A unified framework for spline estimators

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Abstract

This article develops a unified framework to study the asymptotic properties of all periodic spline-based estimators, that is, of regression, penalized and smoothing splines. The explicit form of the periodic Demmler–Reinsch basis in terms of exponential splines allows the derivation of an expression for the asymptotic equivalent kernel on the real line for all spline estimators simultaneously. The corresponding bandwidth, which drives the asymptotic behavior of spline estimators, is shown to be a function of the number of knots and the smoothing parameter. Strategies for the selection of the optimal bandwidth and other model parameters are discussed.

Keywords: B-spline; Equivalent kernel; Euler–Frobenius polynomial; Exponential spline; Demmler–Reinsch basis.

1 Introduction

Consider a nonparametric regression model for the data pairs \((y_i, x_i)\)

\[ y_i = f(x_i) + \epsilon_i \quad (i = 1, \ldots, N), \tag{1} \]
with the standard assumptions on the random errors, that is \( E(\epsilon_i) = 0 \) and \( E(\epsilon_i \epsilon_j) = \sigma^2 \delta_{ij} \) with \( \sigma^2 > 0 \) and \( \delta_{ij} \) the Kronecker delta. Any nonparametric linear estimator of \( f \) can be written as \( \hat{f}(x) = n^{-1} \sum_{i=1}^{n} W(x, x_i)y_i \). For kernel estimators the weight function \( W(x, t) = h^{-1}K(x/h, t/h) \) for some bandwidth \( h > 0 \) is given explicitly (Gasser and Müller, 1979) and is called the kernel function. This representation of \( \hat{f} \) allows a straightforward study of its properties.

Another class of nonparametric linear estimators is the spline-based estimators: smoothing splines (Wahba, 1975), regression splines (Agarwal and Studden, 1980) and penalized splines (Ruppert et al., 2003). Penalized splines combine projection onto a low-dimensional spline space with a roughness penalty and circumvent certain practical disadvantages of smoothing and regression splines. For all spline-based estimators the exact form of kernel \( K(x, t) \) is unknown, but it can be sufficiently well approximated for smoothing and regression splines. Such an approximation is called the asymptotic equivalent kernel and is employed to study the local asymptotic properties of spline estimators. Cogburn and Davis (1974) obtained the asymptotic equivalent kernel for smoothing splines on the real line using Fourier techniques. Messer and Goldstein (1993) and Thomas-Agnan (1996), see also Berlien and Thomas-Agnan (2004), extended this kernel to the case of a bounded interval. Eggermont and LaRiccia (2006) refined these results. Other references on equivalent kernels for smoothing splines are Silverman (1984), Nychka (1995) and Abramovich and Grinshtein (1999). Equivalent kernels for regression splines have been derived only on the real line in terms of B-splines of degree three in Huang and Studden (1993).

The asymptotic properties of penalized spline estimators have received attention only recently. Claeskens et al. (2009) show that depending on the number of knots taken, penalized splines have asymptotic behaviour similar either to regression or to smoothing splines. Wang et al. (2011) proved that for a certain number of knots the asymptotic equivalent kernel of penalized spline estimators is asymptotically equivalent to that of the smoothing spline estimators.

In this article we aim to study all spline-based estimators in a unified framework. A new explicit expression for the Demmler–Reinsch basis for periodic splines allows us to derive asymptotic equivalent kernels on the real line for all spline estimators that deliver insights into the local asymptotic behavior of spline estimators, depending on a certain parameter that is a function of the number of knots and the smoothing parameter.

2 Model and equivalent kernels

Consider the nonparametric regression model (1). Let the data be equally spaced on the interval \([0, 1]\), i.e., \( x_i = i/N \) \( (i = 1, \ldots, N) \). The unknown regression function \( f \) is assumed to be sufficiently smooth. More precisely, \( f \in H_{p+1}[0, 1] = \{ f : f \in C^p, \int_0^1 (f^{(p+1)}(x))^2 dx < \infty \} \). To estimate \( f \in H_{p+1}[0, 1] \), first define a partition of \([0, 1]\) into \( K \leq N \) equidistant intervals \( \tau_K = \{ 0 = \tau_0 < \tau_1 < \cdots < \tau_{K-1} < \tau_K = 1 \} \).
with \( \tau_i = i/K \) (\( i = 0, \ldots, K \)). The spline space \( S(p; \Xi_K) \) of degree \( p > 0 \) based on \( \Xi_K \) consists of functions \( s \in C^{p-1}[0,1], \) such that \( s \) is a degree \( p \) polynomial on each \( [\tau_i, \tau_{i+1}) \) (\( i = 0, \ldots, K - 1 \)). The spline estimator \( \hat{f} \) is the solution to

\[
\min_{s \in S(p; \Xi_K)} \left[ \frac{1}{N} \sum_{i=1}^{N} (Y_i - s(x_i))^2 + \lambda \int_{0}^{1} \{s^{(q)}(x)\}^2 \, dx \right], \quad \lambda \geq 0, \quad 0 < q \leq p. \tag{2}
\]

For \( K = N \) and \( p = 2q - 1 \) the solution to (2) is the smoothing spline estimator. If \( \lambda = 0 \) and \( K \ll N, \) (2) yields the regression spline estimator, and a general estimator with \( K < N, \) \( p + 1 > q > 0 \) and \( \lambda > 0 \) is the penalized spline estimator. A solution to (2) can be written as \( \hat{f}(x) = N^{-1} \sum_{i=1}^{n} W^{(0,1)}(x, x_i) Y_i, \) where the bandwidth \( h = h(n) > 0 \) decays to zero such that \( nh(n) \to \infty. \) The weight function \( W^{(0,1)}(x, t) \) depends on the observations \( x_i \) and on \( N \) and therefore is called the effective kernel. Let \( W^{(0,1)}(x, t) \) denote an approximation to \( W^{(1,1)}(x, t), \) which is independent of \( x_i, \) \( N \) and such that \( E \left\{ \sup_{x,q} |\hat{f}(x) - N^{-1} \sum_{i=1}^{N} W^{(0,1)}(x, x_i) Y_i| \right\} \) is negligible compared to the bias of \( \hat{f}. \)

Then, \( \mathcal{W}^{(0,1)}(x, t) \) is called the asymptotic equivalent kernel for \( \hat{f}. \) Typically, \( \mathcal{W}^{(0,1)}(x, t) \) is found as a sum \( \mathcal{W}^{(0,1)}(x, t) = \mathcal{W}(x, t) + \mathcal{W}^b(x, t). \) Here, \( \mathcal{W}(x, t) \) corresponds to the asymptotic equivalent kernel on the real line and \( \mathcal{W}^b(x, t) \) is the asymptotic boundary kernel, which decays exponentially away from the boundaries. In particular, \( \hat{f}(x) \approx N^{-1} \sum_{i=1}^{N} \mathcal{W}(x, x_i) Y_i \) for \( x \) away from the boundaries.

The available results on equivalent kernels for spline estimators can be summarised as follows. For smoothing splines \( \mathcal{W}^{(0,1)}_{ss}(x, t) \) has been approximated by the Green’s function for the Euler equations

\[
f(x) + \lambda (-1)^q f^{(2q)}(x) = g(x), \quad x \in (0,1), \quad \lambda > 0,
\]

\[
f^{(j)}(0) = f^{(j)}(1) = 0 \quad (j = q, \ldots, 2q - 1). \tag{3}
\]

The solution to (3) is found in two steps. First, a fundamental solution is obtained as the Green’s function of Euler equation (3) with \( \lim_{|x| \to \infty} f^{(j)}(x) = 0 \) (\( j = q, \ldots, 2q - 1 \)). This Green’s function is the asymptotic equivalent kernel \( \mathcal{W}_{ss}(\cdot, t) \) on the real line and is known explicitly for each \( q. \) In particular, scaling with \( h = \lambda^{1/(2q)} > 0 \) gives

\[
h \mathcal{W}_{ss}(hx, ht) = \mathcal{K}_{ss}(x, t) = \sum_{j=0}^{q-1} \frac{i \exp \{i x - t \} \exp \{i \pi (2j + 1)/(2q)\}}{2q \exp \{i \pi (2q - 1)(2j + 1)/(2q)\}}, \quad x, t, \in \mathbb{R}. \tag{4}
\]

Here and subsequently \( i = (-1)^{1/2}. \) At the second step the boundary conditions are matched, which leads to the corresponding boundary kernel \( \mathcal{W}^b_{ss}(x, t). \) An explicit expression for this boundary kernel for \( q = 1, 2 \) can be found, for example in [Thomas-Agnan (1996)]. For \( q > 2 \) derivation of \( \mathcal{W}^b_{ss}(x, t) \) becomes very tedious.

