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A NEW METHOD WITH ERROR BOUND TO ESTIMATE SECOND DERIVATIVES FROM SCATTERED DATA

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RÉSUMÉ. Une méthode originale est développée afin d'estimer le laplacien d'une fonction à valeurs connues sur un ensemble aléatoire de points. Une borne d'erreur théorique est obtenue, ainsi que le taux de convergence vers la dérivée seconde. Les résultats théoriques sont corroborés par quelques calculs numériques.

ABSTRACT. A new method is proposed for estimating numerically from scattered data the second derivative of a function. It uses the convolution of the data with well chosen even functions. Theoretical error bounds and numerical results establish the validity and effectiveness of the method. Moreover, the order of convergence derived from the theory is corroborated by numerical examples.

1. Introduction

In the literature, techniques to estimate derivatives are used to simulate physical phenomena governed by differential equations. Here we introduce a method to estimate, from data at disordered points $\{x_i\}_{i=1}^N$ in an open interval $]a, b[\subset [a, b] = I$, the second derivative of a (twice differentiable) real function. Our approach is inspired by smoothed particle hydrodynamics (SPH) developed by Lucy [18] and by Gingold and Monaghan [13, 20, 21] to simulate astrophysical phenomena. This meshfree method allowed them to calculate from scattered data the Laplacian of a function and to transform the original Navier-Stokes equation to that of a system of ordinary differential equations (with respect to time) which was then solved numerically [5, 9, 16, 23, 26]. More recently, SPH was used to simulate fluid motion encountered in every day life [6, 10, 11, 15, 22, 24, 28, 29]. The numerical precision of SPH in estimating a Laplacian depends in large part on the Laplacian of the kernel [8, 17, 23] with which the scattered data is convoluted. It also depends on the summation method used to numerically estimate the convolution. Obviously, all numerical methods used in estimating an integral are subject to a high level of inaccuracy when the density of the disordered points is low. These weaknesses inherent to SPH are compounded by the complexity of the few theoretical error bounds found in the literature [4, 19, 25, 27]. By contrast, our approach based on elementary principles yields simple useful theoretical error bounds and better numerical results when estimating a second derivative. In this article we

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restrict ourselves to one-dimensional spaces. In a later paper, our technique will be extended to higher dimensions to estimate a Laplacian.

2. Preliminaries

By a *kernel*, we mean a family (indexed by $h > 0$) of bounded piecewise smooth (*i.e.*, infinitely differentiable) even functions $k_h : \mathbb{R} \to [0, \infty[$ with support in $[-h, h]$ and such that we have for every $r \in \mathbb{R}$,

$$k_h(r) = \frac{1}{2}\left[k_h(r-) + k_h(r+)\right], \tag{1}$$

where $k_h(r-) = \lim_{s\downarrow 0} k_h(r-s)$ and $k_h(r+) = \lim_{s\downarrow 0} k_h(r+s)$ exist at all points $r \in \mathbb{R}$, for all $h > 0$,

$$\int_{-\infty}^{\infty} k_h(r)\, dr = 1, \tag{2}$$

and

$$\|k_h\|_\infty = O\left(h^{-1}\right) \tag{3}$$

where $\|\cdot\|_\infty$ designates the essential supremum norm over I. For any kernel k_h we have

$$\int_{-\infty}^{\infty} r^i k_h(r)\, dr = \begin{cases} 1 & \text{if } i = 0, \\ 0 & \text{if } i = 1, \\ O\left(h^2\right) & \text{if } i = 2. \end{cases} \tag{4}$$

This identity for $i = 0$ is simply condition (2) imposed on a kernel. The fact that $r \to r k_h(r)$ is an odd function yields (4) for $i = 1$. Furthermore

$$\int_{-\infty}^{\infty} r^2 k_h(r)\, dr = 2\int_0^{\infty} r^2 k_h(r)\, dr \le \frac{2h^3}{3}\|k_h\|_\infty$$

and so by (3) we get (4) for $i = 2$.

The family δ_h $(h > 0)$ of functions defined on $\mathbb{R}$ by

$$\delta_h(r) = \begin{cases} 1/2h & \text{if } -h < r < h, \\ 1/4h & \text{if } r = \pm h, \\ 0 & \text{otherwise,} \end{cases} \tag{5}$$

(and used in [2, 3] to approximate first and second derivatives from scattered data) is an example of a kernel. So are the well-known families of continuous functions

$$k_{h,6}(r) = \begin{cases} \dfrac{35}{32h^7}\left(h^2 - r^2\right)^3 & \text{if } -h \le r \le h, \\ 0 & \text{otherwise,} \end{cases} \tag{6}$$

and

$$k_{h,D}(r) = \begin{cases} \dfrac{3}{4h^3}(h^2 - r^2) & \text{if } -h \le r \le h, \\ 0 & \text{otherwise,} \end{cases} \tag{7}$$

