

Computing a family of reproducing kernels for statistical applications*

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For an open subset Ω of \mathbb{R} , an integer m , and a positive real parameter τ , the Sobolev spaces $H^m(\Omega)$ equipped with the norms: $\|u\|^2 = \int u(t)^2 dt + (1/\tau^{2m}) \int u^{(m)}(t)^2 dt$ constitute a family of reproducing kernel Hilbert spaces. When Ω is an open interval of the real line, we describe the computation of their reproducing kernels. We derive explicit formulas for these kernels for all values of m in the case of the whole real line, and for $m = 1$ and $m = 2$ in the case of a bounded open interval.

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1. Introduction

1.1. Motivation

It is often the case that statisticians or applied probabilists encounter the theory of reproducing kernel Hilbert spaces (RKHS) in their studies (see for example Weinert [11]). Each specific application usually requires the use of an adapted RKHS. Some of them are very well documented in the literature [4, 5], but we have come across cases where the expression of the kernel function of the space was not available, as for example in Delecroix et al. [6] for the nonparametric estimation of functions under shape restrictions. We believe that the method of derivation as well as the actual expression of these kernels may be of interest to other authors.

The rest of this introduction is devoted to the description of the spaces of interest. In section 2, we establish that, in the case of the whole real line, the kernels are Fourier

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transforms of simple functions and can be obtained through easy contour integration. In section 3, we turn to the case of a bounded open interval. We first establish the relationship between the kernel on the interval (a, b) associated with τ and the kernel on the interval $(0, 1)$ associated with another value of this parameter. Then, to determine the kernel on $(0, 1)$, we derive a system of differential equations of order $2m$ with initial conditions, and give its solutions for $m = 1$ and $m = 2$. The appendix contains a collection of intermediate steps in these computations.

1.2. The spaces and their norms

Let Ω denote an open subset of \mathbb{R} , and $H^m(\Omega)$ the classical real Sobolev space, i.e., the set of elements u of $L^2(\Omega)$ whose weak derivatives $u^{(k)}$ in the sense of generalized functions belong to $L^2(\Omega)$ for any integer k between 1 and m . For classical properties of these spaces, we refer the reader to Adams [1]. We just recall here that each element u of $H^m(\Omega)$ is equal almost everywhere to a unique absolutely continuous function on Ω with ordinary derivatives absolutely continuous up to order $m - 1$, and last derivative defined almost everywhere in the ordinary sense and square integrable. We will identify elements of $H^m(\Omega)$ with this unique representor. The classical norms for these spaces are:

$$\|u\|^2 = \sum_{j=0}^m \int_{x \in \Omega} (u^{(j)}(t))^2 dt. \quad (1)$$

For the particular application we had in mind in Delecroix et al. [6], the following norms seemed more appropriate:

$$\|u\|^2 = \int (u(t))^2 dt + \frac{1}{\tau^{2m}} \int (u^{(m)}(t))^2 dt. \quad (2)$$

They are simpler to interpret as a weighted sum of the L^2 norms of u and its last derivative $u^{(m)}$, the parameter τ regulating the balance. The norms defined by (2) are topologically equivalent to the ones defined by (1), by virtue of the Sobolev inequalities (see Agmon [2]), which can be applied to the case of the real line or the case of a bounded open interval.

Let us also recall a few facts about reproducing kernel Hilbert space theory. Let Dkx , the derivative functional of order k at x , be defined by:

$$\forall x \in \Omega, \forall u \in H^m(\Omega), \quad Dkx(u) = u^{(k)}(x). \quad (3)$$

A reproducing kernel Hilbert space is a Hilbert space in which the evaluation functionals $D0x$ are continuous functionals for all $x \in \Omega$. Let dkx in $H^m(\Omega)$ denote the representors of the functionals Dkx , in the sense that:

$$\forall x \in \Omega, \forall u \in H^m(\Omega), \quad Dkx(u) = \langle u, dkx \rangle. \quad (4)$$