For regression splines the asymptotic equivalent kernel on \( \mathbb{R} \) \( \mathcal{W}_{rs}(x, t) \) was obtained by [Huang and Studden (1993)] for \( p = 3 \) only as a \( L_2 \) projection kernel on a spline space.
defined on \( \mathbb{R} \). More precisely, for \( f \in L^2(\mathbb{R}) \),

\[
\int_{-\infty}^{\infty} W_{rs}(\cdot, t)f(t)dt = \arg \min_{s \in S(p, \mathbb{Z})} \int_{-\infty}^{\infty} \{s(x) - f(x)\}^2 dx.
\]

The spline space \( S(p, \mathbb{Z}) = \{s(x) : s(x) = \sum_{i=\infty}^{\infty} N_i(x)\theta_i, \ \theta = (\theta_i)_{i \in \mathbb{Z}} \in l_2\} \), where \( N_i(x) \) denotes a B-spline centered at \( i \), is the \( L^2(\mathbb{R}) \) subspace of splines with integer knots. With \( h = K^{-1} \) Huang and Studden (1993) give the expression for \( h W_{rs}(hx, ht) = K_{rs}(x, t) \) in terms of normalised cubic B-splines. In contrast to the asymptotic equivalent kernel for smoothing splines, \( K_{rs}(x, t) \) is not translation-invariant. The boundary kernel for regression splines \( W_{bs}(x, t) \) has not been obtained.

The derivations of \( W_{ss}(x, t) \) and \( W_{rs}(x, t) \) seem to differ greatly both technically and conceptually. In the following we derive the asymptotic equivalent kernel on the real line \( W(x, t) \) for all spline estimators in a unified framework for general \( p, q, K \) and \( \lambda \), and study the pointwise asymptotic properties of all spline estimators away from the boundaries.

### 3 Periodic spline spaces

Let us first introduce some notation. Let

\[
Q_{p-1}(z) = \sum_{l=\infty}^{\infty} \text{sinc}\{\pi(z + l)\}^{p+1},
\]

a polynomial of \( \cos(\pi z) \) of degree \( (p - 1) \), which can be expressed in terms of Euler–Frobenius polynomials \( \Pi_p(\cdot) \) [Schoenberg, 1973]:

\[
Q_{p-1}(z) = \begin{cases} 
\exp\{iz\pi(p-1)\} \Pi_p\{\exp(-2i\pi z)\}/p!, & p \text{ odd,} \\
\exp\{iz\pi(p-1)\} \bar{\Pi}_p(z)/p!, & p \text{ even,}
\end{cases}
\]

for

\[
\bar{\Pi}_p(z) = \cos(\pi z/2)^{p+1} \Pi_p\{\exp(-\pi iz)\} - (-1)^{p/2}i \sin(\pi z/2)^{p+1} \Pi_p\{-\exp(-\pi iz)\}.
\]

Further, we make use of the exponential splines [Schoenberg, 1973]

\[
\Phi_p(t, z) = z^{|t|} (1 - z^{-1})^p \sum_{j=0}^{p} \binom{p}{j} \frac{t^{|j|}}{p!} \frac{\Pi_j(z)}{(z - 1)^j}, \quad z \neq 0, \ z \neq 1,
\]

(6)
where \( \{ t \} \) denotes the fractional part of \( t \) and \( \lfloor t \rfloor \) is the largest integer not greater than \( t \). With the convention \( 0^0 = 1 \), one can also define \( \Phi_p(t, 1) = 1 \). Note that

\[
\Phi_p \{ t, \exp(2\pi it) \} = \frac{\exp(2\pi iz)}{\exp(\pi iz(p + 1))} \sum_{l=-\infty}^{\infty} (-1)^{(p+1)} \text{sinc} \{ \pi (z + l) \}^{p+1} \exp(2\pi ilt). \tag{7}
\]

Next, we define

\[
Q_{p,M}(z) = \frac{1}{N} \sum_{i=1}^{N} \left| \Phi_p \left\{ i/M + (p + 1)/2, \exp(-2\pi iz) \right\} \right|^2, \tag{8}
\]

where \( M = N/K \). For \( M = 1 \) we find \( Q_{p,1}(z) = Q_{p-1}^2(z) \), since \( \Phi \left\{ (p + 1)/2, \exp(2\pi iz) \right\} = \Phi_{p-1}(z) \) from (7). If \( M = N/K > 1 \), then \( Q_{p,M}(z) \) varies between \( Q_{2p}(z) \) and \( Q_{2p-1}^2(z) \), depending on \( M \). In particular, it can be shown that \( Q_{p,M}(z) = Q_{2p}(z) + c \sin(\pi z)^{p+1} M^{-p+1} \), for a constant \( c > 0 \).

Now we state a lemma giving the explicit expression for the complex-valued Demmler and Reinsch (1975) basis for the periodic spline space \( S_{\text{per}}(p; \mathbb{Z}_K) = \{ s : s \in S(p; \mathbb{Z}_K) \text{ and } s^{(j)}(0) = s^{(j)}(1), \ j = 0, \ldots, p-1 \} \).

**Lemma 1** The functions

\[
\psi_i(x) = \frac{\Phi_p \{ Kx + (p + 1)/2, \exp(-2\pi i i/K) \}}{\{Q_{p,M}(i/K)\}^{1/2}} \quad (i = 1, \ldots, K), \quad x \in \mathbb{R}, \tag{9}
\]

form the complex-valued Demmler-Reinsch basis in \( S_{\text{per}}(p; \mathbb{Z}_K) \), i.e.,

\[
\frac{1}{N} \sum_{i=1}^{N} \psi_i(l/N)\overline{\psi_j(l/N)} = \delta_{i,j}, \tag{10}
\]

\[
\int_0^1 \overline{\psi_i^{(q)}(x)} \psi_j^{(q)}(x) dx = \nu_i \delta_{i,j} \quad (i, j = 1, \ldots, K) \tag{11}
\]

and the eigenvalues

\[
\nu_i = (2\pi i)^{2q} \text{sinc}(\pi i/K)^{2q} \frac{Q_{2p-2q}^2(i/K)}{Q_{p,M}(i/K)}. \tag{12}
\]

Moreover, the functions

\[
\phi_i(x) = \frac{\Phi_p \{ Kx + (p + 1)/2, \exp(-2\pi i i/K) \}}{\{Q_{2p}(i/K)\}^{1/2}} \quad (i = 1, \ldots, K),
\]
satisfy
\[
\int_0^1 \phi_i(x)\overline{\phi_j(x)}\,dx = \delta_{i,j} = \frac{1}{\mu_i} \int_0^1 \phi_i^{(q)}(x)\overline{\phi_j^{(q)}(x)}\,dx
\]  
(13)
for \(\mu_i = (2\pi i)^{2q}\text{sinc}(\pi i/K)^{2q}Q_{2p-2q}(i/K)/Q_{2p}(i/K)\).

The basis functions \(\psi_i(x)\) is the scaled discrete Fourier transform of periodic B-splines \(\psi_i(x)K\{Q_p,M(i/K)\}^{1/2} = \sum_{i=1}^K B_i(x) \exp(-2\pi i l/K)\). A similar basis up to a scaling factor for \(N = K\) has been considered by Lee et al. (1992) and Zheludev (1998).

Even though the Demmler–Reinsch basis for periodic smoothing splines was employed by Cogburn and Davis (1974) and Craven and Wahba (1978), no explicit expressions for \(\psi_i\) and \(\nu_i\) were given there. For \(K = N\) and \(p = 2q-1\), \(\nu_i = (2\pi i)^{2q}\text{sinc}(\pi i/K)^{2q}Q_{2p-2q}(i/K)^{-1}\) and at the data points \(l/N\), the Demmler–Reinsch basis reduces to \(\psi_i(l/N) = \exp(-2\pi i l)\).

Thus, any \(s \in S_{\text{per}}(p,\mathbb{T}_K)\) can be represented as \(s(x) = \sum_{i=1}^K \beta_i \psi_i(x)\) and the solution to (2) over the special class of periodic splines \(S_{\text{per}}(p,\mathbb{T}_K)\) results in

\[
\hat{f}_{\text{per}}(x) = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^K \psi_j(x)\overline{\psi_j(x_i)}(1 + \lambda \nu_i)^{-1},
\]

where \(W_{\text{per}}^{(0,1)}(x,t) = \sum_{i=1}^K \psi_i(x)\overline{\psi_i(t)}(1 + \lambda \nu_i)^{-1}\), with \(\psi_i(t)\) denoting the complex conjugate, is the effective kernel for periodic spline estimators, which depends on \(N\) via \(Q_p,M\). The corresponding asymptotic equivalent kernel is \(W_{\text{per}}^{[0,1]}(x,t) = \sum_{i=1}^K \phi_i(x)\overline{\phi_i(t)}(1 + \lambda \mu_i)^{-1}\), and is such that

\[
\int_0^1 W_{\text{per}}^{[0,1]}(\cdot,x)f(x)\,dx = \min_{s \in S_{\text{per}}(p,\mathbb{T}_K)} \left[ \int_0^1 \{s(x) - f(x)\}^2\,dx + \lambda \int_0^1 \{s(\cdot)\}^2\,dx \right].
\]

Both \(W_{\text{per}}^{[0,1]}(x,t)\) and \(W_{\text{per}}^{[0,1]}(x,t)\) are known explicitly.

