Jitka Poměnková Remarks on optimum kernels and optimum boundary kernels

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REMARKS ON OPTIMUM KERNELS AND OPTIMUM BOUNDARY KERNELS*

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Abstract. Kernel smoothers belong to the most popular nonparametric functional estimates used for describing data structure. They can be applied to the fix design regression model as well as to the random design regression model. The main idea of this paper is to present a construction of the optimum kernel and optimum boundary kernel by means of the Gegenbauer and Legendre polynomials.

Keywords: kernel, optimum kernel, optimum boundary kernel

MSC 2010: 62G08

1. INTRODUCTION

Kernel estimations, as part of nonparametric functional estimates, provide a simple tool for finding a structure in data. Special types of polynomial functions, kernels, are used for an estimation of the resultant regression function. The quality of the estimate heavily depends on the kernel used, especially on its smoothness. We can show that smoother kernels produce nice-looking curves.

The aim of this paper is to present the construction of minimum variance kernels and smooth kernels by means of the Legendre and Gegenbauer polynomials. We deal with the problem of finding smooth optimum kernels which minimize the leading terms of the asymptotic mean square error which is a suitable measure of the kernel quality. The optimum boundary kernels, which can be used for the construction of estimates at the edge points, represent a special type of optimum kernels.

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In this paper we are going to treat the problem of finding kernels minimizing the asymptotic mean square error which are called optimum kernels and optimum boundary kernels. Derivation of the optimum kernels formula as well as the optimum boundary kernels formula is presented in graphical and numerical form. Using optimum kernels in the case of kernel estimate construction usually gives a better nice looking—estimate. It can be measured by the asymptotic mean square error. Optimum boundary kernels can be used in the case of edge effects, i.e., when the kernel estimate has big bias at the edge points. Using these kernels it is possible to remove edge effects. The proof of an identity important for the formula derivation is also presented. At the end some illustrating charts of the simulation function, showing the effect of using the chosen minimum variance kernel, optimum kernel and optimum boundary kernel, will be attached.

2. Basic terms and definitions

First, the definitions of a kernel and a smooth kernel are recalled. Denote by $C^{\mu}[-1,1]$ the set of μ times continuously differentiable real valued functions on [-1,1]. Let ν , k be nonnegative even integers, $0 \leq \nu \leq k$, $K \in \text{Lip}[-1,1]$, support(K) = [-1,1] and let K satisfy the moment conditions

(i)
$$K(-1) = K(1) = 0$$

(ii) $\int_{-1}^{1} x^{j} K(x) dx = \begin{cases} 0, & 0 < j < k \\ 1, & j = 0, \\ \beta_{k} \neq 0, & j = k. \end{cases}$

Then the function K is called a *kernel* of order (ν, k) and we write $K \in M_{\nu,k}$. The smoothness of the kernel function will be quantified as follows.

Let us denote for any integer $\mu \ge 1$

$$M^{\mu}_{\nu,k} = \{ K \colon K \in M_{\nu,k} \cap C^{\mu}[-1,1]; \ K^{(j)}(-1) = K^{(j)}(1) = 0, \ j = 0, \dots, \mu - 1 \}.$$

Then the kernels are called smooth kernels and we write $K \in M^{\mu}_{\nu,k}$. (For details and practical applications see [4], [15], [10].)

Let us denote

$$C_n^{\alpha}(x) = \sum_{r=0}^n c_{n,r}^{\alpha} x^r$$
 and $P_k(x) = \sum_{i=0}^k p_i^k x^i$.

Recall that the Gegenbauer polynomials $C_n^{\alpha}(x)$, $\alpha > -1/2$, $n \ge 1$ are orthogonal on [-1, 1] with respect to the weight function $w(x) = (1 - x^2)^{\alpha - 1/2}$ and

$$\int_{-1}^{1} (1-x^2)^{\alpha-1/2} C_n^{\alpha}(x) C_m^{\alpha}(x) \, \mathrm{d}x = \begin{cases} 0, & m \neq n, \\ \frac{\pi 2^{1-2\alpha} \Gamma(n+2\alpha)}{n! (\alpha+n) (\Gamma(\alpha))^2}, & \alpha \neq 0, n = m. \end{cases}$$