(for all $h > 0$) referred to in the literature as *poly6* and *dome-shaped* [14, 16], respectively. (Though $k_{h,D}$ is not differentiable at $x = \pm h$, it has the advantage of requiring fewer operations to evaluate than does $k_{h,6}$.) Given a twice continuously differentiable function $f : \mathbb{R} \to \mathbb{R}$ and a kernel k_h, classic SPH uses the second derivative k_h'' (when it exists) to estimate f'' by way of the convolution $f * k_h''$. This is justified whenever the equality

$$f'' * k_h = f * k_h'' \tag{8}$$

holds. Integrating twice by parts yields (8) for $k_h = k_{h,6}$. Kernel (5) does not satisfy (8) since $\delta_h'' = 0$ almost everywhere. Neither does kernel (7). For example, if $f(x) = x^2$ then $\left(k_{h,D}'' * f\right)(0) = -1$ while $(k_{h,D} * f'')(0) = 2$. In this article we generalize the technique based on (8) by substituting in place of k_h'' $(h > 0)$ a family λ_h $(h > 0)$ of real bounded piecewise smooth even functions of mean zero on $\mathbb{R}$ with support in $[-h, h]$ and for which, for every $r \in \mathbb{R}$,

$$\lambda_h(r) = [\lambda_h(r+) + \lambda_h(r-)]/2, \tag{9}$$

where $\lambda_h(r+)$ and $\lambda_h(r-)$ exist at all points $r \in \mathbb{R}$, for all $h > 0$,

$$\int_{-\infty}^{\infty} r^2 \lambda_h(r)\, dr = 2, \tag{10}$$

and

$$\|\lambda_h\|_\infty = O\left(h^{-3}\right). \tag{11}$$

We shall call such a family of functions a *Laplacian kernel* and observe that

$$\int_{-\infty}^{\infty} r^i \lambda_h(r)\, dr = \begin{cases} 0 & \text{if } i = 0, 1, 3, \\ 2 & \text{if } i = 2, \\ O\left(h^2\right) & \text{if } i = 4. \end{cases} \tag{12}$$

(This is the case when $\lambda_h = k_h''$ for any kernel k_h satisfying (8)).

In this paper, we will approximate f'' by the convolution $f * \lambda_h$ which will in turn be approximated by $f_{n'} * \lambda_h$, where $f_{n'}$ is an appropriate piecewise Lagrange polynomial interpolation (of degree $n' - 1$) of f based on a given set of data $\{(x_i, f(x_i))\}_{i=1}^N \subset \mathbb{R}^2$ at n' consecutive points in the disordered set $\{x_i\}_{i=1}^N \subset \mathbb{R}$. In this way we use to advantage the smoothing effect of integration in the vicinity of the nodes x_i. Finally, $f_{n'} * \lambda_h$ will be estimated by Boole's rule. In the process, useful new bounds are derived for the error in approximating f'' by the convolution $f_{n'} * \lambda_h$ evaluated via Boole's rule. These error bounds along with some numerical results on the order of convergence as $h \downarrow 0$ will establish the theoretical validity and numerical effectiveness of our method. In what follows we write $\|\cdot\|_1$ to denote the usual L^1 norm on the class of Lebesgue integrable functions on $\mathbb{R}$. The family of bounded piecewise smooth real functions of compact support on $\mathbb{R}$ is an important subset of this class.

Example 2.1. The family of continuous even functions

$$\lambda_h(r) = \begin{cases} \dfrac{105}{16h^7}(6h^2r^2 - 5r^4 - h^4) & \text{if } -h \le r \le h, \\ 0 & \text{otherwise,} \end{cases} \tag{13}$$

(for all $h > 0$) obtained from (6) by $\lambda_h(r) = k''_{h,6}(r)$ for all $r \neq \pm h$ and extended to all $\mathbb{R}$ by (9) is used in classic SPH to estimate a second derivative by way of (8). We have

(14) $$\|\lambda_h\|_\infty = 105/16h^3,$$

(15) $$\|\lambda_h\|_1 = \frac{84}{25h^2}\sqrt{5}$$

and

$$\int_{-\infty}^{\infty} r^i \lambda_h(r)\, dr = \begin{cases} 0 & \text{if } i = 0, 1, 3, \\ 2 & \text{if } i = 2, \\ 4h^2/3 & \text{if } i = 4. \end{cases}$$

Thus (13) is a Laplacian kernel. As we shall see, Laplacian kernels like (13), obtained by taking the second derivative (almost everywhere) of a kernel, need not provide optimal results when estimating a second derivative even when (8) holds. We note that

$$\lambda_h(r) = \begin{cases} -\dfrac{3}{2h^3} & \text{if } -h \le r \le h, \\ 0 & \text{otherwise,} \end{cases}$$

based on the second derivative (almost everywhere) of kernel (7) is not a Laplacian kernel since, as already noted, $\int_{-h}^{h} r^2 k''_{h,D}(r)\, dr = -1 \neq 2$.