4 Asymptotic equivalent kernels on \(\mathbb{R}\)

Let

\[
W(x,t) = \int_0^1 \phi(u,x)\overline{\phi(u,t)}\,du,
\]

where \(\mu(u) = (2\pi u)^{2q}\text{sinc}(\pi u/K)^{2q}Q_{2p-2q}(u/K)/Q_{2p}(u/K)\) and \(\phi(u,x) = \Phi_p\{Kx + (p+1)/2, \exp(-2\pi i u/K)\}\{Q_{2p}(u/K)\}^{-1/2}\). As shown in the proof of Lemma 3, \(W_{\text{per}}^{[0,1]}(x,t)\) can be obtained by folding back \(W(x,t)\), that is \(W_{\text{per}}^{[0,1]}(x,t) = \sum_{l=-\infty}^\infty W(x,t+l)\). In particular, for a periodic function \(f\) one finds \(\int_0^1 W_{\text{per}}^{[0,1]}(x,t)f(t)\,dt = \int_{-\infty}^\infty W(x,t)f(t)\,dt\). Subsequently, we refer to \(W(x,t)\) as the asymptotic equivalent kernel for spline estimators on \(\mathbb{R}\). The following lemma gives the explicit expression for \(W(x,t)\).
Lemma 2 Let

\[ P_{2p}(u) = \Pi_{2p}(u) + (-1)^q \lambda K^{2q}(1-u)^{2q}\Pi_{2p-2q+1}(u)/(2p-2q+1)! \]  

be a polynomial of degree 2p where \( \Pi_p(u) \) is the Euler–Frobenius polynomial. Let also \( r_j, r_j^{-1}, j = 1, \ldots, p \) be the roots of \( P_{2p}(u) \) with \( |r_j| < 1 \). Then, denoting \( P_{2p}(r_j) = \partial P_{2p}(u)/\partial u |_{u=r_j} \), \( d_{x,t} = [K x - \{(p+1)/2\}] - [K t - \{(p+1)/2\}] \) and representing \( z^p - d_{x,t} \Phi_p \{K x + (p+1)/2, z\} \Phi_p \{K t + (p+1)/2, z^{-1}\} = \sum_{i=0}^{2p} \alpha_l(\{K x\}, \{K t\})z^l \) for some functions \( \alpha_l(t_1, t_2) \) and \( x, t \in \mathbb{R} \), results in

\[ \mathcal{W}(x, t) = K \sum_{j=1}^{p} \sum_{l=0}^{2p} \alpha_l(\{K x\}, \{K t\})r_j^{[d_{x,t}+l-1]+(2p-2l)(d_{x,t}+l\leq 0)}, \]  

where \( \mathbb{I}(A) \) is an indicator function, which is equal to 1 if \( A \) is true and 0 otherwise.

For \( p = q = 1 \) a simple equivalent kernel \( \mathcal{W}(x, t) \) has a simple representation, for larger \( p \) and \( q \) it becomes much more involved. For \( p = q = 1 \) one finds \( r_1 = 1 - \{(3 + 36\lambda K^2)/3\}/(6\lambda K^2 - 1) \), \( P_{2p}(r_1) = \{(2 + 12\lambda K^2)/3\}^{1/2} \), \( \alpha_2(t_1, t_2) = \alpha_0(t_2, t_1) = t_1 - t_1 t_2 \) and \( \alpha_1(t_1, t_2) = 1 - \alpha_0(t_1, t_2) - \alpha_0(t_2, t_1) \). Expression (15) for the asymptotic equivalent kernel on \( \mathbb{R} \) is valid for any combinations of \( p, q, K \) and \( \lambda \). The next lemma gives the order of this kernel. Let \( \mu_m(\mathcal{W}) = \int_{-\infty}^{\infty} t^m \mathcal{W}(x, t) dt \).

Lemma 3 For \( x, t \in \mathbb{R} \), \( d = \min\{p+1, 2q\} \) and \( m \in \mathbb{N}_0 \),

\[ \mu_m(\mathcal{W}) = \begin{cases} 1, & m = 0, \\ 0, & m = 1, \ldots, d - 1, \\ -\mathbb{I}(d = 2q) \cdot 2q \lambda (2q)!, & m = d, \end{cases} \]

with \( \mathcal{B}_{p+1}(x) \) a \((p+1)\)-th degree Bernoulli polynomial.

To establish the correspondence between our results and the known asymptotic equivalent kernels on \( \mathbb{R} \) for smoothing and regression spline estimators, we must first determine an appropriate bandwidth, which is universal for all spline estimators. Let us define the variable \( k_q = \lambda^{1/(2q)} \pi K \), which characterizes the type of the spline estimator. In particular, \( k_q = 0 \) corresponds to the regression spline estimator, \( k_q = \lambda^{1/(2q)} \pi N \) to the smoothing spline estimator and all intermediate values characterize penalized spline estimators. With this, we introduce the bandwidth \( h(k_q) \), which is universal for all spline estimators, given by

\[ h(k_q)^{-1} = \int_{0}^{K} \frac{dx}{1 + \lambda (\pi x)^{2q}} = \lambda^{-1/(2q)} \pi^{-1} \int_{0}^{k_q} \frac{dx}{1 + x^{2q}}. \]

Bandwidth \( h(k_q) \) is a smooth function of \( k_q \) with a rather complicated closed form expression available for each \( q \). In our subsequent developments we use the following rep-
presentation.

\[ h(k_q)^{-1} = \lambda^{-1/(2q) \pi^{-1}} \begin{cases} k_q c_1, & k_q < 1, \\ \pi c_2, & k_q \geq 1, \end{cases} \]  

(16)

with constants \( c_1 = c_1(k_q) = 2 \mathcal{F}_1\{1, 1/(2q)\}; \{1 + 1/(2q)\}, -k_q^{2q} \) and \( c_2 = c_2(k_q) = \bar{c}_2 - \pi^{-1} k_q^{1-2q} 2 \mathcal{F}_1\{1, 1-1/(2q)\}; \{2-1/(2q)\}, -k_q^{-2q} / (2q-1) \), where \( \bar{c}_2 = \pi^{-1} \text{sinc}\{\pi/(2q)\}^{-1} \) is independent of \( k_q \) and \( 2 \mathcal{F}_1 \) denoting the hypergeometric series (Abramowitz and Stegun, 1972). Both \( c_1(k_q) \) and \( c_2(k_q) \) are convergent and vary slowly with \( k_q \), namely \( c_1(k_q) \in (\pi/4, 1] \) for any \( k_q < 1 \) and \( c_2(k_q) \in (1/4, 1/2] \) for any \( k_q \geq 1 \). For the regression spline estimators, \( k_q = 0 \), the bandwidth \( h(0) = K^{-1} \) and for the smoothing spline estimators, \( k_q \to \infty \), the bandwidth \( h(\infty) = \lambda^{1/(2q)}/\bar{c}_2 \).

This separation into two cases for \( k_q < 1 \) and \( k_q \geq 1 \) was introduced by Claeskens et al. (2009). If \( k_q < 1 \), then the asymptotic behaviour of the penalized spline estimator is similar to that of the regression spline estimator, while \( k_q \geq 1 \) corresponds to asymptotic behaviour similar to that of smoothing splines.

Let \( \mathcal{K}(x, t) \) denote the scaled version of the equivalent kernel on \( \mathbb{R} \), i.e.,

\[ h(k_q) \mathcal{W} \{ h(k_q) x, h(k_q) t \} = \mathcal{K}(x, t). \]

**Theorem 1** The equivalent kernel for spline estimators on \( \mathbb{R} \) with \( p = 2q - 1 \) satisfies

\[
\begin{align*}
& c_1 \mathcal{K}(c_1 x, c_1 t) = \mathcal{K}_{rs}(x, t) - k_q^{2q} \mathcal{K}_1(x, t), & k_q < 1, \\
& c_2 \mathcal{K}(c_2 x, c_2 t) = \mathcal{K}_{ss}(t-x) + k_q^{-2q} \mathcal{K}_2(x, t), & k_q \geq 1,
\end{align*}
\]

where \( \mathcal{K}_1(x, t) \) and \( \mathcal{K}_2(x, t) \) are bounded functions given in the proof, \( \mathcal{K}_{rs}(x, t) \) is the asymptotic regression spline equivalent kernel on \( \mathbb{R} \), i.e.,

\[ \mathcal{K}_{rs}(x, t) = \sum_{j=1}^{p} \sum_{l=0}^{2p_j} \frac{\alpha_l \{x_j, \{t\}\}}{P_{2p_l}(r_j)} r_j^{d_{x,t} + l - 1} \big( d_{x,t} + l \big)^{(2p_l-2)I(d_{x,t} + l \leq 0)}, \]

with \( \alpha_l \), \( r_j \), \( d_{x,t} \), \( P_{2p_l}(u) = \Pi_{2p_l}(u) \) defined in Lemma 2 and \( \mathcal{K}_{ss}(x, t) \) the asymptotic smoothing spline equivalent kernel on \( \mathbb{R} \) as given in (4).