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The Gegenbauer polynomials satisfy the recurrent relations

$$C_{n+1}^{\alpha}(x) = \frac{2(\alpha+n)}{n+1} x C_n^{\alpha}(x) - \frac{2\alpha+n-1}{n+1} C_{n-1}^{\alpha}(x), \quad n \ge 1,$$

$$C_0^{\alpha}(x) \equiv 1, \quad C_1^{\alpha}(x) = 2\alpha x,$$

$$C_n^{\alpha}(x) = \frac{1}{2(\alpha+n)} \left(\frac{\mathrm{d}}{\mathrm{d}x} C_{n+1}^{\alpha}(x) - \frac{\mathrm{d}}{\mathrm{d}x} C_{n-1}^{\alpha}(x)\right), \quad n \ge 1,$$

$$C_n^{\alpha}(-x) = (-1)^n C_n^{\alpha}(x), \quad x \in [-1,1],$$

$$C_n^{\alpha}(1) = (-1)^n C_n^{\alpha}(-1) = \frac{\Gamma(n+2\alpha)}{n!\Gamma(2\alpha)},$$

$$(1-x^2) C_k^{3/2}(x) = \frac{(k+1)(k+2)}{2k+3} (P_k(x) - P_{k+1}(x)),$$

where P_k is the Legendre polynomial of order k [14].

Horová [5] showed that

$$\nu c_{k,\nu}^{\alpha} = 2 \sum_{r=\nu-1}^{k-1} (\alpha+r) c_{k,\nu-1}^{\alpha},$$

where $\nu, k \in \mathbb{N}$ and $(\nu + k)$ is even, $0 \leq \nu \leq k - 2$.

3. Optimum kernel construction

The kernel choice has a strong impact on statistical properties of the corresponding estimates, since it affects the leading terms of the average mean square error. This error depends on kernels by means of certain functionals. Granovsky, Müller and Pfeifer [3] wrote that under some regularity conditions (including the *k*th order differentiability of the estimated curve for a given k > 0) and after inserting the asymptotically optimal smoothing parameters, the asymptotically leading term of the average mean square error ($\overline{\text{AMSE}}$) in the nonparametric regression analysis is proportional to the functional $T(K)^{2/(2k+1)}$, where

$$T(K) = \left(\int_{-1}^{1} K^{2}(x) \, \mathrm{d}x\right)^{k-\nu} \left|\int_{-1}^{1} x^{k} K(x) \, \mathrm{d}x\right|^{2\nu+1}.$$

By minimizing T(K), such a suitable form of the kernel can be found that the value of $\overline{\text{AMSE}}$ used as an estimate quality measure will be as small as possible.

The solution of the variational problem

minimum
$$C_K = \int_{-1}^1 K^2(x) \,\mathrm{d}x, \quad K \in M_{\nu,k},$$

is called the minimum variance kernel (see [2], [6]).

In order to minimize the functional T(K) on the set $M_{\nu,k}$ it was proposed in [1] to impose on K an additional side condition, called the *minimality of sign changes* on the kernel function:

$$K \in N_{k-2} = \{ f \in L^2 : f \text{ has exactly } k-2 \text{ sign changes on } R \}.$$

Now, we shall study the kernels of order (ν, k) with the support [-1, 1] optimal in the following sense (see [9]):

(i) $K \in N_{k-2}$,

(ii)
$$T(K) = \left(\int_{-1}^{1} K^2(x) \, dx\right)^{k-\nu} \left|\int_{-1}^{1} x^k K(x) \, dx\right|^{2\nu+1} = C_K^{k-\nu} |\beta_k|^{2\nu+1}$$
 is minimum.