Example 2.2. For any given kernel k_h we introduce the family of odd functions k_h^1 $(h > 0)$ defined by the divided difference formula

(16) $$k_h^1(r) = \frac{1}{h}\left[k_{h/2}\left(r + \frac{h}{2}\right) - k_{h/2}\left(r - \frac{h}{2}\right)\right].$$

Thus by (1) we have

$$k_h^1(r) = \begin{cases} k_{h/2}(h/2)/2h & \text{if } r = -h, \\ k_{h/2}(r + h/2)/h & \text{if } -h < r < 0, \\ -k_{h/2}(r - h/2)/h & \text{if } 0 < r < h, \\ -k_{h/2}(h/2)/2h & \text{if } r = h, \\ 0 & \text{otherwise.} \end{cases}$$

The equality

(17) $$\left\|k_h^1\right\|_\infty = O\left(h^{-2}\right)$$

follows by virtue of (3) and the equality

(18) $$\left\|k_h^1\right\|_1 = \frac{2}{h^2}$$

follows from (2). We also have

(19) $$\int_{-\infty}^{\infty} r^i k_h^1(r)\, dr = \begin{cases} 0 & \text{if } i = 0, 2, \\ -1 & \text{if } i = 1, \\ O\left(h^2\right) & \text{if } i = 3. \end{cases}$$

Identity (19) for $i = 0, 2$ is a consequence of the fact that $r^i k_h^1(r)$ is an odd function of r. For $i = 1$ we have

$$\int_{-\infty}^{\infty} r k_h^1(r)\, dr = \frac{1}{h}\left[\int_{-h}^{0} r k_{h/2}\left(r+\frac{h}{2}\right) dr - \int_0^h r k_{h/2}\left(r-\frac{h}{2}\right) dr\right].$$

The change of variable $\rho = r + h/2$ gives

$$\begin{aligned}\int_{-h}^{0} r k_{h/2}\left(r+\frac{h}{2}\right) dr &= \int_{-h/2}^{h/2}\left(\rho-\frac{h}{2}\right) k_{h/2}(\rho)\, d\rho \\ &= \int_{-h/2}^{h/2} \rho k_{h/2}(\rho)\, d\rho - \frac{h}{2}\int_{-h/2}^{h/2} k_{h/2}(\rho)\, d\rho \\ &= -h/2.\end{aligned}$$

Similarly

$$\int_0^h r k_{\frac{h}{2}}\left(r-\frac{h}{2}\right) dr = h/2$$

and so (19) holds for $i = 1$. Finally, for $i = 3$ we have

$$\int_{-\infty}^{\infty} r^3 k_h^1(r)\, dr = 2\int_0^{\infty} r^3 k_h^1(r)\, dr \le 2\left\|k_h^1\right\|_\infty \int_0^{\infty} r^3 dr = \frac{h^4}{2}\left\|k_h^1\right\|_\infty$$

and so, by virtue of (17), (19) is proved. Using (16) we now define the family of even functions

$$k_h^2 = \frac{1}{h}\left[k_{h/2}^1\left(r+\frac{h}{2}\right) - k_{h/2}^1\left(r-\frac{h}{2}\right)\right] \tag{20}$$

which can also be written as

$$k_h^2(r) = \begin{cases} k_{h/4}(h/4)/h^2 & \text{if } r = \pm h, \\ 2k_{h/4}(|r| - 3h/4)/h^2 & \text{if } h/2 < |r| \le h, \\ -2k_{h/4}(|r| - h/4)/h^2 & \text{if } 0 < |r| < h/2, \\ -4k_{h/4}(h/4)/h^2 & \text{if } r = 0, \\ 0 & \text{otherwise,} \end{cases}$$

and so

$$\left\|k_h^2\right\|_\infty = O\left(h^{-3}\right) \tag{21}$$

because of (17) and

$$\left\|k_h^2\right\|_1 = \frac{1}{h}\int_{-h}^{0} k_{h/2}^1\left(r+\frac{h}{2}\right) dr + \frac{1}{h}\int_0^h k_{h/2}^1\left(r-\frac{h}{2}\right) dr = \frac{8}{h^2} \tag{22}$$

by (18). We also have

$$\int_{-\infty}^{\infty} r^i k_h^2(r)\, dr = \begin{cases} 0 & \text{if } i = 0, 1, 3, \\ 2 & \text{if } i = 2, \\ O\left(h^2\right) & \text{if } i = 4. \end{cases} \tag{23}$$

Identity (23) for $i = 1, 3$ is a consequence of the fact that $r^i k_h^2(r)$ is an odd function of r. The case $i = 0$ follows by virtue of (19) and (20). For $i = 2$ we have

$$\int_{-\infty}^{\infty} r^2 k_h^2(r)\, dr = \frac{1}{h}\left[\int_{-h}^{0} r^2 k_{h/2}^1\left(r + \frac{h}{2}\right) dr - \int_0^h r^2 k_{h/2}^1\left(r - \frac{h}{2}\right) dr\right]. \tag{24}$$

