishes at the ends of the support and is asymptotically close to the optimal kernel. Thus we agree with Hastie and Loader (1993) that in the interior of the data interval, the local polynomial regression is the best way to estimate $f^{(q)}$.

To combine estimation in the interior and boundary region we should make sure that they produce the same estimate at the touch point. In the continuum limit

case, this holds (see Theorem 6) because the equivalent kernel of the local polynomial regression turns out the polynomial of order p . This still holds in the equispaced data case if t_0 is one of the data points or the midpoint of two data points. In such a case, Theorem 5 guarantees that for $t = t_0$ the linear weighting $2h - x$ produces the same estimator as the Bartlett-Priestley weighting, $h^2 - (x - h)^2$. For an arbitrary pattern of data points, the equivalent polynomial of the local polynomial regression with Bartlett-Priestley weighting is generally of order $2 + (p - 1) = p + 1$. Thus, estimates $\widehat{f}_{\text{boundary}}^{(q)}(t_0)$ and $\widehat{f}_{\text{interior}}^{(q)}(t_0)$ will differ. This discrepancy is eliminated by setting

$$\widehat{f}^{(q)}(t) = \widehat{f}_{\text{boundary}}^{(q)}(t) - \frac{t}{t_0} \left[\widehat{f}_{\text{boundary}}^{(q)}(t_0) - \widehat{f}_{\text{interior}}^{(q)}(t_0) \right].$$

The correction term in the brackets vanishes identically for equispaced data and is asymptotically small as $N \rightarrow \infty$.

9 Comparison of Different Estimators

We compare, in the continuum limit, the performance of our boundary kernels and local polynomial regression with Bartlett-Priestley weighting. The latter estimator is equivalent to the boundary kernel $K(t, x) = \frac{1}{h} G\left(\frac{t}{h} - 1, \frac{x}{h} - 1\right)$ where

$$G(z, y) = P_q(y) + (2q + 3)zP_{q+1}(y) - (1 + (2q + 3)z + b(z))P_{q+2}(y) + b(z)P_{q+3}(y),$$

and $P_q, P_{q+1}, P_{q+2}, P_{q+3}$ are the Legendre polynomials. For the touch point, $z = 0$, we have $b(0) = 0$. In particular, if $q = 0$ then $b(z) = \frac{9z^2}{10z^2 - 8z + 1}$.

Figure 1 plots $R(t)/R(t_0)$ (the MSE at estimation point t normalized to the MSE at the touch point) as a function of t for the optimal boundary kernel when $h(t) = h_0(t)$. When the estimation point approaches the edge, MSE is $4(q + 1)^2$ times larger than in the interior. Figure 2 compares the ratio of the MSE for the Bartlett-Priestley weighting of local polynomial regression with the optimal kernel. For kernels of type (0,2), there is an improvement of at most five percent. For type (4,6), the performance ratio increases to 21% at its highest. The difference is largest when

$t > 0.5$. For smaller t , the half parabola of the Bartlett-Priestley weighting resembles the equivalent linear weighting of the optimal kernel, and thus the MSEs are similar.

Figures 1 and 2 are calculated assuming $h(t) = h_0(t)$. We now consider the case where the kernel halfwidth is different than the optimal halfwidth. This case occurs when $|f^{(p)}|^2$ is estimated poorly or when $h(t)$ is determined by other requirements. Figure 3 plots the ratio of the MSE of the Bartlett-Priestley weighting to that of our kernel for $h(t) = \frac{1}{2}h_0(t)$ and $h(t) = 2h_0(t)$. We see that both kernels perform similarly when $h(t)$ is less than $h_0(t)$. However, when $h(t)$ is greater than $h_0(t)$, the optimal kernel performs much better than the Bartlett-Priestley weighting. This occurs because the optimal kernel has better bias protection.

Figure 4 gives the same plot for the asymptotically optimal kernel (or, equivalently, for the asymptotically optimal linear weighting in local polynomial regression). The difference in performance is less because the shape of the asymptotically optimal kernel is independent of $h(t)/h_0(t)$. For some values of t , the Bartlett-Priestley weighting actually outperforms the asymptotically optimal weighting. This occurs because the asymptotically optimal kernel is optimal only when $h(t) = h_0(t)$. Figure 4 shows that the performance of the two weightings is similar for $h(t) \leq h_0(t)$. However, the asymptotically optimal weighting has an appreciable advantage over the Bartlett-Priestley weighting for $h(t) > h_0(t)$.