The optimal polynomials K are of order k with real roots in [-1, 1], including -1 and 1. The explicit formulas are given in terms of the Legendre polynomials

$$K(x) = \frac{(-1)^{\nu}\nu!}{2} \sum_{r=\nu}^{k} (2r+1)p_{\nu}^{r}P_{r}(x) + \beta_{k} \frac{(2k+1)}{2}p_{k}^{k}P_{k}(x), \quad x \in [-1,1],$$

where

$$\beta_k = \int_{-1}^1 x^k K(x) \, \mathrm{d}x = \frac{(-1)^{\nu+1} \nu!}{(2k+1)p_k^k} \sum_{r=\nu}^k (2r+1)p_\nu^r.$$

Horová [5] proved that

$$\frac{\mathrm{d}}{\mathrm{d}x}K(x) = \tilde{K}(x), \quad x \in (-1,1),$$

where $\tilde{K} \in M_{\nu+1,k+1}$ is the minimum variance kernel $(0 \leq \nu \leq k-2, (\nu+k) \text{ even})$.

Theorem. The functional T(K) is invariant with respect to the transformation H_{δ} : $L^2 \to L^2$, H_{δ} : $K(\cdot) \to (\delta^{\nu+1})^{-1}K(\cdot/\delta)$, i.e. the relation $T(K) = T(K_{\delta})$ holds.

Proof. We prove the following functional equality

$$T(K) = \left(\left(\int_{-1}^{1} K^{2}(x) \, \mathrm{d}x \right)^{k-\nu} \left| \int_{-1}^{1} x^{k} K(x) \, \mathrm{d}x \right|^{2\nu+1} \right)^{2/(2k+1)},$$

$$T(K_{\delta}) = \left(\left(\int_{-1}^{1} \frac{1}{\delta^{2(\nu+1)}} K^{2}\left(\frac{x}{\delta}\right) \, \mathrm{d}x \right)^{k-\nu} \left| \int_{-1}^{1} x^{k} \frac{1}{\delta^{\nu+1}} K\left(\frac{x}{\delta}\right) \, \mathrm{d}x \right|^{2\nu+1} \right)^{2/(2k+1)},$$

In both terms of the functional $T(K_{\delta})$, the same substitution $u = x/\delta$, $x = u\delta$, $dx = \delta du$ is used. Then, for the first term we have

$$\left(\int_{-1}^{1} \frac{1}{\delta^{2(\nu+1)}} K^{2}\left(\frac{x}{\delta}\right) \mathrm{d}x\right)^{k-\nu} = \left(\int_{-1/\delta}^{1/\delta} \frac{\delta}{\delta^{2(\nu+1)}} K^{2}(u) \mathrm{d}u\right)^{k-\nu}$$
$$= \frac{1}{\delta^{(2\nu+1)(k-\nu)}} \left(\int_{-1/\delta}^{1/\delta} K^{2}(u) \mathrm{d}u\right)^{k-\nu}$$

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and for the second

$$\left| \int_{-1}^{1} x^{k} \frac{1}{\delta^{\nu+1}} K\left(\frac{x}{\delta}\right) \mathrm{d}x \right|^{2\nu+1} = \left| \int_{-1/\delta}^{1/\delta} \frac{\delta(u\delta)^{k}}{\delta^{\nu+1}} K(u) \mathrm{d}u \right|^{2\nu+1}$$
$$= |\delta^{k-\nu}|^{2\nu+1} \left| \int_{-1/\delta}^{1/\delta} u^{k} K(u) \mathrm{d}u \right|^{2\nu+1}.$$

This yields

$$\begin{split} T(K_{\delta}) &= \left(\frac{1}{\delta^{(2\nu+1)(k-\nu)}} \left(\int_{-1/\delta}^{1/\delta} K^{2}(u) \,\mathrm{d}u\right)^{k-\nu} |\delta^{k-\nu}|^{2\nu+1} \left|\int_{-1/\delta}^{1/\delta} u^{k} K(u) \,\mathrm{d}u\right|^{2\nu+1}\right)^{2/(2k+1)} \\ &= \left(\frac{|\delta^{(k-\nu)}|^{2\nu+1}}{\delta^{(2\nu+1)(k-\nu)}} \left(\int_{-1/\delta}^{1/\delta} K^{2}(u) \,\mathrm{d}u\right)^{k-\nu} \left|\int_{-1/\delta}^{1/\delta} u^{k} K(u) \,\mathrm{d}u\right|^{2\nu+1}\right)^{2/(2k+1)} \\ &= \left(\left(\int_{-1/\delta}^{1/\delta} K^{2}(u) \,\mathrm{d}u\right)^{k-\nu} \left|\int_{-1/\delta}^{1/\delta} u^{k} K(u) \,\mathrm{d}u\right|^{2\nu+1}\right)^{2/(2k+1)}. \end{split}$$
Thus, the equality $T(K) = T(K_{\delta})$ holds.