The change of variable $\rho = r + h/2$ yields

$$\begin{aligned}\int_{-h}^{0} r^2 k_{h/2}^1(r + h/2)\, dr &= \int_{-h/2}^{h/2}\left(\rho - \frac{h}{2}\right)^2 k_{h/2}^1(\rho)\, d\rho \\ &= \int_{-h/2}^{h/2} \rho^2 k_{h/2}^1(\rho)\, d\rho - h\int_{-h/2}^{h/2} \rho k_{h/2}^1(\rho)\, d\rho \\ &\quad + \frac{h^2}{4}\int_{-h/2}^{h/2} k_{h/2}^1(\rho)\, d\rho\end{aligned}$$

and so (19) and the fact that $k_{h/2}^1(\rho)$ is an odd function of ρ gives

$$\int_{-h}^{0} r^2 k_{h/2}^1(r + h/2)\, dr = h.$$

Similarly

$$\int_0^h r^2 k_{h/2}^1(r - h/2)\, dr = -h$$

and so, by (24), we get (23) for $i = 2$. Finally, for $i = 4$, we have

$$\int_{-\infty}^{\infty} r^4 k_h^2(r)\, dr \le 2\left\|k_h^2\right\|_\infty \int_0^h r^4 dr = \frac{2h^5}{5}\left\|k_h^2\right\|_\infty$$

and so we get (23) for $i = 4$, by virtue of (21). Thus we have proved (23) and so $\lambda_h = k_h^2$ is a Laplacian kernel. In particular, each of the three families of functions

$$\delta_h^2(r) = \begin{cases} 2/h^3 & \text{if } r = \pm h, \\ 4/h^3 & \text{if } h/2 < |r| < h, \\ -4/h^3 & \text{if } 0 < |r| < h/2, \\ 0 & \text{otherwise,} \end{cases}$$

$$k_{h,6}^2(r) = \begin{cases} 35840\left[(h/4)^2 - (|r| - 3h/4)^2\right]^3 \Big/ h^9 & \text{if } h/2 < |r| < h, \\ -35840\left[(h/4)^2 - (|r| - h/4)^2\right]^3 \Big/ h^9 & \text{if } 0 < |r| < h/2, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$k_{h,D}^2(r) = \begin{cases} 96\left[(h/4)^2 - (|r| - 3h/4)^2\right] \Big/ h^5 & \text{if } h/2 < |r| < h, \\ -96\left[(h/4)^2 - (|r| - h/4)^2\right] \Big/ h^5 & \text{if } 0 < |r| < h/2, \\ 0 & \text{otherwise,} \end{cases} \tag{25}$$

constitute a Laplacian kernel. We note that (12) for $i = 4$ can be written explicitly as

$$\int_{-\infty}^{\infty} r^4 k_h^2(r)\,dr = \begin{cases} 3h^2/2 & \text{if } k_h = \delta_h, \\ 4h^2/3 & \text{if } k_h = k_{h,6}, \\ 7h^2/5 & \text{if } k_h = k_{h,D}, \end{cases}$$

which are all $O\left(h^2\right)$. Furthermore, we have

$$\left\|k_h^2\right\|_\infty = \begin{cases} 4/h^3 & \text{if } k_h = \delta_h, \\ 35/4h^3 & \text{if } k_h = k_{h,6}, \\ 6/h^3 & \text{if } k_h = k_{h,D}. \end{cases} \tag{26}$$

Equations (16) and (20) can be generalized inductively to

$$k_h^j = \frac{1}{h}\left[k_{h/2}^{j-1}\left(r + \frac{h}{2}\right) - k_{h/2}^{j-1}\left(r - \frac{h}{2}\right)\right]$$

for $j = 1, 2, 3, \ldots$ The derivative $f^{(j)}$ can then be approximated by way of the convolution $f * k_h^j$. Thus, for $j = 3$, k_h^3 verifies the necessary properties to estimate f'''.

Let $C(I)$ denote the class of all real functions on the interval $I = [a, b]$ which can be extended to continuous real functions on an open interval containing I. In general $C^j(I)$ $(j = 1, 2, 3, \ldots)$ denotes the class of functions in $C(I)$ which can be extended to j-times continuously differentiable functions on an open interval containing I. As we shall see, the Laplacian kernels given so far verify

$$f \in C^n(I) \Rightarrow \left\|f'' - f * \lambda_h\right\|_\infty = \begin{cases} O(h) & \text{if } n = 3, \\ O\left(h^2\right) & \text{if } n = 4. \end{cases} \tag{27}$$

Example 2.3. If S_h is the step function given by

$$S_h(r) = \begin{cases} -27/8h^3 & \text{if } 2h/3 < |r| < h, \\ 189/8h^3 & \text{if } h/3 < |r| < 2h/3, \\ -81/4h^3 & \text{if } -h/3 < |r| < h/3, \\ -27/16h^3 & \text{if } r = \pm h, \\ 27/16h^3 & \text{if } r = \pm h/3, \\ 81/8h^3 & \text{if } r = \pm 2h/3, \\ 0 & \text{otherwise}, \end{cases} \tag{28}$$

then

$$\left\|S_h\right\|_\infty = 189/8h^3 \tag{29}$$

and

$$\left\|S_h\right\|_1 = 63/2h^2. \tag{30}$$

Later we shall see that

$$f \in C^n(I) \Rightarrow \left\|f'' - f * S_h\right\|_\infty = O\left(h^{n-2}\right) \tag{31}$$

for $n = 3, \dots, 6$. This will follow from

$$\int_{-\infty}^{\infty} r^i S_h(r)\, dr = \begin{cases} 2 & \text{if } i = 2, \\ 0 & \text{if } i = 0, 1, 3, 4, 5, \\ -14h^4/27 & \text{if } i = 6, \end{cases} \tag{32}$$

which is easy to show. Clearly, (32) implies that S_h is a Laplacian kernel.