Müller (1991), Müller and Wang (1994) suggest boundary modifications of the optimal interior kernels. Their modifications are done under the constraint that the kernel vanishes at both endpoints of its support. We agree with Hastie and Loader (1993, p.140) and Jones (1994, p.10) that this requirement is artificial in the boundary region. The Müller boundary kernel of type $(q, q + 2)$ is the unique polynomial of order $q + 3$ which satisfies simultaneously the moment conditions and the two boundary conditions: $K(t, 0) = 0$ and $K(t, 2h) = 0$. This kernel is $K(t, x) = \frac{1}{h^{q+1}}G\left(\frac{t}{h} - 1, \frac{x}{h} - 1\right)$ where

$$G(z, y) = \gamma_q \cdot [P_q(y) + (2q + 3)zP_{q+1}(y) - P_{q+2}(y) - (2q + 3)zP_{q+3}(y)] .$$

The requirement that the kernel vanishes at the left end point leads to a significantly larger MSE (especially when we are estimating close to the edge).

The comparison of MSE for the Müller kernel and for our optimal boundary kernel is given on Figure 5. The Müller kernel has noticeably larger risk.

10 Conclusion

In Section 3, we have derived a smoothing kernel which minimizes the leading order expected mean square error for a given pattern of data points x_i . In Section 4, we have described a fast algorithm to compute the estimate in the case when the kernel halfwidth is constant in the boundary region. In Section 5, we have found an explicit formula for the optimal boundary kernel of type $(q, q + 2)$ in the continuum limit (when the data points are spaced approximately regularly and their number tends to infinity). We also have defined the asymptotically optimal boundary kernel which is an approximation of the optimal kernel where dependence on $f^{(p)}(t)$ is eliminated. Both kernels are polynomials of order $q + 2$ whose coefficients depend on t . When the estimation point is the first or the last in the dataset, the minimal possible MSE is $4(q + 1)^2$ larger in comparison with the estimation in the interior. These boundary kernels can also be used for prediction with a minimum of MSE. In Section 6, we have proved that a kernel estimator of type (q, p) is equivalent to a local polynomial regression estimator of order $p - 1$ with some non-negative weighting if and only if the kernel has at most $p - 1$ sign changes in its support. In Section 7, we have shown that the asymptotically optimal boundary kernel of type $(q, q + 2)$ is equivalent to a local polynomial regression with non-negative linear weighting whose slope depends on the estimation point. In Section 8, we have described how to apply the optimal boundary kernels and weightings to discrete data with arbitrarily placed points. In Section 9, we compare MSE of our kernel estimators versus local polynomial regression with the Bartlett-Priestley weighting. The optimal boundary kernel takes into account changes in $f^{(p)}(t)$ and thus always outperforms the local polynomial regression. The

asymptotically optimal boundary kernel is more robust than the local polynomial regression with respect to misspecification of the halfwidth (caused by possible errors in estimating $f^{(p)}$).

Appendix A. Legendre Polynomials

Let P_0, P_1, \dots be the Legendre polynomials on $[-1, 1]$:

$$P_0(y) = 1, \quad P_1(y) = y, \quad P_i(y) = \frac{1}{i}[(2i-1)yP_{i-1}(y) - (i-1)P_{i-2}(y)].$$

Set

$$m_{ij} = \int_{-1}^1 P_i(y) \frac{1}{j!} y^j dy = \begin{cases} \frac{2^{i+1} \left(\frac{i+j}{2}\right)!}{(i+j+1)! \left(\frac{j-i}{2}\right)!} & \text{if } j \geq i, j \equiv i \pmod{2}; \\ 0, & \text{otherwise.} \end{cases}$$

In particular, $m_{q,q} = \frac{1}{\gamma_q}$ and $m_{q-1,q+1} = \frac{1}{2\gamma_q}$, where $\gamma_q = \frac{1}{2} \prod_{i=1}^q (2i+1)$.

For the interval $[-h_L, h_R]$, we define $\bar{P}_i(x) = P_i\left(2\frac{h_L+x}{h_L+h_R} - 1\right) = P_i\left(z + \frac{x}{h}\right)$, where $h = \frac{1}{2}(h_L + h_R)$, $z = \frac{h_L}{h} - 1 = \frac{h_L - h_R}{h_L + h_R}$. Then

$$\int_{-h_L}^{h_R} \bar{P}_i(x) \bar{P}_j(x) dx = h \int_{-1}^1 P_i(y) P_j(y) dy = \frac{2h}{2i+1} \delta_{ij}.$$

Define

$$C_{ij} = \left(\frac{1}{h}\right)^{j+1} \int_{-h_L}^{h_R} \bar{P}_i(x) \frac{x^j}{j!} dx = \sum_{k=0}^j \frac{(-1)^{j-k} z^{j-k}}{(j-k)!} \int_{-1}^1 P_i(y) \frac{y^k}{k!} dy.$$

Since $m_{ik} = 0$ with $i > k$, we have $C_{ij} = 0$ if $i > j$, and $C_{ij} = \sum_{k=i}^j \frac{(-1)^{j-k} z^{j-k}}{(j-k)!} m_{ik}$ if $i \leq j$. For the case of $p = q + 2$, this gives

$$C_{qq} = m_{qq}, \quad C_{q,q+1} = -zm_{q,q}, \quad C_{q,q+2} = m_{q,q+2} + \frac{1}{2}z^2 m_{q,q},$$

$$C_{q+1,q+2} = -zm_{q+1,q+1}, \quad C_{q+1,q+1} = m_{q+1,q+1}, \quad C_{q+2,q+2} = m_{q+2,q+2}.$$

Equation (3.2) reduces to $b_q = \frac{1}{C_{qq}} = \gamma_q$ and $b_{q+1} = -\frac{1}{C_{q+1,q+1}} C_{q,q+1} b_q = (2q+3)z\gamma_q$.