These representors exist by the Riesz representation theorem as soon as Dkx is continuous. The function $K(x, y) = d0x(y)$ is known as the kernel of the space, and the reader is referred to Aronszajn [3] for more extensive properties. It is known that in the Sobolev spaces $H^m(\Omega)$, the functionals Dkx are well defined and continuous if and only if $m - k > \frac{1}{2}$ (see Wahba and Wendelberger [10]). The computation of dkx from K is straightforward. Our aim in sections 2 and 3 is the computation of K for $H^m(\Omega)$. Let us denote by $K_{m,\tau}^{(a,b)}$ the kernel function of $H^m(\Omega)$ when $\Omega = (a, b)$, and $K_{m,\tau}^\infty$ the kernel function of $H^m(\Omega)$ when $\Omega = \mathbb{R}$.

2. Case of the whole real line

When $\Omega = \mathbb{R}$, the space $H^m(\Omega)$ falls into the family of Beppo-Levi spaces described in Thomas-Agnan [9]. It follows from the results of this paper that the kernel is translation invariant, which can be written with a slight abuse of notation: $K_{m,\tau}^\infty(x, t) = K_{m,\tau}^\infty(t - x)$, and is given by:

$$\mathcal{F}K_{m,\tau}^\infty(\omega) = \frac{1}{1 + (2\pi\omega/\tau)^{2m}}, \quad (5)$$

where \mathcal{F} denotes the Fourier transform (as defined in Thomas-Agnan [9]). Even though the proof can be found in this reference, it is interesting to outline it here in this very simple example. By definition, $K_{m,\tau}^\infty$ satisfies, for all $u \in H^m(\Omega)$,

$$\int_{-\infty}^{\infty} u(t) K_{m,\tau}^\infty(t, x) dt + \frac{1}{\tau^{2m}} \int_{-\infty}^{\infty} u^{(m)}(t) \frac{\partial^m}{\partial t^m} K_{m,\tau}^\infty(t, x) dt = u(x). \quad (6)$$

Using the Parseval identity in these two integrals, and the Fourier inversion formula in the right hand side, one easily concludes that the function $f_x(t) = K_{m,\tau}^\infty(x, t)$ is the solution to the following equation:

$$\mathcal{F}f_x(\omega) + \left(\frac{2\pi\omega}{\tau}\right)^{2m} \mathcal{F}f_x(\omega) = \exp(-2\pi i\omega x). \quad (7)$$

This first shows that $\mathcal{F}f_x(\omega) = \exp(-2\pi i\omega x)\mathcal{F}f_0(\omega)$, and therefore that the kernel is translation invariant, and that $\mathcal{F}f_0$ is given by (5).

From formula (5) and the properties of Fourier transform, one concludes that $K_{m,\tau}^\infty$ can be expressed in terms of $K_{m,1}^\infty$ by:

$$K_{m,\tau}^\infty(t) = \tau K_{m,1}^\infty(\tau t). \quad (8)$$

$K_{m,1}^\infty$ is a kernel which is familiar to the nonparametric statisticians since it is the “asymptotically equivalent” kernel to smoothing splines of order m . The theory for this equivalence can be found in Silverman [8] as well as the analytic expression of this kernel for $\tau = 1$, and $m = 1$ or 2 . After searching the classical mathematical tables, we were unable to find the formula for this Fourier transform for general m , and were led to compute it by contour integration. The result is stated in the following proposition, followed by a short description of this contour integration.

Proposition 1.

$$K_{m,1}^{\infty}(t) = \sum_{k=0}^{m-1} \frac{\exp(-|t| \exp(i\frac{\pi}{2m} + k\frac{\pi}{m} - \frac{\pi}{2}))}{2m \exp((2m-1)(i\frac{\pi}{2m} + i\frac{k\pi}{m}))}. \quad (9)$$

Proof. To compute the integral

$$\int_{-\infty}^{\infty} \frac{\exp(2\pi i \omega x)}{1 + (2\pi \omega)^{2m}} d\omega, \quad \text{for } x \geq 0,$$

integrate on the boundary of the upper half disc of the complex plane $\{|z| \leq R, \operatorname{Im}(z) \geq 0\}$, and let R tend to ∞ . The poles on the upper half plane are

$$\frac{1}{2\pi} \exp\left(i\frac{\pi}{2m} + i\frac{k\pi}{m}\right), \quad \text{for } k = 0, \dots, m-1.$$

The integral is then equal to the product of $2\pi i$ by the sum of the residues of the integrand at these poles, which yields (9). \square

The most frequent cases of application which are $m = 1, 2$ and 3 , are given explicitly in the next corollary and figures 1 and 2 display the graphs of some of these kernels. Low values of τ correspond to flatter kernels.