In general, one can construct, for any given even integer $m \geq 4$, a Laplacian kernel λ_h for which

$$\int_{-\infty}^{\infty} r^i \lambda_h(r)\, dr = \begin{cases} 2 & \text{if } i = 2, \\ 0 & \text{if } i = 0, \dots, m-1, \\ O\left(h^{m-2}\right) & \text{if } i = m. \end{cases} \tag{33}$$

Such a Laplacian kernel yields

$$f \in C^n(I) \Rightarrow \left\| f'' - f * \lambda_h \right\|_\infty = O\left(h^{n-2}\right) \tag{34}$$

for $n = 3, \dots, m$. As we shall see, the error in approximating $f * \lambda_h$ by $f_{n'} * \lambda_h$ for a piecewise Lagrange interpolation polynomial $f_{n'}$ of degree $n' - 1$, followed by the error in approximating $f_{n'} * \lambda_h$ by Boole's rule, renders the construction of a Laplacian kernel for which (34) holds for some even integer $m > 6$ of doubtful value.

3. Interpolation

Given a point $x \in \,]a, b[$, we define

$$\Delta_h f(x) = \sup_{-h \leq w \leq h} |f(x) - f(x - w)| \tag{35}$$

for any $f \in C(I)$ and all $h > 0$ small enough so that $[x - h, x + h] \subset I$. With respect to a given set of distinct points

$$\{x_i\}_{i=1}^N \subset \,]a, b[\,, \qquad x_i < x_{i+1} \quad \text{for } i = 1, \dots, N - 1, \tag{36}$$

let $f \in C(I)$ assume the known value $f(x_i)$ at x_i for all $i = 1, \dots, N$. For $N \geq n' \in \{3, 4, 5\}$ and a point $r \in \,]a, b[\, \subset I = [a, b]$, let $[r]_{n'}$ designate the set of n' consecutive points in $\{x_i\}_{i=1}^N$ closest to r. Using Lagrange's polynomial interpolation formula of degree $n' - 1$ (see [1, 7]) we define $f_{n'}$ to be the piecewise polynomial of degree $n' - 1$ given by

$$f_{n'}(r) = \sum_{i=1}^{N} l_{i,n'}(r)\, f(x_i) \tag{37}$$

where

$$l_{i,n'}(r) = \begin{cases} \displaystyle\prod_{x_j \in [r]_{n'} \setminus \{x_i\}} \left(\frac{r - x_j}{x_i - x_j}\right) & \text{if } x_i \in [r]_{n'}\,, \\ 0 & \text{otherwise.} \end{cases}$$

For all $r \in I$ we have

(38) $$f \in C^{n'}(I) \Rightarrow f(r) - f_{n'}(r) = \prod_{z \in [r]_{n'}} (r - z) f^{(n')}(\overline{r}) / n'!$$

where $\overline{r}$ is some point in the smallest subinterval of I containing the set $[r]_{n'}$ along with the point r (see [1, 7]). It now follows by virtue of (38) that

(39) $$f \in C^{n'}(I) \Rightarrow \|f - f_{n'}\|_\infty \leq d^{n'} \left\| f^{(n')} \right\|_\infty$$

where

(40) $$d = \sup \{|x_{i+1} - x_i| : i = 0, \ldots, N;\ x_0 = a, x_{N+1} = b\}.$$

Clearly d is inversely related to the density of the disordered points.

4. Approximating a second derivative

For arbitrary $x \in]a, b[\subset I = [a, b]$ and all r small enough, Taylor's series expansion yields

(41) $$f \in C^n(I) \Rightarrow f(x - r) = \sum_{j=0}^{n-1} \frac{(-r)^j}{j!} f^{(j)}(x) + \frac{(-r)^n}{n!} f^{(n)}(\overline{x}_r)$$

for some $\overline{x}_r$ between x and $x - r$. In what follows we shall use this formula for various values of $n \in \mathbb{N}$.