Appendix B. Simultaneous Optimization of the Kernel Shape and Halfwidth

Granovsky and Müller (1989) derived the optimal shape of interior kernel of type (q, p) as a function which minimizes the leading order MSE and has $p - 2$ sign changes in the interval of its support. When the support is not symmetric around the estimation point, $p - 2$ sign changes are not enough to meet the moment conditions.

Thus for boundary kernels we have to relax the limitation and allow $p - 1$ sign changes. By Theorem 3, kernels that fit this limitation are equivalent kernels of the local polynomial regression estimators. Therefore, optimization of the kernel shape and support, subject to this limitation, is equivalently optimization of the weighting function for the local polynomial regression in the case when the halfwidth is not fixed.

Theorem 7. *Let t be an estimation point in the left boundary region, and consider the class of boundary kernels of type (q, p) with at most $p - 1$ sign changes in their support. In the continuum limit, the leading order MSE is minimized when the kernel is a polynomial of order p within its support interval and vanishes at the right end of its support.*

The proof of Theorem 7 resembles the proof of the main theorem of Granovsky and Müller (1989). The only difference is that they considered kernels as functions from $L_2(-\infty, \infty)$ while we need $L_2[-t, \infty)$. Their proof shows that the optimal kernel is a continuous function, has finite support, and is a polynomial of order p there. In the case of space $L_2[-t, \infty)$, it implies that the optimal kernel vanishes at the right end of its support.

The kernel defined in Theorem 7 is unique. Indeed, in its Legendre polynomials expansion, $K(t, x) = \frac{1}{h(t)^{q+1}} G\left(\frac{t}{h(t)} - 1, \frac{x}{h(t)} - 1\right)$, $G(z, y) = \sum_{k=q}^p b_k(z) P_k(y)$, coefficients $b_q, b_{q+1}, \dots, b_{p-1}$ are determined from the moment conditions, and the last coefficient is fixed by the requirement to vanish at the right end: $b_p = -(b_q + b_{q+1} + \dots + b_{p-1})$. The leading order MSE for this kernel is a rational function in h . Thus the

optimal halfwidth is a root of a polynomial equation and depends on t and $|f^{(p)}(t)|^2$. For instance, in the case $p = q + 2$,

$$G(z, y) = \gamma_q \cdot [P_q(y) + (2q + 3)zP_{q+1}(y) - (1 + (2q + 3)z)P_{q+2}(y)] ,$$

and the optimal halfwidth equals $h = \beta \cdot h_0(t)$, where β is the maximal root of

$$(2q + 2)\beta^{2q+6} - (4q + 8)\tau\beta^{2q+5} + (2q + 5)\tau^2\beta^{2q+4} - (2q + 2)\beta + (2q + 3)\tau = 0 ,$$

with $\tau = t/h_0(t)$. In the edge estimation case, $t = 0$, we have $\beta = 1$, and therefore the optimum is attained for the halfwidth $h = h_0(0)$. This implies that our edge optimal kernel attains the minimum MSE among all boundary kernels of type $(q, q+2)$ which have at most $q + 1$ sign changes in the support.

For all τ , we have $\beta > \tau$, and the optimal halfwidth, $h(t)$, is always larger than t , so there is no touch point. For any q, p , the optimal boundary kernel of Theorem 7 always has a non-symmetric support and always differs from the optimal interior kernel. This result is natural because the latter has fewer sign changes.

The fact that the optimal kernel of Theorem 7 vanishes at the right end of the support guarantees the continuity of the estimate as a function of t .

The local polynomial regression with the linear weighting $2h - x$, $x \in [0, 2h]$, is equivalent to the optimal kernel of Theorem 7. Indeed, the equivalent kernel is a polynomial of order $1 + (p - 1) = p$ and vanishes at the right end of the support. Thus we have

Corollary 8. *In the case when the halfwidth is not fixed, the leading order MSE of local polynomial regression is minimized for the linear weighting $2h - x$. The optimal halfwidth, $h = h(t)$, depends on $|f^{(p)}(t)|^2$.*

Appendix C. Proofs of Theorems 3, 5, 6

Lemma 9. *Let $K_1(x_i)$ and $K_2(x_i)$ be kernels of type (q, p) with the same estimation point and the same support such that $K_r(x_i) = W(x_i)Q_r(x_i)$, $r = 1, 2$, where*

$W(x_i) \geq 0$ for all data points x_i in the support. If $Q_1(x)$ and $Q_2(x)$ are polynomials of order $p - 1$ then $K_1(x_i) = K_2(x_i)$ for every data point x_i .