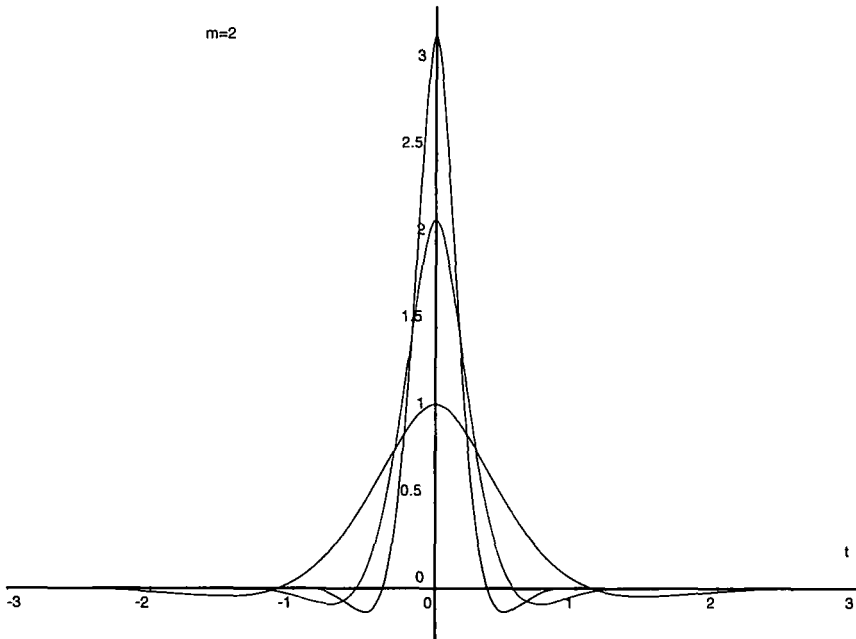
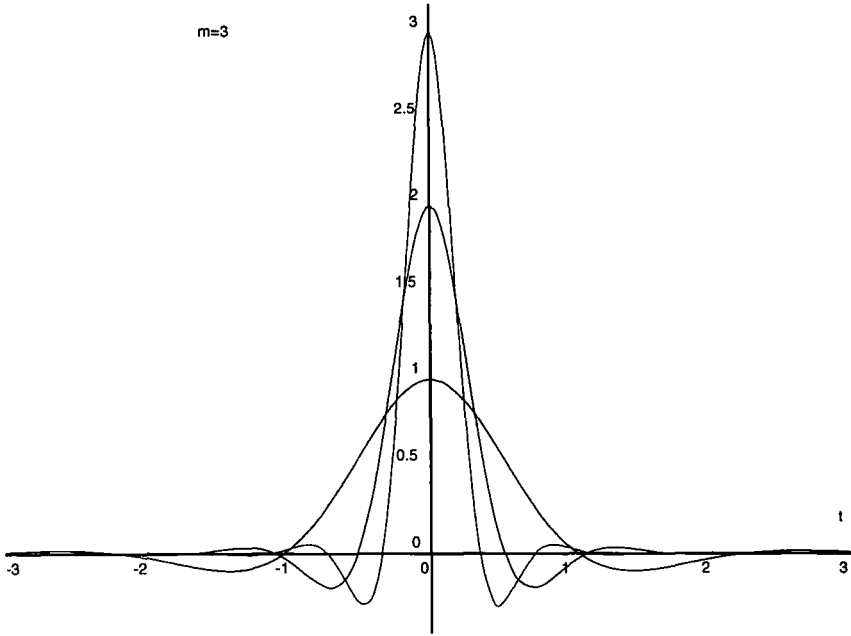


Figure 1. $K_{m,\tau}^{\infty}$ for $m = 2$ and $\tau = 3, 6, 9$.