Thus, the equality $T(K) = T(K_{\delta})$ holds.

The following table provides optimum kernels for some k and for ν = 0,1 (for $\nu=2$ see [12]). Selected graphs are given in Figs. 1–4.

$\nu = 0$				
k	$K_{ m opt}$			
2	$-\frac{3}{4}(x^2-1)$			
4	$\frac{15}{32}(x^2-1)(7x^2-3)$			
6	$-\frac{105}{256}(x^2-1)(33x^4-30x^2+5)$			
8	$\frac{315}{4096}(x^2-1)(715x^6-1001x^4+385x^2-35)$			
10	$-\frac{3465}{65536}(x^2-1)(4199x^8-7956x^6+4914x^4-1092x^2+63)$			

$\nu = 1$				
k	$K_{ m opt}$			
3	$\frac{15}{4}x(x^2-1)$			
5	$-\frac{105}{32}x(x^2-1)(9x^2-5)$			
7	$\frac{315}{256}x(x^2-1)(143x^4-154x^2+35)$			
9	$-\frac{3465}{4096}x(x^2-1)(1105x^6-1755x^4+819x^2-105)$			
11	$\frac{45045}{65536}x(x^2-1)(260015x^8-14212x^6+10098x^4-2772x^2+231)$			

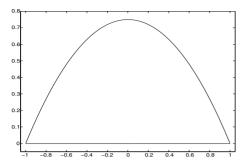


Figure 1. Optimum kernel of order (0, 2).

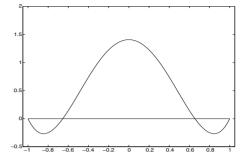
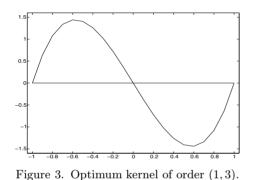


Figure 2. Optimum kernel of order (0, 4).



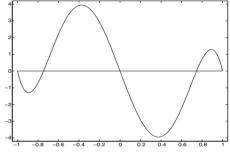


Figure 4. Optimum kernel of order (1, 5).

4. Optimum kernels with asymmetric support

The following result of Horová [7] gives the explicit form of the left optimum boundary kernel:

(1)
$$K_{\text{opt},L}(x) = (-1)^{\nu} \nu ! 2^{\nu+1} \left(1 - \left(\frac{2x - q_i + 1}{q_i + 1} \right)^2 \right) \\ \times \sum_{r=\nu}^{k-1} \frac{C_r^{3/2} \left(\frac{2x - q_i + 1}{q_i + 1} \right)}{a_r(q_i + 1)} \left(\sum_{j=\nu}^r c_j^r \frac{(1 - q_i)^{j-\nu}}{(1 + q_i)^j} \begin{pmatrix} j \\ \nu \end{pmatrix} \right),$$

where

(2)
$$a_r = \int_{-1}^{1} (1 - x^2) (C_r^{3/2}(x))^2 \, \mathrm{d}x$$

and $c_r^{3/2}$ is the coefficient of the polynomial $C_r^{3/2}(x) = \sum_{j=0}^r c_j^r x^r$. Further, r_i , $i = 1, \ldots, \frac{1}{2}(k-\nu)$ is the nonnegative root of the polynomial $d^{\nu}/dx^{\nu}C_{k-1}^{3/2}(x)$ and $q_i = (1-r_i)/(1+r_i)$, $i = 1, \ldots, \frac{1}{2}(k-\nu)$. These kernels are polynomials of degree k+1.