Proof. Since K_1 and K_2 satisfy the same moment conditions, their difference is orthogonal to any polynomial $P(x_i)$ of order $p - 1$: $\sum_i (K_1(x_i) - K_2(x_i))P(x_i) = 0$. When we choose $P(x_i) = Q_1(x_i) - Q_2(x_i)$, we have $\sum_i W(x_i)(Q_1(x_i) - Q_2(x_i))^2 = 0$. Since $W(x_i) \geq 0$, it implies $W(x_i)(Q_1(x_i) - Q_2(x_i)) = 0$ for every x_i .

Proof of Theorem 3. Let a kernel $K(x_i)$ have $m \leq p - 1$ sign changes in the interval of its support. We enumerate the sign changes: z_1, z_2, \dots, z_m . Namely, if the l th sign change occurs at x_j or between x_j and x_{j+k} , we set $z_l = x_j + \varepsilon$ where $\varepsilon < \min\{x_2 - x_1, x_3 - x_2, \dots, x_N - x_{N-1}\}$. Now we define $P(x) = (-1)^s \prod_{l=1}^m (x - z_l)$, $W(x_i) = K(x_i)/P(x_i)$. The function $W(x_i)$ has no sign changes. We choose s to make all of the values $W(x_i)$ non-negative. Let Q be the factor polynomial for the local polynomial regression with the weights $w_i = W(x_i)$. Since $K = WP$ and WQ are kernels of type (q, p) , and P, Q are polynomials of order $p - 1$, Lemma 9 implies that $K(x_i) = W(x_i)P(x_i) = W(x_i)Q(x_i)$ for every data point x_i . Thus K is the equivalent kernel for the local polynomial regression with the weights w_i .

Proof of Theorem 5. It is sufficient to check that weightings $W_1(y) = 1 - y$ and $W_3(y) = 1 - y^2$ have the same equivalent kernel. Let $Q_1(y)$ and $Q_3(y)$ be their respective factor polynomials. Since Q_3 is a polynomial of order $p - 1$, then W_3Q_3 is a polynomial of order $p + 1$. Since W_3 is even and the placement of data points is symmetric, the equivalent kernel, W_3Q_3 , is an even function (if q is even) or an odd function (if q is odd). The difference $p - q$ is even, thus W_3Q_3 can not have term y^{p+1} . Therefore, W_3Q_3 is a polynomial of order p , and the true order of Q_3 is at most $p - 2$. Now we notice that $W_3(y)Q_3(y) = W_1(y)[(1 + y)Q_3(y)]$. Both $(1 + y)Q_3(y)$ and $Q_1(y)$ are polynomials of order $p - 1$. Thus Lemma 9 implies that $W_3(y)Q_3(y) = W_1(y)Q_1(y)$ when $y = \frac{x_i - t}{h}$.

Proof of Theorem 6. First, we show that for every $-1 \leq z \leq 0$, the normalized kernel $G(y) = G(z, y)$, given by Eq. (5.5), has at least one root outside $(-1, 1)$. Indeed,

since $P_k(1) = 1$, $P_k(-1) = (-1)^k$, we have $G(1) = \gamma_q(2q + 3)z(z + 1)$, $G(-1) = \gamma_q(2q + 3)z(z - 1)$. If $z = 0$, we have $G(1) = G(-1) = 0$. If $z = -1$, we have $G(1) = 0$. If $z \neq 0$, $z \neq -1$, we have $\text{sign } G(1) \cdot \text{sign } G(-1) = (-1)^{q+1}$. On the other hand, $G(y)/G(-y) \rightarrow (-1)^q$ as $y \rightarrow \infty$. Therefore, G must have a root $y_0 = y_0(z)$ either in $[1, \infty)$ or in $(-\infty, -1]$. Since G is a polynomial of order p , the number of roots within $(-1, 1)$ is at most $p - 1$. Representing $G(y) = |y - y_0|Q(y)$ and applying the continuous version of Lemma 9, we conclude that the local polynomial regression with the linear weighting $|y - y_0|$, estimation point z , and support $[-1, 1]$, has $G(y)$ as its equivalent kernel. If $z = -1$ (the edge estimation case), then $G(1) = 0$, $y_0 = 1$, and the equivalent linear weighting is $1 - y$. If $z = 0$ (the touch point estimation), then $G(1) = G(-1) = 0$, and either of $1 - y$ and $1 + y$ weightings has G as the equivalent kernel. By the continuous version of Lemma 9, the weighting $1 - y^2$ also has G as its equivalent kernel.