4.1. Approximating f'' by $f * \lambda_h$

For arbitrary Laplacian kernel λ_h, (12) and (41) (for $n = 2$) yield for any $x \in]a, b[$

$$f''(x) - (f * \lambda_h)(x) = \frac{1}{2} \int_{-h}^{h} \left[f''(\overline{x}_r) - f''(x) \right] r^2 \lambda_h(r)\, dr$$

for all $h > 0$ small enough so that $[x - h, x + h] \subset I$. Thus we have, for any given $x \in]a, b[$,

$$\left| f''(x) - (f * \lambda_h)(x) \right| \leq \|\lambda_h\|_\infty \sup_{-h \leq w \leq h} \left| f''(x - w) - f''(x) \right| \int_0^h r^2 dr$$

for all $h > 0$ small enough, and so

(42) $$f \in C^2(I) \Rightarrow \left| f''(x) - (f * \lambda_h)(x) \right| \leq \frac{h^3}{3} \|\lambda_h\|_\infty \Delta_h f''(x)$$

where $\Delta_h f''(x)$ is given by (35) with f'' in place of f. By (11) and (42) we get

(43) $$f \in C^2(I) \Rightarrow f''(x) = \lim_{h \downarrow 0} (f * \lambda_h)(x)$$

and so the right-hand side of (43) is in fact $(f * \delta'')(x)$ where δ'' is the well-known generalized function [12, 30] for which

$$f \in C^2(I) \Rightarrow f''(x) = \left(f * \delta'' \right)(x)$$

for all $x \in]a, b[$.

By (41) we get, for any Laplacian kernel satisfying (33) for some even integer $m \geq n \geq 3$,

$$\left|f''(x) - (f * \lambda_h)(x)\right| = \frac{1}{n!}\left|\int_{-h}^{h} f^{(n)}(\overline{x}_r)\, r^n \lambda_h(r)\, dr\right|$$

and so we obtain the following result.

Theorem 4.1. *Given an integer $n \geq 3$ and a Laplacian kernel λ_h satisfying* (33) *for some even integer $m \geq n$, we have*

$$f \in C^n(I) \Rightarrow \left\|f'' - f * \lambda_h\right\|_\infty \leq \frac{1}{n!}\left\|r^n \lambda_h(r)\right\|_1 \left\|f^{(n)}\right\|_\infty \tag{44}$$

for all $h > 0$ small enough so that $[x-h, x+h] \subset I$.

Since

$$\left\|r^n \lambda_h(r)\right\|_1 \leq 2\left\|\lambda_h\right\|_\infty \int_0^h r^n dr = \frac{2}{n+1} h^{n+1}\left\|\lambda_h\right\|_\infty,$$

we deduce from (44) that

$$f \in C^n(I) \Rightarrow \left\|f'' - f * \lambda_h\right\|_\infty \leq \frac{2}{(n+1)!} h^{n+1}\left\|\lambda_h\right\|_\infty \left\|f^{(n)}\right\|_\infty \tag{45}$$

whenever λ_h satisfies (33) for some even integer $m \geq n$. Since all Laplacian kernels satisfy (12), which is (33) for $m = 4$, we get for $n = 3, 4$ in (45),

$$f \in C^n(I) \Rightarrow \left\|f'' - f * \lambda_h\right\|_\infty \leq \begin{cases} 2h^4\left\|\lambda_h\right\|_\infty \left\|f'''\right\|_\infty / 4! & \text{if } n = 3, \\ 2h^5\left\|\lambda_h\right\|_\infty \left\|f^{(iv)}\right\|_\infty / 5! & \text{if } n = 4, \end{cases} \tag{46}$$

for all $h > 0$ small enough so that $[x-h, x+h] \subset I$. By virtue of (11), (46) yields (27) under the stated conditions on h.

Example 4.2. By virtue of (14), (46) yields

$$f \in C^n(I) \Rightarrow \left\|f'' - f * k''_{h,6}\right\|_\infty \leq \begin{cases} 105h\left\|f'''\right\|_\infty / 192 & \text{if } n = 3, \\ 7h^2\left\|f^{(iv)}\right\|_\infty / 64 & \text{if } n = 4, \end{cases} \tag{47}$$

for all $h > 0$ small enough so that $[x-h, x+h] \subset I$.

Example 4.3. By (26), inequality (46) yields

$$f \in C^3(I) \Rightarrow \left\|f'' - f * \lambda_h\right\|_\infty \leq \begin{cases} h\left\|f'''\right\|_\infty / 3 & \text{if } \lambda_h = \delta_h^2, \\ 35h\left\|f'''\right\|_\infty / 48 & \text{if } \lambda_h = k_{h,6}^2, \\ h\left\|f'''\right\|_\infty / 2 & \text{if } \lambda_h = k_{h,D}^2, \end{cases}$$

for all $h > 0$ small enough so that $[x-h, x+h] \subset I$. Similarly, (46) gives

$$f \in C^4(I) \Rightarrow \left\|f'' - f * \lambda_h\right\|_\infty \leq \begin{cases} h^2\left\|f^{(iv)}\right\|_\infty / 15 & \text{if } \lambda_h = \delta_h^2, \\ 7h^2\left\|f^{(iv)}\right\|_\infty / 48 & \text{if } \lambda_h = k_{h,6}^2, \\ h^2\left\|f^{(iv)}\right\|_\infty / 10 & \text{if } \lambda_h = k_{h,D}^2, \end{cases} \tag{48}$$

for all $h > 0$ small enough.