Theorem 1 implies that if \( k_q < 1 \), then the asymptotic equivalent kernel on \( \mathbb{R} \) for spline estimators is dominated by \( \mathcal{K}_{rs}(x, t) \), the asymptotic equivalent regression spline kernel on \( \mathbb{R} \), while for \( k_q \geq 1 \) \( \mathcal{K}(x, t) \) is dominated by \( \mathcal{K}_{ss}(x, t) \), which agrees with the findings of Claeskens et al. (2009). Moreover, if \( p = 2q - 1 \), then \( \mathcal{K}(x, t) \) varies smoothly between \( \mathcal{K}_{rs}(x, t) \) and \( \mathcal{K}_{ss}(x, t) \), appropriately scaled, both having the same order. In particular, \( \lim_{k_q \to \infty} c_2 \mathcal{K}(c_2 x, c_2 t) = \bar{c}_2^{-1} \mathcal{K}_{ss}\{x - t\}/\bar{c}_2 \) and \( \lim_{k_q \to 0} c_1 \mathcal{K}(c_1 x, c_1 t) = \mathcal{K}_{rs}(x, t) \).

Figure 1 depicts the penalized spline kernel \( \mathcal{K}(x, t) \) at \( t = 0 \) and \( t = 0.3 \) as a function of
Figure 1: Equivalent kernels $K(x, 0)$ (left) and $K(x, 0.3)$ (right) for $p = q = 1$ (top) and $p = 2q - 1 = 3$ (bottom) and different values of $k_q$. The grey line corresponds to the smoothing spline kernel, the bold line to the regression spline kernel, the dashed and dotted lines to the penalized spline kernel with $k_q = 1$ and $k_q = 5$, respectively.

$x$ for different values of $k_q$ and for $p = 1, 3$. The case $k_q = 0$ corresponds to $K_{rs}(x, t)$. As $k_q$ grows, $K(x, t)$ becomes more symmetric and for $k_q = 5$ is already indistinguishable from the smoothing spline kernel.

From Lemma 2 the expression for $K(x, t)$ can be obtained for any combination of $p$ and $q$. However, if $p \neq 2q - 1$, then no smooth transition between two scenarios with $k_q < 1$ and $k_q \geq 1$ is possible. In this case the orders of the asymptotic equivalent regression and smoothing spline kernels will be different and, hence, the asymptotic rates of the corresponding estimators, see also discussion on the parameter choice in Section 6. To keep the exposition clear, in the next section we focus on the case $p = 2q - 1$. 
5 Local asymptotics of spline estimators

The following theorem gives the pointwise bias and variance of all spline estimators away from the boundaries.

**Theorem 2** Let the model (1) hold and \( \hat{f}(x) \in S(2q - 1; K) \) be the solution to (2) with \( x_i = i/N \) (i = 1, . . . , N) and \( K = \{i/K\}_{i=0}^K \). Then for \( f \in \mathcal{H}_{2q}[0, 1] \), such that \( f^{(2q)} \) is Hölder continuous with \( |f^{(2q)}(x) - f^{(2q)}(t)| \leq L|x-t|^{\alpha}, \ x, t \in [0, 1], \ L > 0 \) and \( \alpha \in (0, 1] \), for any \( x \in I_q = [\delta_q h(q_k) \log \{h(q_k)^{-1}\}, 1 - \delta_q h(q_k) \log \{h(q_k)^{-1}\}] \), we have

\[
E\left\{ \hat{f}(x) \right\} - f(x) = (-1)^{q+1} h(q_k)^{2q} \frac{f^{(2q)}(x)}{(2q)!} C(q_k, x) + o \{h(q_k)^{2q}\} \tag{17}
\]

\[
\text{var} \left\{ \hat{f}(x) \right\} = \frac{\sigma^2}{Nh(q_k)} \int_{-\infty}^{\infty} K \{x/h(q_k), t\}^2 dt + o \{N^{-1} h(q_k)^{-1}\} \tag{18}
\]

where

\[
C(q_k, x) = \begin{cases} 
  c_1^q \left[ (-1)^q \mathcal{B}_{2q} \{Kx\} + (2q)! \pi^{-2q} k^{2q}_q \right], & k_q < 1 \\
  c_2^q \left[ (2q)! \pi^{-2q} k^{2q}_q \right], & k_q \geq 1
\end{cases}
\]

and \( \int_{-\infty}^{\infty} K \{x/h(q_k), t\}^2 dt < C^2/\log(\gamma^{-1}), \) for some \( C \in (0, \infty) \) and \( \gamma \in (0, 1) \), both depending on \( k_q \), explicitly given in the proof of Lemma 4 in the Appendix. The constant \( \delta_q \) in \( I_q \) depends only on \( q \) and \( \gamma \) and it is such that \( \delta_q > 2q \log_q(1/e) \).

If \( f \) is a periodic function, that is \( f \in \mathcal{P}_{2q}[0, 1] = \{f : f \in C^{2q}(\mathbb{R}), f^{(j)}(0 + l) = f^{(j)}(1 + l), \ l \in \mathbb{Z}, j = 0, \ldots, 2q - 1\} \) and \( \hat{f}(x) = \hat{f}_{\text{per}}(x) \in S_{\text{per}}(2q - 1; K) \), then (17) and (18) hold uniformly for all \( x \in [0, 1] \).

It is easy to see that the limiting cases of expression (17) and (18) for \( k_q = 0 \) and \( k_q \to \infty \) coincide with the known results on regression and smoothing splines. \cite{Li and Ruppert, 2008} obtained pointwise bias and variance of penalized spline estimators with a slightly different penalty matrix for the special cases \( p = 0.1 \) with \( q = 1, 2 \) and \( k_q > 1 \). These results also agree with the corresponding equations (17) and (18), up to the expression for the bandwidth, which is given up to a constant only.

An asymptotic optimal bandwidth at any \( x \in I_q \) can be obtained from Theorem 2.

**Corollary 1** Under the assumptions of Theorem 2 the asymptotic optimal bandwidth depending on \( k_q \) for \( f \in \mathcal{H}_{2q}[0, 1] \) at any \( x \in I_q \) and for \( f \in \mathcal{P}_{2q}[0, 1] \) at any \( x \in [0, 1] \) is

\[
h_{\text{opt}}(k_q, x) = \left[ \frac{N - 4qC(q_k, x)^2 \{f^{(2q)}(x)\}^2}{\sigma^2(2q)!^2 \int_{-\infty}^{\infty} K \{x/h(q_k), t\}^2 dt} \right]^{-1/(4q+1)}.
\]

The proof is straightforward from (17) and (18).
6 Choice of parameters

Several parameters for penalized spline estimators must be chosen in practice, i.e., \( p, q, K \) and \( \lambda \). Theorems [1] and [2] allow us to make the following practical recommendations.

Theorem [1] implies that setting \( p = 2q - 1 \) provides a smooth transition between two asymptotic scenarios, that is \( k_q < 1 \) and \( k_q \geq 1 \). In this case, according to Theorem [2], the convergence rate of spline estimators in both scenarios is the same and \( k_q \) enters only the constants, see definition of \( C(k_q, x) \) in Theorem [2]. Hence, it is convenient to choose \( q \) and set \( p = 2q - 1 \) to make the rate of convergence of the estimator independent on the number of knots chosen. The choice of \( q \) depends on the smoothness of the underlying regression function \( f \), but \( q = 2 \) is typically taken in practice.

A second issue is the choice of tuning parameters. For regression or smoothing splines, there is only one tuning parameter, \( K \) or \( \lambda \), respectively, which is typically chosen to minimize an unbiased estimator of the empirical \( L_2 \) risk of the estimator, for example the generalized cross validation criterion. However, in practice one typically prefers to use penalized splines with \( K \ll N \), but still with a penalty tuned by \( \lambda \), so that two parameters need to be selected. A typical approach in practice is to fix \( K \) arbitrarily and then choose \( \lambda \). Ruppert (2002) ran a large simulation study, recommending using \( \min\{N/4, 35\} \) knots in practice. The results of Theorem [2] suggest that first fixing \( K \) and then choosing \( \lambda \) can be problematic. Indeed, if \( K \) is selected so that \( k_q < 1 \), then the bandwidth \( h(k_q) \) would depend on \( K \) with \( \lambda \) entering only \( c_1(k_q) \). Hence, in this case \( \lambda \) cannot be estimated consistently. We argue that both parameters should be chosen simultaneously. One can fix a reasonable value of \( k_q \) and search only over those \( K \)'s and \( \lambda \)s that give this particular \( k_q \). Since for \( p = 2q - 1 \) the convergence rate is independent of \( k_q \), the difference between estimators with different \( k_q \) values would vanish with the growing sample size. The constant \( C(k_q, x) \) from Theorem [2] is a smooth increasing function of \( k_q \), so smaller values could be preferable. However, \( k_q < 1 \) values lead to the regression spline-type estimators, for which not only the number of knots but also their locations is crucial. Hence, fixing \( k_q \) slightly larger than unity in practice would help to avoid the dependence on knot location.