Figure 2. $K_{m,\tau}^\infty$ for $m = 3$ and $\tau = 3, 6, 9$.**Corollary 1.**

$$\begin{aligned}
 K_{1,1}^\infty(t) &= \frac{1}{2} e^{-|t|}, \\
 K_{2,1}^\infty(t) &= \frac{1}{2} e^{-|t|/\sqrt{2}} \sin\left(|t|\frac{\sqrt{2}}{2} + \frac{\pi}{4}\right), \\
 K_{3,1}^\infty(t) &= \frac{1}{6} \left\{ e^{-|t|} + 2e^{-|t|/2} \sin\left(|t|\frac{\sqrt{3}}{2} + \frac{\pi}{6}\right) \right\}.
 \end{aligned}$$

3. Case of a bounded open interval*3.1. Reducing the problem to the unit interval*

By definition (4), the kernel $K_{m,\tau}^{(0,1)}$ must satisfy, for all $u \in H^m(0, 1)$,

$$\int_0^1 u(t) K_{m,\tau}^{(0,1)}(t, x) dt + \frac{1}{\tau^{2m}} \int_0^1 u^{(m)}(t) \frac{\partial^m}{\partial t^m} K_{m,\tau}^{(0,1)}(t, x) dt = u(x). \quad (10)$$

After the change of variables $t = (s - a)/(b - a)$, for $s \in (a, b)$, and letting

$$v(s) = u\left(\frac{s - a}{b - a}\right) \quad \text{and} \quad y = a + (b - a)x,$$

equation (10) yields for all $v \in K_{m,\tau}^{(a,b)}$:

$$\int_a^b v(s) K_{m,\tau}^{(0,1)} \left(\frac{s-a}{b-a}, \frac{y-a}{b-a} \right) \frac{1}{b-a} ds + \frac{1}{\tau^{2m}} \int_a^b (b-a)^m v^{(m)}(s) \frac{\partial^m}{\partial s^m} K_{m,\tau}^{(0,1)} \left(\frac{s-a}{b-a}, \frac{y-a}{b-a} \right) \frac{1}{b-a} ds = v(y). \quad (11)$$

It is then easy to conclude by definition of $K_{m,\tau}^{(a,b)}$ that:

Proposition 2.

$$K_{m,\mu}^{(a,b)}(s, y) = \frac{1}{b-a} K_{m,\tau}^{(0,1)} \left(\frac{s-a}{b-a}, \frac{y-a}{b-a} \right), \quad \text{where } \tau = \mu(b-a). \quad (12)$$

This formula relates $K_{m,\mu}^{(a,b)}$ to $K_{m,\tau}^{(0,1)}$ and therefore it is enough to compute the kernels on the unit interval.

3.2. Computation of $K_{m,\tau}^{(0,1)}$

In the bounded interval case, the kernels are not translation invariant, and it is convenient to introduce the right and left kernels as follows:

$$K_{m,\tau}^{(0,1)}(x, t) = \begin{cases} L_x(t), & \text{for } t \leq x, \\ R_x(t), & \text{for } t \geq x. \end{cases} \quad (13)$$

Because of the fundamental symmetry property of reproducing kernels (see Aronszjan [3]), it is enough to know the left kernel since:

$$\text{for } t \geq x, \quad R_x(t) = L_t(x). \quad (14)$$

Then let us return to equation (10) and perform m consecutive integrations by parts in the second integral. For any function g with $2m$ derivatives in an open subinterval (α, β) , we can write:

$$\int_{\alpha}^{\beta} u^{(m)}(t) g^{(m)}(t) dt = (-1)^m \int_{\alpha}^{\beta} u(t) g^{(2m)}(t) dt + \sum_{k=m}^{2m-1} (-1)^{k+m} [u^{(2m-1-k)} g^{(k)}]_{\alpha}^{\beta}$$