Example 4.4. Inequality (45) yields, by virtue of (29),

$$f \in C^n(I) \Rightarrow \left\| f'' - f * S_h \right\|_\infty \leq \begin{cases} 63h \left\| f''' \right\|_\infty /32 & \text{if } n = 3, \\ 63h^2 \left\| f^{(iv)} \right\|_\infty /160 & \text{if } n = 4, \\ 21h^3 \left\| f^{(v)} \right\|_\infty /320 & \text{if } n = 5, \\ 3h^4 \left\| f^{(vi)} \right\|_\infty /320 & \text{if } n = 6, \end{cases} \tag{49}$$

for all $h > 0$ small enough so that $[x-h, x+h] \subset I$. This proves (31).

4.2. Approximating $f * \lambda_h$ by interpolating f

We now establish an error bound when approximating $f * \lambda_h$ by $f_{n'} * \lambda_h$ where $N \geq n' \in \{3, 4, 5\}$. In particular, the piecewise polynomial interpolation f_5 (of degree 4) associated with f is given by (37). Whenever $[x-h, x+h] \subset I$, we have

$$\begin{aligned} \left| (f * \lambda_h)(x) - (f_{n'} * \lambda_h)(x) \right| &\leq \int_{x-h}^{x+h} \left| f(r) - f_{n'}(r) \right| \left| \lambda_h(x-r) \right| dr \\ &\leq \left\| f - f_{n'} \right\|_\infty \left\| \lambda_h \right\|_1 \end{aligned}$$

and so we get the following result by virtue of (39).

Theorem 4.5. *Given a point* $x \in \,]a, b[\, \subset I = [a, b]$*,* $h > 0$ *small enough so that* $[x-h, x+h] \subset I$ *and a Laplacian kernel* λ_h*, then for all* $f \in C^{n'}(I)$ *(where* $N \geq n' \in \{3, 4, 5\}$*) we have*

$$\left\| f * \lambda_h - f_{n'} * \lambda_h \right\|_\infty \leq d^{n'} \left\| f^{(n')} \right\|_\infty \left\| \lambda_h \right\|_1 \tag{50}$$

where d *is given by* (40).

Example 4.6. If $\lambda_h = k''_{h,6}$, then (50) gives

$$f \in C^{n'}(I) \Rightarrow \left\| f * k''_{h,6} - f_{n'} * k''_{h,6} \right\|_\infty \leq \frac{84}{25h^2} \sqrt{5} d^{n'} \left\| f^{(n')} \right\|_\infty \tag{51}$$

by virtue of (15).

Example 4.7. If $\lambda_h = k_h^2$ for arbitrary kernel k_h, then (50) gives

$$f \in C^{n'}(I) \Rightarrow \left| \left(f * k_h^2 \right)(x) - \left(f_{n'} * k_h^2 \right)(x) \right| \leq \frac{8d^{n'}}{h^2} \left\| f^{(n')} \right\|_\infty \tag{52}$$

by virtue of (22).

Example 4.8. For $\lambda_h = S_h$, we have (30) and so

$$f \in C^{n'}(I) \Rightarrow \left| (f * S_h)(x) - (f_n * S_h)(x) \right| \leq \frac{63d^{n'}}{2h^2} \left\| f^{(n')} \right\|_\infty \tag{53}$$

by virtue of (50).

4.3. Approximating $f_5 * \lambda_h$ (and so f'') by Boole's rule

We have, for any real function g on an interval $[\alpha, \beta]$, the Boole sum

$$\begin{aligned} BOOLE_\alpha^\beta(g) = \frac{(\beta - \alpha)}{90} &\left[7g(\alpha) + 32g\left(\frac{\beta + 3\alpha}{4} \right) \right. \\ &\left. + 12g\left(\frac{\alpha + \beta}{2} \right) + 32g\left(\frac{3\beta + \alpha}{4} \right) + 7g(\beta) \right]. \end{aligned} \tag{54}$$

By Boole's rule [1, 7], for any interval $[\alpha, \beta]$ and any $g \in C^6([\alpha, \beta])$, there exists $\xi \in [\alpha, \beta]$ such that

$$\int_\alpha^\beta g(r)\,dr - BOOLE_\alpha^\beta(g) = -\frac{(\beta-\alpha)^7}{1935360} g^{(vi)}(\xi). \tag{55}$$