To illustrate this discussion we ran a simulation study with two functions, \( f_1(x) = \sin(6\pi x) \) and \( f_2(x) = \sin(2\pi x)^2 \exp(x) \). We set \( n \in \{300, 1000\} \), \( \sigma = 0.1 \), \( p = 3 \), \( q = 2 \) and consider \( k_q \in \{0.5, 1, 1.2, 1.5, 5\} \). We restricted the range of \( K \) to \( K = 2, \ldots, 50 \) and set \( \lambda = \{k_q/(\pi K)\}^{2q} \) for each given \( k_q \) and all values \( K \). Finally, we evaluated the generalized cross validation criterion \( \text{GCV}(k_q) \), \( k_q \in \{0.5, 1, 1.2, 1.5, 5\} \), for each \( k_q \) choosing those \( K \) and \( \lambda \), that minimize \( \text{GCV}(k_q) \). This procedure is very fast, since the only values of \( K \) and \( \lambda \) considered are such that \( \lambda^{1/(2q)}\pi K \) equals a particular number, which leads to a search over a very sparse grid. Table [6] reports the results from \( M = 500 \) Monte Carlo simulations; here \( A_N(f) = (NM)^{-1} \sum_{j=1}^{N} \sum_{i=1}^{M} \{\hat{f}_i(x_j) - f(x_j)\}^2 \), with \( \hat{f}_i(\cdot) \) denoting the estimator of \( f \) in the \( i \)-th Monte Carlo replication. Choosing \( k_q \) slightly larger than unity leads to a somewhat better average mean squared error, but the differences between spline estimators with different \( k_q \)'s are marginal.
Table 1: $A_N(f_1)$ and $A_N(f_2)$ depending on $N$ and $k_q$. All entries are multiplied by $10^4$.

| $N$   | $A_N(f_1)$ | $A_N(f_2)$ |
|-------|------------|------------|
| 300   | 6.781      | 5.212      |
|       | 6.720      | 5.158      |
|       | 6.662      | 5.139      |
|       | 6.519      | 5.206      |
|       | 6.798      | 5.896      |
| 1000  | 2.124      | 1.564      |
|       | 2.119      | 1.560      |
|       | 2.113      | 1.556      |
|       | 2.098      | 2.018      |

7 Discussion

We have obtained equivalent kernels and local asymptotic results for spline estimators of sufficiently smooth $f$s away from the boundaries, assuming equidistant knots and observations. For periodic functions all the results hold uniformly over $[0, 1]$. Two issues remain undiscussed. First, non-equidistant design for knots and observations and second, the boundary behaviour of spline estimators of general smooth functions.

The equidistant design assumption is dominant in the literature on equivalent kernels, since it allows a clear exposition. However, it can easily be relaxed, as in [1]. In particular, if the design points $x_i$ ($i = 1, \ldots, N$) have a limiting density $g(x)$ and the sequence of knots $\tau_i$ is such that $\int_{\tau_{i-1}}^{\tau_i} p(x)dx = 1/K$, for a positive continuous density $p(x)$ on $[0, 1]$, then the equivalent kernel for a general spline estimator satisfies

$$W(x, t) = \frac{1}{g(x)h(k_q(x))} K \left[ \frac{x}{h(k_q(x))}, \frac{t}{h(k_q(x))} \right],$$

where $k_q(x) = k_q p(x)^{1-1/(2q)}$ and $h(k_q(x))^{-1} = \int_0^K \left\{ 1 + k_q(x)^{2q}(t/K)^{2q} \right\}^{-1} dt$. The asymptotic results of Theorem 2 should then be read as follows: $k_q$ is everywhere replaced by $k_q(x)$ and the variance in (18) will be additionally scaled by $1/g(x)$.

The boundary behaviour of general spline estimators remains open. It can be studied after derivation of a boundary kernel $W_b(x, t)$, such that the equivalent kernel on $[0, 1]$ is $W^{[0,1]}(x, t) = W(x, t) + W_b(x, t)$. While such a boundary kernel is known for smoothing splines, it is not available for regression and penalized spline estimators, since the Green’s function approach of smoothing splines cannot be applied. In general, it is known that regression spline estimators do not have boundary effects, while smoothing spline estimators have a larger bias at the boundaries. Considering the results of Theorem 1, one can make a conjecture on the boundary behaviour of general spline estimators. Since $K(x, t)$ varies smoothly between $K_{rs}(x, t)$ and $K_{ss}(x, t)$, one can expect that additional boundary terms in $K^{[0,1]}$ also vary smoothly between $K^{[0,1]}_{rs}(x, t)$ and $K^{[0,1]}_{ss}(x, t)$, so that the boundary effects of spline estimators grow as $k_q \to \infty$. This is another reason to select a smaller $k_q > 1$ in practice.
Appendix. Technical details

.1 Proof of Lemma 1

Inserting the Fourier series of a periodic B-spline into the discrete Fourier transform of B-splines, we find

\[
\sum_{i=1}^{K} B_i(x) \exp(-2\pi i l/K) = \sum_{m=-\infty}^{\infty} \exp(-2\pi i x) \text{sinc}(\pi m/K)^{p+1} \sum_{i=1}^{K} \exp\{2\pi i (m - l)/K\} \\
= K \sum_{n=-\infty}^{\infty} \exp\{-2\pi i (l + nK)x\} \text{sinc}\{\pi(l/K + n)\}^{p+1} \\
= \{Q_{p,M}(i/K)\}^{1/2} \psi_i(x),
\]

where in the last equality the representation

\[
\psi_i(x) = \{Q_{p,M}(i/K)\}^{1/2} \sum_{l=-\infty}^{\infty} \text{sinc}\{\pi(i/K + l)\}^{p+1} \exp\{-2\pi i x(i + lK)\}. \tag{19}
\]

has been used, which follows from (7), and \(n = (m - l)/K\). The properties of the discrete Fourier transform ensure that the functions \(\psi_i(x)\) \((i = 1, \ldots, K)\) are also the basis in \(S(p; \mathbb{T}_K)\). Property (10) follows immediately from the definition of \(Q_{p,M}(z)\). To show property (11) one can use again the representation in (19) to find

\[
\{Q_{p,M}(i/K)\}^{1/2} \phi_i^{(q)}(x) = (-2\pi i)^q \sum_{l=-\infty}^{\infty} \text{sinc}\{\pi(i/K + l)\}^{p+1-q} \exp\{-2\pi i x(i + lK)\},
\]

which implies the assertion and proves the lemma. Property (13) of functions \(\phi_i\) follows similarly from the definition of \(Q_{2p}(z)\). \(\square\)

.2 Proof of Lemma 2

Let us show that

\[
W(x, t) = \sum_{l=-\infty}^{\infty} W(x, t + l). \tag{20}
\]

This can be proved by showing that the Fourier coefficients of both functions coincide. The Fourier coefficients of \(W(x, t)\) as a function of \(t\) at a fixed \(x\) can be found from

\[
W(x, t) = \sum_{l=-\infty}^{\infty} \sum_{i=1}^{K} \text{sinc}\{\pi(i/K + l)\}^{p+1} \phi_i(x) \frac{Q_{2p}(i/K)}{Q_{2p}(i/K)\}^{1/2(1 + \lambda \mu_i)} \exp\{2\pi i t(i + lK)\}.
\]
Since $Q_2p(i/K) = Q_2p(i/K + l)$, $\mu_i = \mu_{i+lK}$ and $\phi_i(x) = \phi_{i+lK}(x)$, we obtain

$$a_i(x) = \frac{\sin\{\pi(l/K)^{p+1}\phi_i(x)}{Q_2p(l/K)^{1/2}(1 + \lambda\mu_l)}, \quad l \in \mathbb{Z},$$

(21)

for $W(x, t) = \sum_{i=\infty} a_i(x) \exp(2\pi i t)$. From the Poisson summation formula

$$\int_0^1 \sum_{j=-\infty} a_i(x) \exp(-2\pi i t)dt = \int_{-\infty} a_i(x) \exp(-2\pi i t)dt$$

(22)

follows the equality of $l$th Fourier coefficients of $\sum_{j=-\infty} W(x, t + j)$ and of the Fourier transform of $W(x, t)$. Applying the Poisson summation formula again we obtain

$$W(x, t) = \int_0^K \sum_{l=-\infty} \sin\{\pi(u/K + l)^{p+1}\phi(u, x)}{Q_2p(u/K)^{1/2}(1 + \lambda\mu(u))} \exp(2\pi i t(u + lK))du$$

$$= \int_{-\infty} \sin\{\pi(u/K)^{p+1}\phi(u, x)}{Q_2p(u/K)^{1/2}(1 + \lambda\mu(u))} \exp(2\pi i tu)du.$$  

(23)

From (22), (23) and the inverse Fourier transform follows the equality of the Fourier coefficients of $\sum_{j=-\infty} W(x, t + j)$ and $a_i(x)$ in (21), which proves (20).