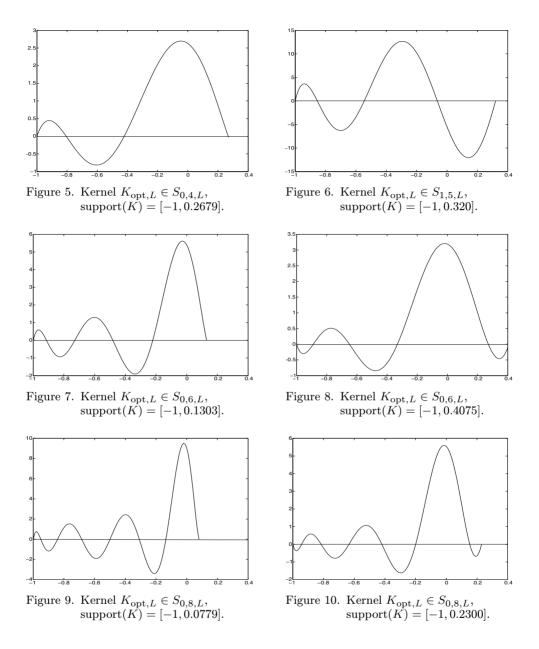
The left optimum boundary kernel $K_{\text{opt},L}$ satisfies $K_{\text{opt},L} \in S_{\nu,k,L}$, where

$$S_{\nu,k,L} = \begin{cases} K \in C^{1}[-1,q], \text{ support}(K) = [-1,q], \ 0 < q < 1, \\ K(-1) = K(q) = 0, \\ \\ \int_{-1}^{q} x^{j} K(x) \, \mathrm{d}x = \begin{cases} 0 & 0 \leq j < k, \ j \neq \nu, \\ (-1)^{\nu} \nu! & j = \nu, \\ \\ \beta_{k} & j = k. \end{cases}$$

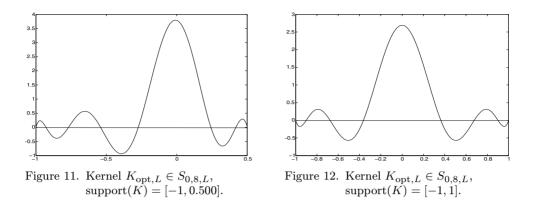
The right optimum boundary kernel can be constructed in the same way, but with the support [-q, 1]. For the left optimum boundary kernel deviation see [14].

Let us have a look at some formulas and figures for the left optimum boundary kernel $K_{\mathrm{opt},L}$:

Left optimum boundary kernel				
$K_{\text{opt},L} \in S_{0,4,L}, \text{ support}(K) = [-1, 0.2679]$				
$K_{\text{opt},L}(x) = 58.3549x^5 + 85.4375x^4 - 0.0332x^3 - 32.7080x^2 - 2.9910x + 2.6291$				
$K_{\text{opt},L} \in S_{0,6,L}, \text{ support}(K) = [-1, 0.1303]$				
$K_{\text{opt},L}(x) = 10^4 (0.3107x^7 + 0.9405x^6 + 1.0040x^5 + 0.4011x^4)$				
$+7.1680 \cdot 10^{-17} x^3 - 0.0290 x^2 - 0.0016 x + 0.0005)$				
$K_{\text{opt},L} \in S_{0,6,L}, \text{support}(K) = [-1, 0.4075]$				
$K_{\text{opt},L}(x) = -177.4043x^7 - 237.8810x^6 + 131.8714x^5 + 241.9009x^4$				
$-6.9026 \cdot 10^{-15}x^3 - 54.7696x^2 - 2.0280x + 3.1887$				
$K_{\text{opt},L} \in S_{0,8,L}, \text{ support}(K) = [-1, 0.0779]$				
$K_{\text{opt},L}(x) = 10^5 (1.0074x^9 + 4.2709x^8 + 7.3114x^7 + 6.3922x^6 + 2.9240x^5)$				
$+0.5931x^4 - 6.5125 \cdot 10^{-16}x^3 - 0.0140x^2 - 0.0005x + 0.0001)$				
$K_{\text{opt},L} \in S_{0,8,L}, \text{support}(K) = [-1, 0.2290]$				
$K_{\text{opt},L}(x) = 10^4 (-1.1042x^9 - 3.6208x^8 - 4.0740x^7 - 1.3609x^6 + 0.5880x^5$				
$+0.4191x^4 + 6.5070 \cdot 10^{-16}x^3 - 0.0291x^2 - 0.0008x + 0.0006)$				
$K_{\text{opt},L} \in S_{0,8,L}, \text{support}(K) = [-1, 0.5019]$				
$K_{\text{opt},L}(x) = 10^3 (0.5923x^9 + 0.6862x^8 - 0.9995x^7 - 1.3576x^6 + 0.2463x^5$				
$+0.5957x^4 + 2.6257 \cdot 10^{-16}x^3 - 0.0906x^2 - 0.0017x + 0.0038)$				
$K_{\text{opt},L} \in S_{1,5,L}, \text{ support}(K) = [-1, 0.3139]$				
$K_{\text{opt},L}(x) = 10^3 (-1.0375x^6 - 1.6271x^5 - 6.0590 \cdot 10^{-16}x^4 + 0.7944x^3$				
$+0.1277x^2 - 0.0824x - 0.0053)$				