Assuming the left and right kernels do have this extra smoothness property, which will be checked a posteriori, we can apply this identity to $g = L_x$ on $(\alpha, \beta) = (0, x)$ and to $g = R_x$ on $(\alpha, \beta) = (x, 1)$, and plug it back into equation (10) to get:

$$\begin{aligned} & \int_0^x \left[L_x + \frac{(-1)^m}{\tau^{2m}} L_x^{(2m)} \right] (t) dt + \int_x^1 \left[R_x + \frac{(-1)^m}{\tau^{2m}} R_x^{(2m)} \right] (t) dt \\ & + \sum_{k=m}^{2m-1} (-1)^{k+m} \left\{ [u^{(2m-1-k)} L_x^{(k)}]_0^x + [u^{(2m-1-k)} R_x^{(k)}]_x^1 \right\} = u(x). \end{aligned} \quad (15)$$

Identifying the terms with the right hand side of (10), one gets the following result:

Proposition 3. The left and right kernels L_x and R_x are entirely determined by the following system of differential equations:

$$\begin{aligned} L_x + \frac{(-1)^m}{\tau^{2m}} L_x^{(2m)} &= 0, \\ R_x + \frac{(-1)^m}{\tau^{2m}} R_x^{(2m)} &= 0, \end{aligned} \quad (16)$$

with the boundary conditions:

$$\begin{aligned} L_x^{(k)}(0) &= 0 \quad \text{for } k = m, \dots, 2m-1, \\ R_x^{(k)}(1) &= 0 \quad \text{for } k = m, \dots, 2m-1, \end{aligned} \quad (17)$$

and

$$L_x^{(k)}(x) - R_x^{(k)}(x) = \begin{cases} 0, & \text{for } k = 0, \dots, 2m-2, \\ (-1)^{m-1} \tau^{2m}, & \text{for } k = 2m-1. \end{cases} \quad (18)$$

From equations (16), one concludes that L_x and R_x can be expressed as follows:

$$\begin{aligned} L_x(t) &= \sum_{j=1}^m l_j \exp(\gamma_j t) \cos(\lambda_j t) + l_{j+m} \exp(\gamma_j t) \sin(\lambda_j t), \\ R_x(t) &= \sum_{j=1}^m r_j \exp(\gamma_j t) \cos(\lambda_j t) + r_{j+m} \exp(\gamma_j t) \sin(\lambda_j t), \end{aligned} \quad (19)$$

where

$$\gamma_j = \sin\left(\frac{\pi}{2m} + \frac{j\pi}{m}\right) \quad \text{and} \quad \lambda_j = \cos\left(\frac{\pi}{2m} + \frac{j\pi}{m}\right).$$

The $4m$ unknowns l_j , r_j , $j = 1, \dots, 2m$ are entirely determined by the system of $4m$ linear equations (17) and (18).

Specializing now to the case $m = 1$, and combining with the result of proposition 2, we give the solution in the next corollary and the system of four linear equations in the appendix.

Corollary 2. The left kernel corresponding to $K_{1,\tau}^{(a,b)}$ is given by:

$$\text{for } t \leq x, \quad L_x(t) = \frac{\tau}{\sinh \tau(b-a)} \cosh \tau(b-x) \cosh \tau(t-a). \quad (20)$$

This kernel can be found in the case $\tau = 1$ in Duc-Jacquet [7].

In the case $m = 2$, we introduce the following four functions in order to express the final result:

$$b_1(z) = \exp\left(\frac{\sqrt{2}}{2}z\right) \cos\left(\frac{\sqrt{2}}{2}z\right),$$

$$\begin{aligned}
b_2(z) &= \exp\left(\frac{\sqrt{2}}{2}z\right) \sin\left(\frac{\sqrt{2}}{2}z\right), \\
b_3(z) &= \exp\left(-\frac{\sqrt{2}}{2}z\right) \cos\left(\frac{\sqrt{2}}{2}z\right), \\
b_4(z) &= \exp\left(-\frac{\sqrt{2}}{2}z\right) \sin\left(\frac{\sqrt{2}}{2}z\right).
\end{aligned} \tag{21}$$

For the same purpose, we will write the left kernel in the following form:

$$L_x(t) = \sum_{j=1}^4 \sum_{k=1}^4 l_{jk} b_j(\tau t) b_k(\tau x), \tag{22}$$

where the 16 coefficients l_{jk} are given in the next corollary, and the system of eight linear equations in the appendix.