Next we aim to represent and $W(x, t)$ as a ratio of two polynomials of exponential functions. The basis functions $\phi_i(x)$ and $\phi(u, x)$, as well as $Q$ polynomials, can be expressed in terms of the Euler–Frobenius polynomials of exponential functions, as shown in Section 2. With this

$$W(x, t) = \int_0^K \frac{\exp(-2\pi i d_x t u/K)\sum_{l=0}^{2p} \alpha_l(\{Kx\}, \{Kt\}) \exp(-2\pi i u/K)du}{P_{2p}(\{Kx\})}. $$

The coefficients of the partial fractional decomposition of $1/P_{2p}$ are $1/P_{2p}'(r_j)$ and $1/P_{2p}'(r_j^{-1})$ correspondant to the roots $r_j$ and $r_j^{-1}$ for $j = 1, \ldots, p$. From the representation of $P_{2p}$ as a function of $\cos^2(\pi i/K) = \{\exp(-2\pi i/K) + \exp(2\pi i/K) + 2\}/4$ follows that $P_{2p}'(r_j^{-1}) = -r_j^{2-2p}P_{2p}'(r_j^{-1})$. Then

$$W(x, t) = \sum_{j=1}^{p} \sum_{l=0}^{2p} \alpha_l(\{Kx\}, \{Kt\}) / P_{2p}(r_j) R(j, l),$$

for

$$R(j, l) = \int_0^K \left[ \frac{\exp\{-2\pi i (\frac{d_x t + l}{u/K})u/K\} - r_j^{2p-2}\exp\{-2\pi i (\frac{d_x t + l}{u/K})u/K\}}{\exp(-2\pi i u/K) - r_j} \right] du.$$  

Solution to $R(j, l)$ follows from the Cauchy integral formula, where the contour integral
is taken counter-clockwise

\[
R(j, l) = \begin{cases} 
\frac{K}{2\pi i} \oint_{|z|=1} \left( \frac{z^{d_{x,t}+l-1}}{z-r_j} - \frac{r_j^{2p-2}z^{d_{x,t}+l-1}}{z-r_j} \right) dz = Kr_j^{d_{x,t}+l-1}, & (d_{x,t} + l) > 0 \\
\frac{K}{2\pi i} \oint_{|z|=1} \left( \frac{z^{d_{x,t+l-1}}}{z-r_j} - \frac{r_j^{2p-2}z^{d_{x,t}+l-1}}{z-r_j} \right) dz = Kz^{-d_{x,t+l}+2p-1}, & (d_{x,t} + l) \leq 0
\end{cases}
\]

.3 Proof of Lemma 3

From (23) and symmetry of the kernel follows that

\[
W(x, t) = \int_{-\infty}^{\infty} a(u, x) \exp \left( -2\pi i tu \right) du,
\]

with

\[
a(u, x) = \frac{\text{sinc} \left\{ \pi \left( u/K \right) \right\}^{p+1} \phi(u, x)}{Q_{2p} \left( u/K \right) ^{1/2} \left\{ 1 + \mu(u) \right\}}.
\]

Properties of the Fourier transform ensure that

\[
\int_{-\infty}^{\infty} (2\pi i t)^m W(x, t) \exp(2\pi i tu) dt = \frac{\partial^m}{\partial u^m} \left\{ a(u, x) \right\}.
\]

Evaluating derivative of \( a(u, x) \) at \( u = 0 \) and grouping the terms we represent

\[
\int_{-\infty}^{\infty} (2\pi i t)^m W(x, t) dt = I_1 + I_2 + I_3,
\]

where

\[
I_1 = \frac{\partial^m}{\partial u^m} \left\{ \begin{array}{c}
\exp(2\pi i xu) \frac{\text{sinc} \left( \pi u/K \right)^{2p+2}}{Q_{2p} \left( u/K \right) ^{1/2} \left\{ 1 + \lambda \mu(u) \right\}} \\
u=0
\end{array} \right\},
\]

\[
I_2 = \frac{\partial^m}{\partial u^m} \left\{ \begin{array}{c}
\left\{ \text{sinc} \left( \pi u/K \right) \text{sinc} \left( \pi u/K \right) \right\}^{p+1} Q_{2p} \left( u/K \right) ^{1/2} \left\{ 1 + \lambda \mu(u) \right\} \\
\sum_{l \neq 0} \exp \left\{ 2\pi i x (u + lK) \right\} \left\{ (-1)^l \pi (u/K + l) \right\} ^{p+1} \\
u=0
\end{array} \right\},
\]

\[
I_3 = \frac{\partial^m}{\partial u^m} \left\{ \begin{array}{c}
\lambda \mu(u) \text{sinc} \left( \pi u/K \right)^{p+1} \phi(u, x) \\
Q_{2p} \left( u/K \right) ^{1/2} \left\{ 1 + \lambda \mu(u) \right\} \\
u=0
\end{array} \right\}.
\]

The idea is to represent each of these components as a product of the \( \sin \left( \pi u/K \right)^n, n \in \mathbb{Z} \) and some function that is differentiable at 0. Then, we use that \( Q_{2p}(0) = \phi(0, x) = 1 \), \( \mu(0) = 0 \),

\[
\frac{\partial^m}{\partial u^m} \sin \left( \pi u/K \right)^n \bigg|_{u=0} = \begin{cases} 0, & m = 0, \ldots, n-1, \\
n! \left( \pi/K \right)^n, & m = n,
\end{cases}
\]

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and the Fourier series of the periodic Bernoulli polynomials $B_{p+1}(\{x\}) = (-1)^p (p + 1)! \sum_{s \neq 0} \exp(-2\pi isx)/(2\pi is)^{p+1}$.

Putting it all together and noting that $Q_{2p}(z) = \text{sinc}(\pi z)^{2p+2} + \sum_{l \neq 0} \text{sinc}\{\pi(z + l)\}^{2p+2}$, we get $I_1 = (2\pi ix)^m (m = 0, \ldots, p + 1)$. The expression for $I_2$ follows immediately from its representation

$$I_2 = \begin{cases} 0, & m = 0, \ldots, p, \\
-(2\pi i/K)^{p+1}B_{p+1}(\{Kx + \frac{p+1}{2}\}), & m = p + 1. 
\end{cases}$$

To find $I_3$, we use $\mu(u) = (2K)^{2q} \sin(\pi u/K)^{2q}Q_{2p-2q}(u/K)/Q_{p,M}(u/K)$

$$I_3 = \begin{cases} 0, & m = 0, \ldots, 2q - 1, \\
-\lambda (2\pi)^{2q} (2q)!, & m = 2q. 
\end{cases}$$

To get the result for $\int_{-\infty}^{\infty} (t - x)^m W(x, t) dt$ one needs to expand $(t - x)^m$ and use (24).

\[ \Box \]

.4 Proof of Theorem 1

The asymptotic equivalent kernel on $\mathbb{R}$ can be written as

$$W(x, t) = \int_{0}^{K} \frac{\phi(u, x)/\phi(u, t)}{1 + \lambda \mu(u)} du = \Re \int_{0}^{1/2} \frac{2K\phi(Ku, x)/\phi(Ku, t)}{1 + \lambda \mu(Ku)} du.$$

First consider $0 \leq k_q < 1$. Scaling $W(x, t)$ with $c_1^{-1}K^{-1}$ leads to

$$c_1 K(c_1 x, c_1 t) = \Re \int_{0}^{1/2} 2\phi(Ku, x/K)/\phi(Ku, t/K) du - \int_{0}^{1/2} \frac{2\lambda \mu(Ku)\phi(Ku, x/K)/\phi(Ku, t/K)}{1 + \lambda \mu(Ku)} du = K_{rs}(x, t) - k_q^{2q}K_1(x, t),$$

where $\Re$ denotes the real part of a complex number, $K_{rs}(x, t)$ is the equivalent regression spline kernel on $\mathbb{R}$ and

$$K_1(x, t) = \Re \int_{0}^{1/2} 2\sin(\pi u)^{2q}Q_{2q-2}(u)\phi(Ku, x/K)/\phi(Ku, t/K) du$$

$$\leq \frac{2^{2q}Q_{2q-2}(1/2)}{\pi^{2q}Q_{2q-2}(1/2)} K_{rs}(x, t).$$

Using $Q_{lq-2}(1/2) = 2\pi^{lq}(2^{lq} - 1)\zeta(lq)$ for the Riemann zeta function $\zeta(lq) = \sum_{i=1}^{\infty} i^{-lq}$, one can get explicit bounds for each $q$. 