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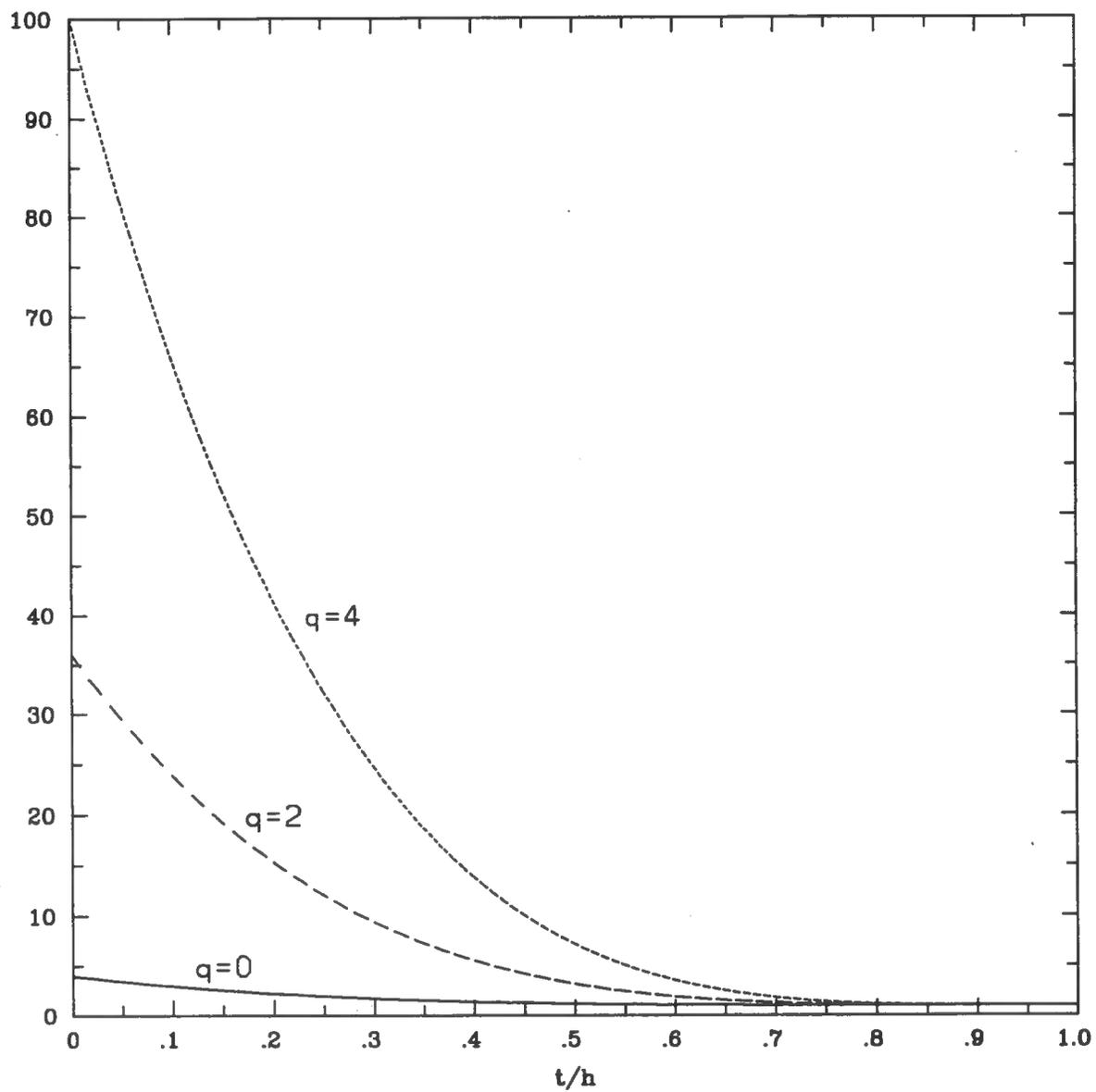


Figure 1. Ratio of EMSEs of the optimal boundary kernel to the optimal interior kernel, $h=h_0$