As an illustration, in Fig. 12 we can also see that formula (1) for the left optimum boundary kernels (kernels with asymmetric support) is used for kernel construction with symmetric support [-1, 1]. In this way, the optimum kernel of the corresponding order is obtained. That is, the kernel $K_{\text{opt},L} \in S_{0,8,L}$, support(K) = [-1, 1], is the kernel $K \in M_{0,8}^1$ as well.



5. Application

The algorithm described in the preceding part was used for finding the optimum kernel and the optimum boundary kernel for an estimate of the simulated function

$$f(x) = 12 - 18x \cdot \cos(7^x - 5),$$

 $\sigma^2 = 12$. In this case a special type of estimate, the Gasser-Müller estimate, was chosen for data structure estimation. Plug in method was used for optimum bandwidth choice in all cases. For details of the construction of the Gasser-Müller estimate see [11]. The edge effect was removed by using optimum boundary kernels, but other possible techniques can also be used (reflection technique or cyclic model), see [8].

The first estimate of the function f(x) was obtained using the minimum variance kernel

$$K(x) = \frac{15}{128}(15 - 70x^2 + 64x^4), \quad K \in M_{0,6}^0$$

with $\alpha = 0.05$ and the bandwidth h = 0.17 (Fig. 13).

The second estimate of the function f(x) was obtained using the optimum variance kernel

$$K(x) = \frac{35}{256} (15 - 105x^2 + 189x^4 - 99x^6), \quad K \in M^1_{0,6},$$

 $\alpha=0.05$ and the bandwidth h=0.25 (Fig. 14).

The last estimate of the function f(x) was made using the optimum variance kernel $K \in M_{0,6}^1$ and the optimum boundary kernels $K_{\text{opt},L} \in S_{0,6,L}$, $K_{\text{opt},L} \in S_{0,6,R}$ for removing edge effects, $\alpha = 0.05$ and the bandwidth h = 0.25 (Fig. 15). The corresponding formulas are written in the text above.

Numerical illustration of the effect of the kernel type choices used for the Gasser-Müller estimate described above is presented in the following table. For comparison,

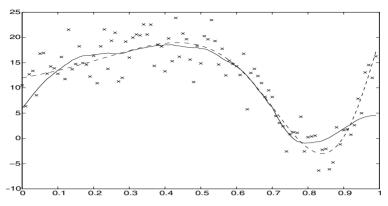


Figure 13. An estimate of the function f(x) using the minimum variance kernel (the solid line is the estimate, the dashed line is the function f(x)).

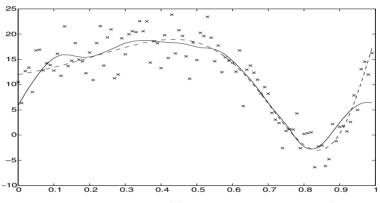


Figure 14. An estimate of the function f(x) using the optimum kernel (the solid line is the estimate, the dashed line is the function f(x)).

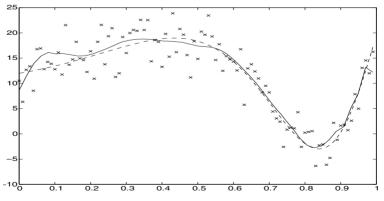


Figure 15. An estimate of the function f(x) using the optimum kernel and the optimum boundary kernels (the solid line is the estimate, the dashed line is the function f(x)).

the values of the $\overline{\text{AMSE}}$ for some other possible kernels are also given. We can see that the optimum kernel and optimum boundary kernels give in all cases the best results for the chosen kernel type (Fig. 15).