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For $k_q \geq 1$ we first introduce the notation: $1 + \lambda\mu(Ku) = \{1 + \lambda(2\pi Ku)^{2q}\}\{1 + r_1(u)\}; \phi(Ku,x)\phi(Ku,t) = \exp\{2\pi i Ku(x-t)\}\{1+r_2(x,t,u)\}; r_q(x,t,u) = \{r_2(x,t,u) - r_1(u)\}\{1 + r_1(u)\}^{-1}$. Scaling $\mathcal{W}(x,t)$ with $c_2^{-1}\lambda^{1/(2q)}$ results in

$$
c_2K(c_2x,c_2t) = \int_{-\infty}^{\infty} \exp\{2\pi i u(t-x)\} \frac{1}{1 + (2\pi u)^{2q}} du + \Re \int_0^{k_q/2} 2 \exp\{2\pi i u(t-x)\} \frac{1}{1 + (2u)^{2q}} r_q(u/k_q) \frac{du}{u} 
- \Re \int_{k_q/2}^{\infty} 2 \exp\{2\pi i u(t-x)\} \frac{1}{1 + (2u)^{2q}} \frac{du}{u} = K_{ss}(x,t) + k_q^{-2q+1}K_2(x,t),
$$

where $K_{ss}(x,t)$ is the smoothing spline kernel on $\mathbb{R}$ and

$$
\pi K_2(x,t) = k_q^{2q-1}\Re \int_0^{k_q/2} \frac{2 \exp\{2\pi i u(t-x)\}}{1 + (2u)^{2q}} r_q(u/k_q) \frac{du}{u} - \int_1^{\infty} \frac{\cos\{k_q u(t-x)\}}{k_q^{-2q} + u^{2q}} du.
$$

The second component of $\pi K_2(x,t)$ is obviously bounded by 1. Now, let us consider $r_q(u/k_q)$. First,

$$
r_1(u/k_q) = \frac{(2u)^{2q}}{1 + (2u)^{2q}} \left\{ \frac{\sin((\pi u/k_q)^{2q}Q_{2q-2}(u/k_q))}{Q_{4q-2}(u/k_q)} - 1 \right\},
$$

where $Q_{2q-2}(u/k_q)\sin((\pi u/k_q)^{2q}/Q_{4q-2}(u/k_q)) - 1 = 2\zeta(2q)(u/k_q)^{2q} + 4\zeta(4q)(u/k_q)^{4q} + \ldots$ is a positive number for any $u$. Further,

$$
r_2(x,t,u/k_q) \leq \frac{Q_{2q}^2}{Q_{4q-2}(u/k_q)}Q_{4q-2}(u/k_q)^{-1} - 1 = 4\zeta(2q)(u/k_q)^{2q} + 8\zeta(4q)(u/k_q)^{4q} + \ldots
$$

With this, $r_q(x,t,u/k_q) \leq 4\zeta(2q)(u/k_q)^{-2q} + \ldots$ and hence, the first term in $\pi K_2(x,t)$ is also bounded for any $k_q \geq 1$.

Finally, $K_{ss}(x,t)$ is given in [Thomas-Agnan (1996)] and $K_{rs}(x,t)$ is obtained from (15), scaling $\mathcal{W}(x,t)$ with $K$ and setting $P_{2p}(u) = \Pi_{2p}(u)$. \hfill \square

.5 Proof of Theorem 2

The following lemma will be used in the proof of Theorem 2

**Lemma 4** Kernel $\mathcal{K}(x,t)$, $x,t \in \mathbb{R}$ decays exponentially, i.e., there are constants $0 < C < \infty$ and $0 < \gamma < 1$ such that $|\mathcal{K}(x,t)| < C\gamma^{x-t}$.

**Proof of Lemma 2**

Since $\mathcal{K}(x,t)$ is defined as a scaled with $h(k_q)$ function $\mathcal{W}(x,t)$, from (15) and (16) one...
finds for \( k_q < 1 \)

\[
c_1K(c_1x, c_1t) = \sum_{j=1}^p \sum_{l=0}^{2p} \frac{\alpha_l(\{x\}, \{t\})}{P_{2p}(r_j)} r_j^{|x| - |t| + l - 1 + (2p - 2)l(|x| - |t| + l) \leq 0},
\]

while for \( k_q \geq 1 \),

\[
\pi c_2K(\pi c_2x, \pi c_2t) = k_q \sum_{j=1}^p \sum_{l=0}^{2p} \frac{\alpha_l(\{xk_q\}, \{tk_q\})}{P_{2p}(r_j)} r_j^{|xk_q| - |tk_q| + l - 1 + (2p - 2)l(|xk_q| - |tk_q| + l) \leq 0},
\]

where \( P_{2p} \) is given in \((14)\) and \( r_j = r_j(k_q) \) is a root of \( P_{2p} \) with \( |r_j| < 1 \). If \( k_q \) is a bounded constant then \( r_j = r_j(k_q) \rightarrow \exp(-2\pi iu) \), \( u \in (0, 1) \) since

\[
P_{2p}\{\exp(-2\pi iu)\} = \exp(-2\pi i pu) \{Q_{p,M}(u) + (2k_q/\pi)^{2q} \sin(\pi u)^{2q}Q_{2p-2q}(u)\} \neq 0,
\]

where the relationship between Euler–Frobenius and \( Q \)-polynomials has been used. Similarly, \( r_j = r_j(k_q) \rightarrow 0 \) and \( 0 < \gamma < 1 \) can be defined as

\[
\gamma = \begin{cases} 
\sup_{j,k_q} |r_j(k_q)|, & k_q < 1 \\
\sup_{j,k_q} |r_j(k_q)|, & 1 \leq k_q < \infty,
\end{cases}
\]

while

\[
C = \sup_{k_q,j} \frac{p(2p + 1) \sup_{l,x,t} \alpha_l(\{x\}, \{t\})}{|P_{2p}(r_j(k_q))| |r_j(k_q)|^{l+1}} < \infty.
\]

For \( k_q \rightarrow \infty \) it is known from Theorem \([\text{I}]\) that \( \lim_{k_q \rightarrow \infty} K(x,t) = K_{ss}\{x - t\}/c_2 \). To obtain the bound on the smoothing spline kernel \( K_{ss}(x) \), the expression given in Theorem \([\text{I}]\) can be rewritten as

\[
|K_{ss}(x - t)| = \left| -I_{\{q \text{ is odd}\}} \exp(-|x - t|) + \sum_{j=0}^{\lfloor(q-1)/2\rfloor} \exp\left[-|x - t| \sin\left(\pi(2j + 1)/(2q)\right)\right] \times \sin\left[\frac{\pi(2q - 1)(2j + 1)}{2q} - |x - t| \cos\left(\frac{\pi(2j + 1)}{2q}\right)\right]\right| \\
\leq \frac{q + 1}{2q} \exp\left(-|x - t| \sin(\pi 2q)\right),
\]

so one can set \( \gamma = \exp\left[-\sin\{\pi/(2q)\}/c_2\right] \in (0, 1) \), \( C = (q + 1)/(2q c_2) < \infty \) for \( k_q \rightarrow \infty \). \( \square \)

**Proof of Theorem** \([\text{II}]\)

Let \( \hat{f}(x) = N^{-1} \sum_{i=1}^N W^{[0,1]}(x, i/N)Y_i \), \( \hat{f}_{\text{per}}(x) = N^{-1} \sum_{i=1}^N W_{\text{per}}^{[0,1]}(x, i/N)Y_i \). Then, extending \( f \) to the whole real line, such that it still satisfies assumptions of the theorem,
we get

\[
E \left\{ \hat{f}(x) \right\} = \int_{-\infty}^{\infty} W(x, t)f(t)dt + R_1(x) + R_2(x) + O(N^{-1})
\]

\[
E \left\{ \hat{f}_{\text{per}}(x) \right\} = \int_{-\infty}^{\infty} W(x, t)f(t)dt + R_3(x) + O(N^{-1}),
\]

where \( R_1(x) = \int_{0}^{1} \{ W^{[0,1]}(x, t) - W(x, t) \} f(t)dt \), \( R_2(x) = \int_{R \setminus [0,1]} W(x, t)f(t)dt \) and

\( R_3(x) = \int_{0}^{1} \{ W_{\text{per}}^{[0,1]}(x, t) - W_{\text{per}}^{[0,1]}(x, t) \} f(t)dt. \)

Expanding \( f(t) \) in a Taylor series around \( x \) and using Lemma 3 results in

\[
\int_{-\infty}^{\infty} W(x, t)f(t)dt = f(x) + \int_{-\infty}^{\infty} W(x, t)(x - t)^2qf^{(2q)}(\xi_{x,t})\frac{f(2q)(\xi_{x,t})}{(2q)!}dt + O(N^{-1})
\]

\[
= \frac{f^{(2q)}(x)}{(2q)!} \int_{-\infty}^{\infty} W(x, t)(x - t)^2qdt + R_\xi(x) + O(N^{-1})
\]

\[
= h(k_q)^{2q}f^{(2q)}(x)\frac{f^{(2q)}(x)}{(2q)!} \int_{-\infty}^{\infty} K(x, t)(x_h - t_h)^{2q} dt + R_\xi(x) + O(N^{-1}),
\]

where \( \xi_{x,t} \) is a point between \( x \) and \( t \), \( \int_{-\infty}^{\infty} K(x, t)(x_h - t_h)^{2q} dt = -C(k_q, x) \) given in the Theorem 2, \( x_h = x/h(k_q), t_h = t/h(k_q) \) and

\[
R_\xi(x) = h(k_q)^{2q} \int_{-\infty}^{\infty} K(x, t)(x_h - t_h)^{2q} \frac{f^{(2q)}(\xi_{x,t}) - f^{(2q)}(x)}{h(k_q)(2q)!}dt.
\]

It remains to show that error terms \( R_1(x) \), \( R_2(x) \) are negligible for \( x \in I_q \) and \( R_3(x) \), \( R_\xi(x) \) are uniformly negligible.