Corollary 3. The coefficients l_{jk} defining the left kernel of $K_{2,\tau}^{(0,1)}$ through equation (22) are given by:

$$\begin{aligned}
l_{11} &= \delta \{ -\cos(\sqrt{2}\tau) + \sin(\sqrt{2}\tau) + 3\exp(-\sqrt{2}\tau) - 2 \}, \\
l_{12} &= \delta \{ -\cos(\sqrt{2}\tau) - \sin(\sqrt{2}\tau) + \exp(-\sqrt{2}\tau) \}, \\
l_{13} &= \delta \{ -\cos(\sqrt{2}\tau) + 3\sin(\sqrt{2}\tau) - \exp(\sqrt{2}\tau) + 2 \}, \\
l_{14} &= \delta \{ -3\cos(\sqrt{2}\tau) - \sin(\sqrt{2}\tau) - \exp(\sqrt{2}\tau) + 4 \}, \\
l_{21} &= l_{12}, \\
l_{22} &= \delta \{ \cos(\sqrt{2}\tau) - \sin(\sqrt{2}\tau) + \exp(-\sqrt{2}\tau) - 2 \}, \\
l_{23} &= \delta \{ -\cos(\sqrt{2}\tau) + \sin(\sqrt{2}\tau) + \exp(\sqrt{2}\tau) \}, \\
l_{24} &= \delta \{ -\cos(\sqrt{2}\tau) - \sin(\sqrt{2}\tau) - \exp(\sqrt{2}\tau) + 2 \}, \\
l_{31} &= l_{13} - \frac{\sqrt{2}}{4}\tau, \\
l_{32} &= l_{23} + \frac{\sqrt{2}}{4}\tau, \\
l_{33} &= \delta \{ \cos(\sqrt{2}\tau) + \sin(\sqrt{2}\tau) - 3\exp(\sqrt{2}\tau) + 2 \}, \\
l_{34} &= \delta \{ -\cos(\sqrt{2}\tau) + \sin(\sqrt{2}\tau) + \exp(\sqrt{2}\tau) \}, \\
l_{41} &= l_{14} - \frac{\sqrt{2}}{4}\tau, \\
l_{42} &= l_{24} - \frac{\sqrt{2}}{4}\tau,
\end{aligned}$$

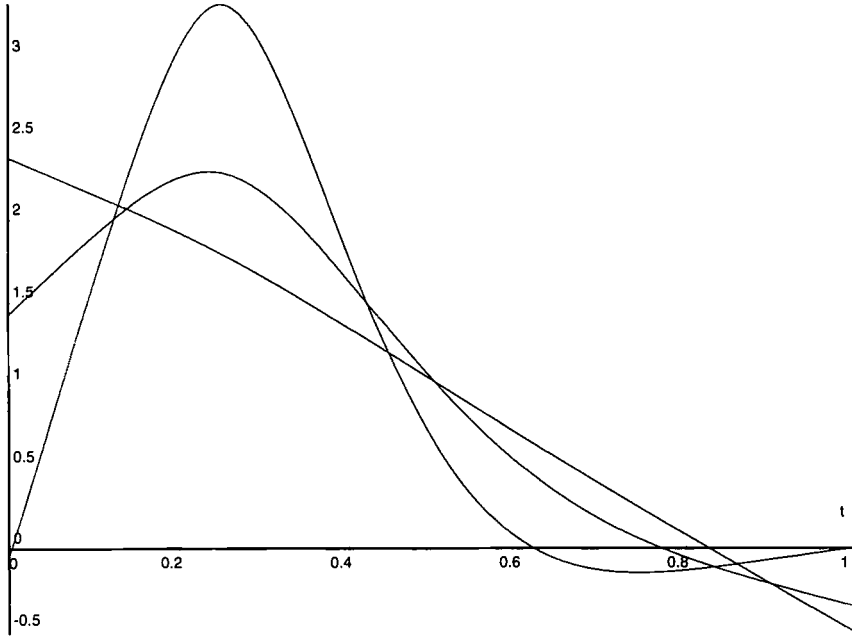


Figure 3. $K_{m,\tau}^{[0,1]}$ for $m = 2$, $\tau = 3, 6, 9$ and $x = 0.25$.