	$K\in M^0_{0,6}$	$K\in M^1_{0,6}$	$K \in M_{0,6}^1, K_{\text{opt},L} \in S_{0,6,L}, K_{\text{opt},L} \in S_{0,6,R}$
AMSE	4.4937	4.0706	1.2549
	$K\in M^0_{0,8}$	$K\in M^1_{0,8}$	$K \in M_{0,8}^1, K_{\text{opt},L} \in S_{0,8,L}, K_{\text{opt},L} \in S_{0,8,R}$
AMSE	3.4021	2.8960	1.2296
	$K\in M^0_{0,10}$	$K\in M^1_{0,10}$	$K \in M_{0,10}^1, K_{\text{opt},L} \in S_{0,10,L}, K_{\text{opt},L} \in S_{0,10,R}$
AMSE	$K \in M^0_{0,10}$ 4.3519	$K \in M^1_{0,10}$ 4.1519	$K \in M^{1}_{0,10}, K_{\text{opt},L} \in S_{0,10,L}, K_{\text{opt},L} \in S_{0,10,R}$ 1.1480
AMSE	- / -	- / -	

For demonstration of the described technique on real data, June average temperatures measured in Prague during the period 1771–1890 were used (see [11]). Note that the period from 1771 to 1890 was renormalized for calculation to the interval $x \in [0, 1]$ according to the assumption of the Gasser-Müller estimate construction. At first, an estimate of the June average temperatures was obtained using optimum variance kernel $K \in M_{0,6}^0$ and the bandwidth h = 0.075 (Fig. 16). At second, an optimum kernel $K \in M_{0,6}^1$ (Fig. 17) and, for removing edge effects, optimum boundary kernels $K_{\text{opt},L} \in S_{0,6,L}, K_{\text{opt},R} \in S_{0,6,R}, \alpha = 0.05$ and the bandwidth h = 0.07(Fig. 18) were used. The corresponding formulas are written in the text above. Value of the bandwidth h was found using the cross-validation method (see [11]).

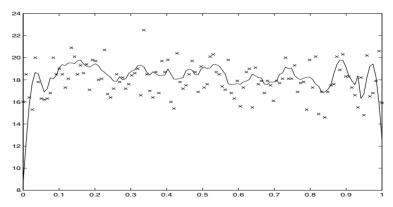


Figure 16. An estimate of June average temperatures measured in Prague using minimum variance kernel.

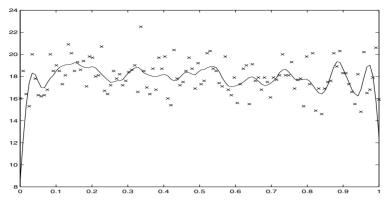


Figure 17. An estimate of June average temperatures measured in Prague using optimum variance kernel.

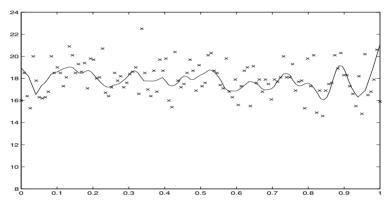


Figure 18. An estimate of June average temperatures measured in Prague using optimum kernel and optimum boundary kernels.

Figs. 16–18 illustrate the effect of different kernel types for the Gasser-Müller estimate construction. Unfortunately, the evaluation of the real data set using $\overline{\text{AMSE}}$ is not possible, as the formula for this type of error, namely

AMSE
$$(\hat{m}, h) = \frac{1}{n} \sum_{i=1}^{n} E(\hat{m}(x_i) - m(x_i))^2,$$

contains an unknown function m. Even though the above results concerning $\overline{\text{AMSE}}$ are only theoretical, they can be used to deduce the behaviour in the case of real data at least qualitatively [13].

In the case of June average temperature estimates using the minimum variance and optimum kernels, it is difficult to distinguish which estimate is better (the difference between the resulting estimates is small, see Figs. 16 and 17). Both the estimates have boundary effects. Therefore, the application of optimum boundary kernels should improve the results as Fig. 18 clearly demonstrates.

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