Using techniques similar to [Huang and Studden (1993)],

\[
R_\xi(x) = h(k_q)^{2q} \sum_{l=-\infty}^{\infty} \int_{x+(l-1)h(k_q)}^{x+lh(k_q)} K(x, t)(x_h - t_h)^{2q} \frac{f^{(2q)}(\xi_{x,t}) - f^{(2q)}(x)}{h(k_q)(2q)!}dt
\]

\[
\leq h(k_q)^{2q+\alpha} CL \sum_{l=-\infty}^{\infty} \int_{x+(l-1)h(k_q)}^{x+lh(k_q)} \gamma^{l-1} |x_h - t_h|^{2q+\alpha} |\xi_{x,t}|^{2q+\alpha} \frac{f^{(2q)}(x)}{h(k_q)(2q)!}dt
\]

\[
\leq h(k_q)^{2q+\alpha} \frac{2CL}{(2q)!} \sum_{l=1}^{\infty} \gamma^{l-1} f^{2q+\alpha} = o \left( h(k_q)^{2q} \right),
\]

where the exponential bound on the kernel from Lemma 4 together with the Hölder continuity of \( f^{(2q)} \) have been used.
To see that $R_3(x) = o \left[\{h(k_q)N\}^{-1}\right]$ for any $x$, use the definitions of both kernels to get

$$|R_3(x)| \leq \|f\|_\infty \int_0^1 \left| \sum_{i=1}^K \phi_i(x) \phi_i(t) Q_{p,M}(i/K) - Q_{2p}(i/K) \right| dt = O \left[\{h(k_q)N\}^{-2q}\right],$$

since $Q_{p,M}(i/K) = Q_{2p}(i/K) + \sin(\pi i/K) 2^q M^{-2q}$ and both $Q_{2p}(i/K), Q_{p,M}(i/K) \in (0,1]$ for any $i = 1, \ldots, K$. Next,

$$|R_2(x)| = \left| \int_{\mathbb{R}\setminus[0,1]} W(x,t) f(t) dt \right| \leq \|f\|_\infty \int_{\mathbb{R}\setminus[0,1]} h(k_q)^{-1/2} |x-t|h(k_q)^{-1} dt$$

$$= \|f\|_\infty \left(\gamma \frac{x^2}{h(k_q)} + \gamma \frac{1-x^2}{h(k_q)}\right) \log(1/\gamma) = o \{h(k_q)^{2q}\},$$

as long as $x \in I_q$ with $\delta_q > 2q \log_\gamma (1/e)$. Finally, for $x \in I_q$,

$$R_1(x) = \int_0^1 \left\{ W^{[0,1]}(x,t) - W(x,t) \right\} f(t) dt$$

$$= \int_0^1 \left\{ W^{[0,1]}(x,t) - W_{\per}^{[0,1]}(x,t) \right\} f(t) dt + R_2(x) + R_3(x)$$

$$= O(N^{-1}) + o \{h(k_q)^{2q}\} + O \left[\{h(k_q)N\}^{-2q}\right],$$

since the difference between projection of function $f$ onto general and periodic spline spaces is zero by definition for $x \in [2q/K, 1-2q/K] \supset I_q$, see Chapter 8.1 in Schumaker (2007).

Now, the variance of $\hat{f}_{\per}(x)$ is given by

$$\text{var}\left\{\hat{f}_{\per}(x)\right\} = \frac{\sigma^2}{N^2} \sum_{i=1}^N W_{\per}^{[0,1]}(x,i/N)^2 = \frac{\sigma^2}{N} \int_0^1 W_{\per}^{[0,1]}(x,t)^2 dt + \frac{\sigma^2}{N} R_4(x) + O(N^{-2}).$$

for $R_4(x) = \int_0^1 \left\{ W_{\per}^{[0,1]}(x,t)^2 - W_{\per}^{[0,1]}(x,t)^2 \right\} dt$. Let us define $K_{\per}(x,t)$ via

$$h(k_q)^{-1} K_{\per}(x,h,t_h) = W_{\per}^{[0,1]}(x,t) = \sum_{l=-\infty}^{\infty} W(x,t+l) = h(k_q)^{-1} \sum_{l=-\infty}^{\infty} \mathcal{K}(x,h,t+l),$$

for $l_h = l/h(k_q)$. Then, using periodicity of $W_{\per}^{[0,1]}(x,t)$

$$\int_0^1 W_{\per}^{[0,1]}(x,t)^2 dt = \int_{x-1/2}^{x+1/2} W_{\per}^{[0,1]}(x,t)^2 dt = \frac{1}{h(k_q)^2} \int_{x-1/2}^{x+1/2} K_{\per}(x,t_h)^2 dt$$

$$= \frac{1}{h(k_q)} \left\{ \int_{-\infty}^{\infty} \mathcal{K}(x,h,t)^2 dt + R_h(x) \right\},$$

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for
\[ h(K)R_k(x) = \int_{x-1/2}^{x+1/2} K_{\text{per}}(x, t_h)^2 dt - \int_{-\infty}^{-K} (x, t_h)^2 dt \]
\[ = \int_{x-1/2}^{x+1/2} \{K_{\text{per}}(x, t_h)^2 - K(x, t_h)^2\} dt \]
\[ - \int_{-\infty}^{-1} K_{\text{per}}(x, t_h)^2 dt - \int_{x+1/2}^{\infty} K(x, t_h)^2 dt. \]

Now, we can make use of \(K_{\text{per}}(x, t) = \sum_{t=-\infty}^{\infty} K(x, t + l)\) and of the exponential decay of \(K(x, t)\) found in Lemma 4 to bound terms in \(h(K)R_k(x)\). That is,
\[ \int_{x-1/2}^{x+1/2} \{K_{\text{per}}(x, t_h)^2 - K(x, t_h)^2\} dt = \int_{x-1/2}^{x+1/2} \sum_{l \neq 0} K(x, t_h + l_h) \left\{ \sum_{l \neq 0} K(x, t_h + l_h) + 2K(x, t_h) \right\} dt \]
\[ \leq C^2 \int_{x-1/2}^{x+1/2} \sum_{l \neq 0} \gamma^{\log(1/(k_q))} \left( \sum_{l \neq 0} \gamma^{\log(1/(k_q))} + 2\gamma^{\log(1/(k_q))} \right) dt \]
\[ \leq h(k_q) C^2 \gamma^{1/h(k_q)} \left\{ 4 + 2h(k_q)^{-1} \log(\gamma^{-1}) \right\}, \]

where \( \sum_{l \neq 0} \gamma^{\log(1/(k_q))} = (\gamma^{\log(1/(k_q))} + \gamma^{\log(1/(k_q))}) / \left\{ 1 - \gamma^{1/(h(k_q))} \right\} \), for \( t \in [x-1/2, x+1/2] \) has been used. Also,
\[ \int_{-\infty}^{x-1/2} K(x, t_h)^2 dt + \int_{x+1/2}^{\infty} K(x, t_h)^2 dt \leq C^2 \int_{-\infty}^{x-1/2} \gamma^{2(x_h-t_h)} dt + \int_{x+1/2}^{\infty} \gamma^{2(t_h-x_h)} dt \]
\[ = h(k_q) C^2 \gamma^{1/h(k_q)} \log(\gamma^{-1}). \]

In a similar fashion one finds \( \int_{-\infty}^{\infty} K(x, t)^2 dt \leq C^2 / \log(\gamma^{-1}) \). Putting it all together gives
\[ |R_k(x)| \leq \frac{C^2 \gamma^{1/h(k_q)}}{\log(\gamma^{-1})} \left[ 1 + 4 + 2h(k_q)^{-1} \log(\gamma^{-1}) / \left\{ \gamma^{1/(h(k_q))} \right\} \right] = O \left\{ h(k_q)^{-1} \gamma^{1/(h(k_q))} \right\} = o(1). \]

The proof for \( \text{var} \{ \hat{f}(x) \} \) follows from
\[ \text{var} \{ \hat{f}(x) \} = \frac{\sigma^2}{N} \sum_{i=1}^{N} W[0,1](x, i/N)^2 = \frac{\sigma^2}{N} \int_{-\infty}^{\infty} W(x, t)^2 dt + \frac{\sigma^2}{N} \{ R_5(x) + R_6(x) \} + O \left( N^{-2} \right) \]
\[ = \frac{\sigma^2}{Nh(k_q)} \int_{-\infty}^{\infty} K(x/h(k_q), t)^2 dt + \frac{\sigma^2}{N} \{ R_5(x) + R_6(x) \} + O \left( N^{-2} \right), \]
where $R_5(x) = \int_0^1 \{ W^{[0,1]}(x,t)^2 - W(x,t)^2 \} \, dt$ and $R_6(x) = \int_{\mathbb{R} \setminus [0,1]} W(x,t)^2 \, dt$. The proof that $R_4(x)$ is uniformly negligible and $R_5(x), R_6(x)$ are negligible for $x \in I_q$ follows exactly the same lines as that for $R_3(x), R_1(x)$ and $R_2(x)$, respectively. □

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