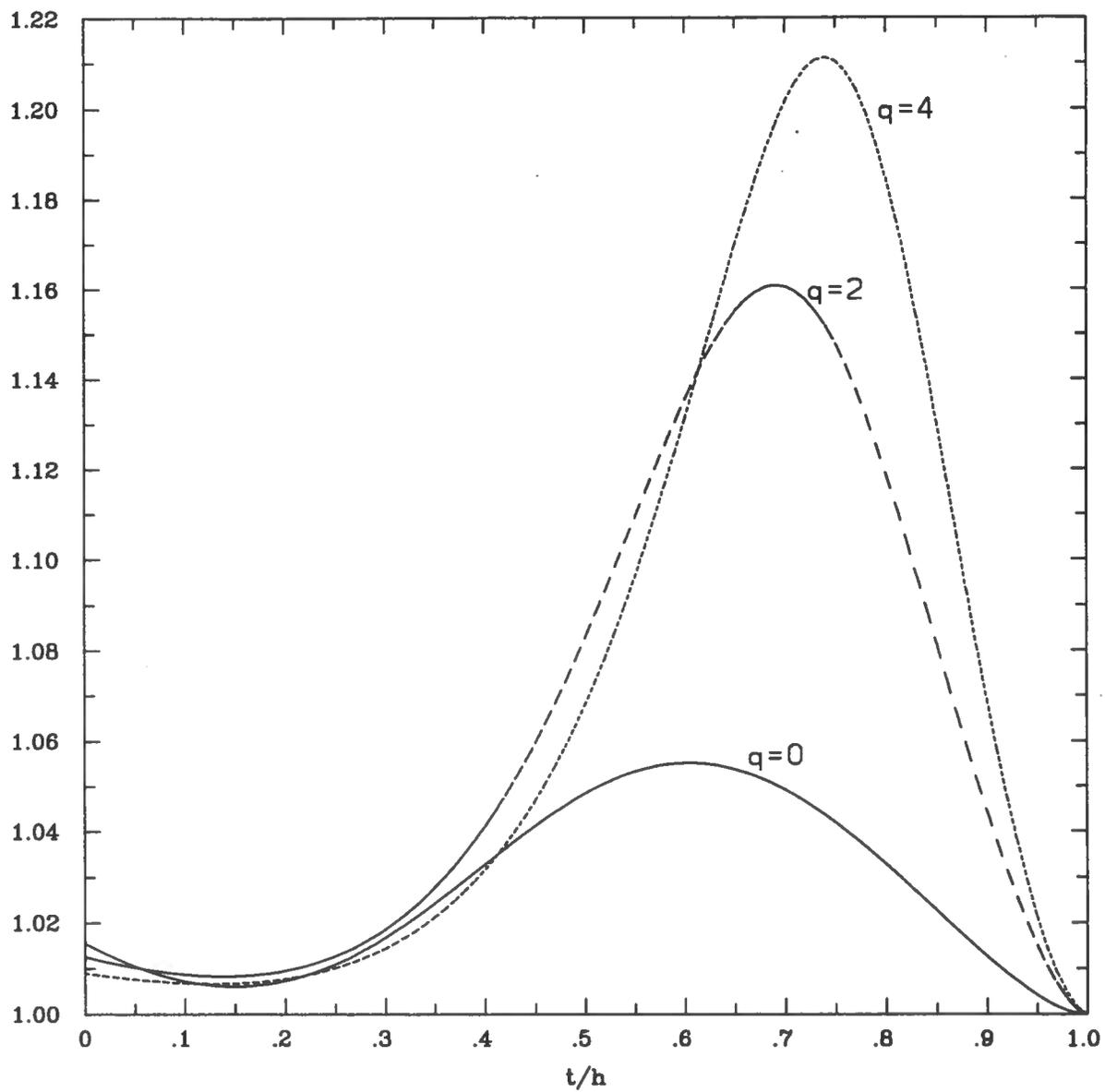


Figure 2. Ratio of EMSEs of Bartlett-Priestley weighting to the optimal kernel, $h=h_0$