$$l_{43} = l_{34},$$

$$l_{44} = \delta \{ -\cos(\sqrt{2}\tau) - \sin(\sqrt{2}\tau) - \exp(\sqrt{2}\tau) + 2 \}, \quad (23)$$

where

$$\delta = \frac{\sqrt{2}\tau}{16(\sin^2(\frac{\sqrt{2}}{2}\tau) - \sinh^2(\frac{\sqrt{2}}{2}\tau))}. \quad (24)$$

The solution of the system of eight linear equations was obtained with the help of the computer algebra system Maple. Nevertheless, for those who wish to compute their own kernel, do not expect the software to yield a nice and good looking solution in a few minutes. When the coefficients of the linear system are, as in our case, functions of x involving products of exponential and trigonometric functions, human intervention still seems to be necessary. The reader will find the Maple code in the appendix. Figures 3 and 4 display the graphs of these kernels in the case $m = 2$, $x = 0.25$ and $x = 0.5$. As before, low values of τ correspond to flatter kernels.

Appendix

A.1. Intermediate steps for $m = 1$

When $m = 1$, the left and right kernels are linear combinations of $\exp(\tau t)$ and $\exp(-\tau t)$:

$$\begin{aligned} L_x(t) &= l_1 \exp(\tau t) + l_2 \exp(-\tau t), \\ R_x(t) &= r_1 \exp(\tau t) + r_2 \exp(-\tau t), \end{aligned} \quad (25)$$

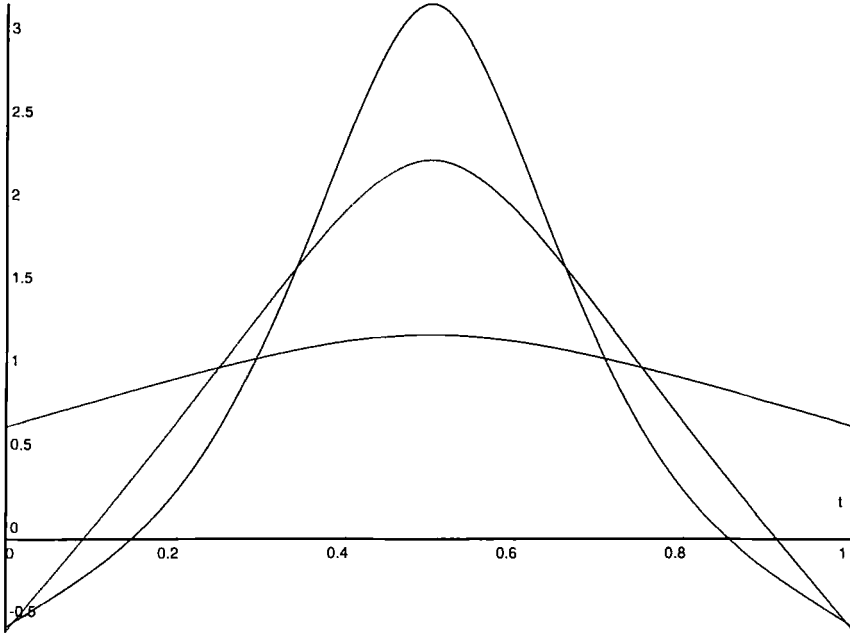


Figure 4. $K_{m,\tau}^{(0,1)}$ for $m = 2$ and $\tau = 3, 6, 9$ and $x = 0.5$.