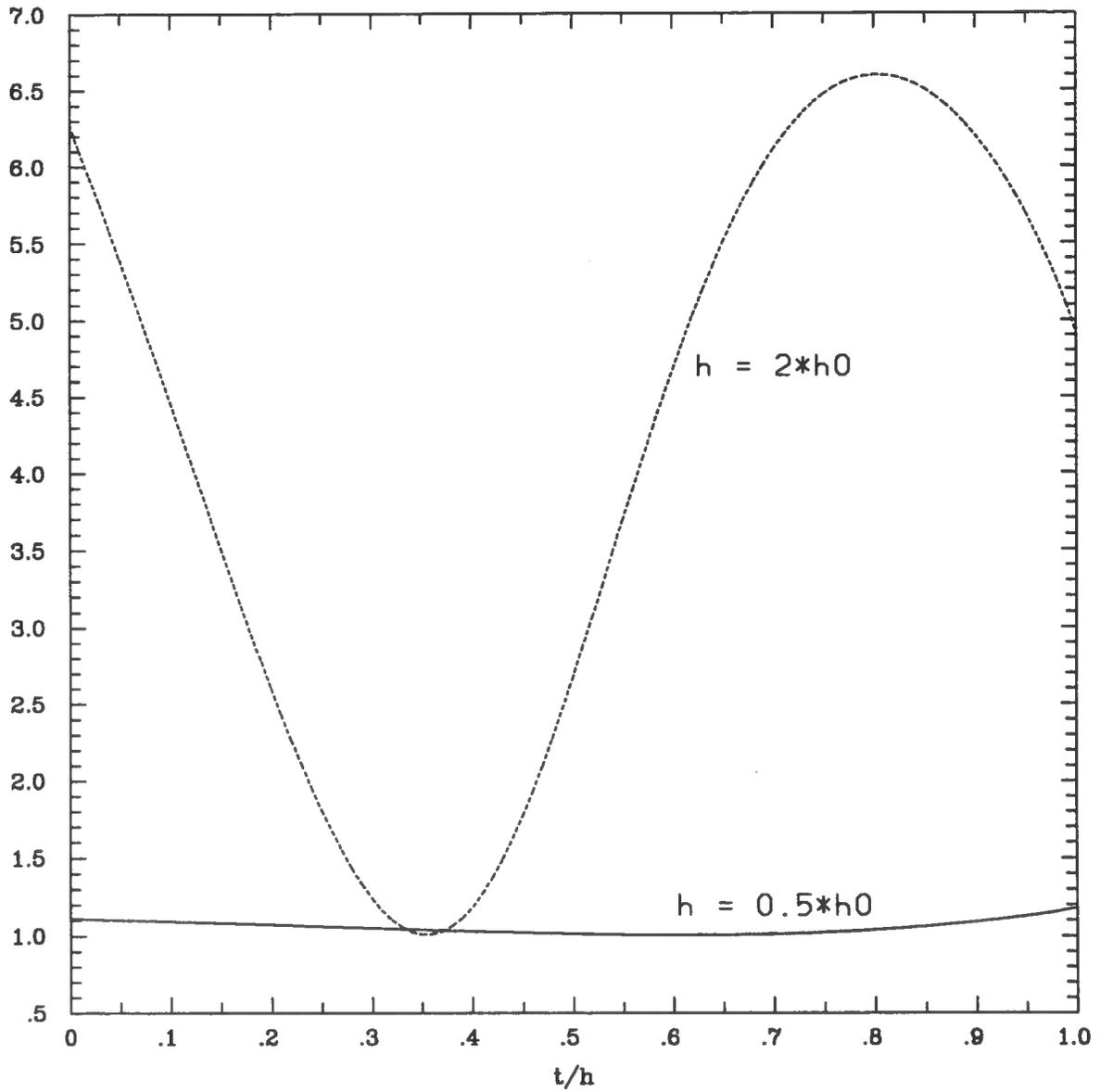


Figure 3. Ratio of EMSEs of Bartlett-Priestley weighting to the optimal kernel, $q=0$