and the linear system defining these coefficients is:

$$\begin{aligned}
 l_1 - l_2 &= 0, \\
 r_1 \exp(\tau) - r_2 \exp(-\tau) &= 0, \\
 l_1 \exp(\tau x) + l_2 \exp(-\tau x) - r_1 \exp(\tau x) - r_2 \exp(-\tau x) &= 0, \\
 (l_1 - r_1) \exp(\tau x) - (l_2 - r_2) \exp(-\tau x) &= \tau.
 \end{aligned} \tag{26}$$

A.2. Intermediate steps for $m = 2$

When $m = 2$, for the purpose of computing the kernel, we write the left and right kernels as follows in terms of the basis functions (21):

$$\begin{aligned}
 L_x(t) &= \sum_{j=1}^4 l_j b_j(\tau t), \\
 R_x(t) &= \sum_{j=1}^4 r_j b_j(\tau t),
 \end{aligned} \tag{27}$$

and the linear system defining these coefficients is:

$$\begin{aligned}
l_2 - l_4 &= 0, \\
-r_1 b_2(\tau) + r_2 b_1(\tau) + r_3 b_4(\tau) - r_4 b_3(\tau) &= 0, \\
-l_1 + l_2 + l_3 + l_4 &= 0, \\
r_1(-b_1(\tau) - b_2(\tau)) + r_2(b_1(\tau) - b_2(\tau)) + r_3(b_3(\tau) - b_4(\tau)) \\
&\quad + r_4(b_3(\tau) + b_4(\tau)) = 0, \\
(l_1 - r_1)b_1(\tau x) + (l_2 - r_2)b_2(\tau x) + (l_3 - r_3)b_3(\tau x) + (l_4 - r_4)b_4(\tau x) &= 0, \quad (28) \\
-(l_1 - r_1)b_2(\tau x) + (l_2 - r_2)b_1(\tau x) + (l_3 - r_3)b_4(\tau x) - (l_4 - r_4)b_3(\tau x) &= 0, \\
(l_1 - r_1)(b_1(\tau x) + b_2(\tau x)) - (l_2 - r_2)(b_1(\tau x) - b_2(\tau x)) \\
&\quad - (l_3 - r_3)(b_3(\tau x) - b_4(\tau x)) - (l_4 - r_4)(b_3(\tau x) + b_4(\tau x)) = \sqrt{2}\tau \\
(l_1 - r_1)(b_1(\tau x) - b_2(\tau x)) + (l_2 - r_2)(b_1(\tau x) + b_2(\tau x)) \\
&\quad - (l_3 - r_3)(b_3(\tau x) + b_4(\tau x)) + (l_4 - r_4)(b_3(\tau x) - b_4(\tau x)) = 0.
\end{aligned}$$

It is clear that the last four equations only involve the unknowns $l_j - r_j$, $j = 1, \dots, 4$. Therefore one can decompose the calculation in two systems of four linear equations. An intermediate result is the expression of these differences:

$$\begin{aligned}
(l_1 - r_1) \exp\left(\frac{\sqrt{2}}{2}\tau x\right) &= \frac{\sqrt{2}}{4}\tau \left[\cos\left(\frac{\sqrt{2}}{2}\tau x\right) + \sin\left(\frac{\sqrt{2}}{2}\tau x\right) \right], \\
(l_2 - r_2) \exp\left(\frac{\sqrt{2}}{2}\tau x\right) &= \frac{\sqrt{2}}{4}\tau \left[-\cos\left(\frac{\sqrt{2}}{2}\tau x\right) + \sin\left(\frac{\sqrt{2}}{2}\tau x\right) \right], \\
(l_3 - r_3) \exp\left(-\frac{\sqrt{2}}{2}\tau x\right) &= \frac{\sqrt{2}}{4}\tau \left[-\cos\left(\frac{\sqrt{2}}{2}\tau x\right) + \sin\left(\frac{\sqrt{2}}{2}\tau x\right) \right], \\
(l_4 - r_4) \exp\left(-\frac{\sqrt{2}}{2}\tau x\right) &= \frac{\sqrt{2}}{4}\tau \left[-\cos\left(\frac{\sqrt{2}}{2}\tau x\right) - \sin\left(\frac{\sqrt{2}}{2}\tau x\right) \right]. \quad (29)
\end{aligned}$$

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