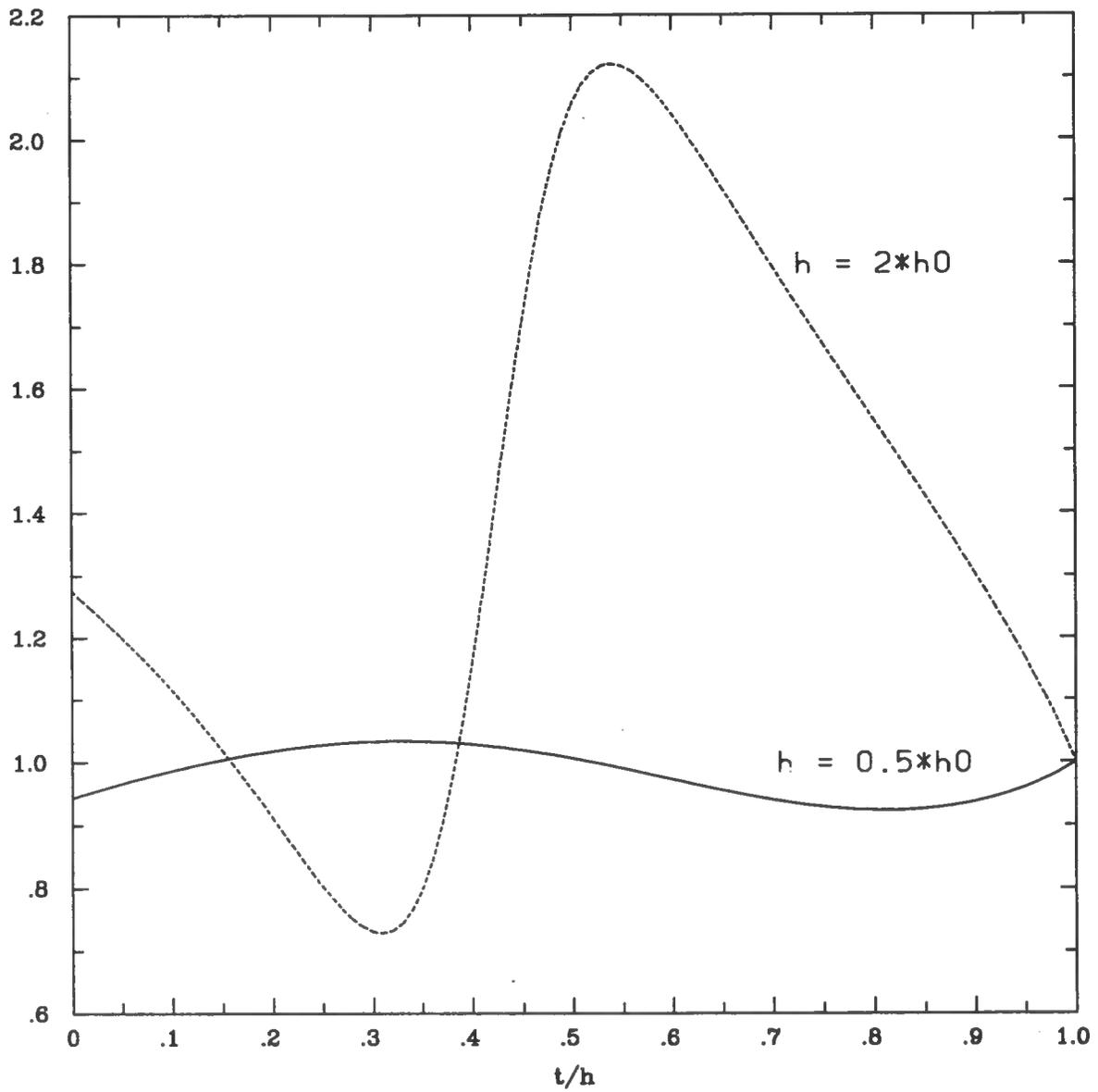


Figure 4. Ratio of EMSEs of Bartlett-Priestley weighting to the asymptotically optimal weighting, $q=0$

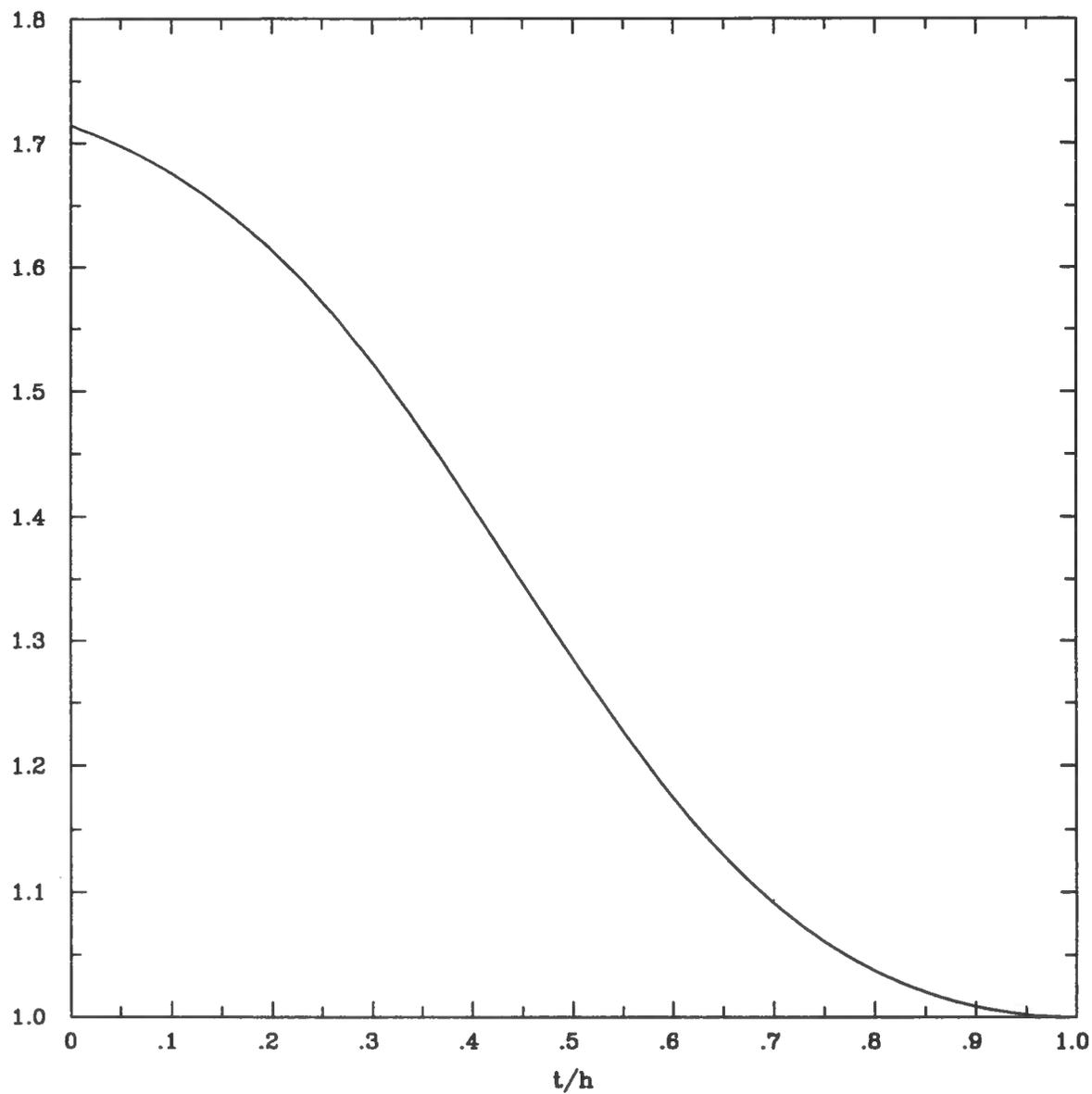


Figure 5. Ratio of EMSEs of the Mueller boundary kernel to the optimal boundary kernel, $q=0$, $h=h_0$