Consider now an arbitrary interval $[u, v] \subset I$ and let $x_{m'}$ and $x_{m''}$ denote the points in $\{x_i\}_{i=1}^N \cap [u, v]$ closest to u and to v, respectively. When $x_{m'}$ and $x_{m''}$ both exist and $x_{m'} \neq x_{m''}$, we define

$$B_u^v(g) = BOOLE_u^{x_{m'}}(g) + \sum_{i=m'}^{m''-1} BOOLE_{x_i}^{x_{i+1}}(g) + BOOLE_{x_{m''}}^v(g),$$

while if $x_{m'}$ exists and $x_{m'} = x_{m''}$, then we put

$$B_u^v(g) = BOOLE_u^{x_{m'}}(g) + BOOLE_{x_{m'}}^v(g),$$

and if no such $x_{m'}$ exists then we simply use (54) for $\alpha = u$ and $\beta = v$. We have

$$\int_u^v = \begin{cases} \int_u^{x_{m'}} + \sum_{i=m'}^{m''-1} \int_{x_i}^{x_{i+1}} + \int_{x_{m''}}^v & \text{if } x_{m'} \neq x_{m''}, \\ \int_u^{x_{m'}} + \int_{x_{m''}}^v & \text{if } x_{m'} = x_{m''}, \\ \int_u^v & \text{if } x_{m'} \text{ does not exist,} \end{cases} \tag{56}$$

and for any $j = 1, 2, 3, \ldots$, we introduce

(57)

$$\Psi_u^v(j) = \begin{cases} (x_{m'} - u)^j + \sum_{i=m'}^{m''-1} (x_{i+1} - x_i)^j + (v - x_{m''})^j & \text{if } x_{m'} \neq x_{m''}, \\ (x_{m'} - u)^j + (v - x_{m'})^j & \text{if } x_{m'} = x_{m''}, \\ (v-u)^j & \text{otherwise.} \end{cases}$$

By (55)–(57) we now have

$$\left| \int_u^v g(r)\,dr - B_u^v(g) \right| \le \frac{\Psi_u^v(7)}{1935360} \left\| g^{(vi)} \right\|_\infty.$$

(Taking $\|\cdot\|_\infty$ to mean the essential supremum rather than the uniform norm eliminates any problem at the few points where g may not be sufficiently differentiable.) Thus by choosing $u = x - h$ and $v = x + h$, we get

$$g \in C^6(I) \Rightarrow \left| \int_{x-h}^{x+h} g(r)\,dr - B_{x-h}^{x+h}(g) \right| \le \frac{\Psi_{x-h}^{x+h}(7)}{1935360} \left\| g^{(vi)} \right\|_\infty. \tag{58}$$

Suppose that g_x is the piecewise smooth function of $r \in I$ given by

$$g_x(r) = f_5(r)\,\lambda_h(x - r) \tag{59}$$

for f_5 the piecewise Lagrange interpolation polynomial defined by (37) and λ_h a Laplacian kernel. Since f_5 is piecewise a polynomial of degree four, Leibniz's rule applied to (59) yields

$$\left\| g_x^{(vi)} \right\|_\infty \le \sum_{j=0}^{4} \binom{6}{j} \left\| f_5^{(j)} \right\|_\infty \left\| \lambda_h^{(6-j)} \right\|_\infty$$

and so (58) becomes

$$\left|\int_{x-h}^{x+h} g_x(r)\,dr - B_{x-h}^{x+h}(g_x)\right| \le \frac{\Psi_{x-h}^{x+h}(7)}{1935360}\sum_{j=0}^{4}\binom{6}{j}\left\|f_5^{(j)}\right\|_\infty \left\|\lambda_h^{(6-j)}\right\|_\infty . \tag{60}$$

For any real numbers $u < v$, we have

$$\Psi_u^v(j) \le (v-u)^j$$

and so

$$\Psi_{x-h}^{x+h}(7) \le 2^7 h^7,$$

which, when applied to (60), yields the following result.

Theorem 4.9. *Given* $x \in \,]a,b[\, \subset I = [a,b]$ *and* $h > 0$ *such that*

$$[x-h, x+h] \subset I,$$

then we have

$$\begin{aligned}\left|\int_{x-h}^{x+h} g_x(r)\,dr - B_{x-h}^{x+h}(g_x)\right| &\le \frac{\Psi_{x-h}^{x+h}(7)}{1935360}\sum_{j=0}^{2}\binom{6}{j}\left\|f_5^{(j)}\right\|_\infty \left\|\lambda_h^{(6-j)}\right\|_\infty \\ &\quad + \frac{h^7}{15120}\sum_{j=3}^{4}\binom{6}{j}\left\|f_5^{(j)}\right\|_\infty \left\|\lambda_h^{(6-j)}\right\|_\infty\end{aligned} \tag{61}$$

where g_x *is given by* (59) *for* f_5 *the piecewise Lagrange interpolation polynomial of degree* 4 *defined by* (37) *and* λ_h *is a Laplacian kernel.*

The triangle inequality

$$\begin{aligned}\left|f''(x) - B_{x-h}^{x+h}(g_x)\right| \le\; &\left|f''(x) - (f*\lambda_h)(x)\right| \\ &+ \left|(f*\lambda_h)(x) - (f_5*\lambda_h)(x)\right| \\ &+ \left|(f_5*\lambda_h)(x) - B_{x-h}^{x+h}(g_x)\right|\end{aligned} \tag{62}$$

is used in the examples that follow to obtain error bounds when approximating $f''(x)$ by $B_{x-h}^{x+h}(g_x)$ for $x \in \,]a,b[\, \subset I = [a,b]$, $h > 0$ such that $[x-h, x+h] \subset I$, $f \in C^n(I)$ $(n \in \{5,6\})$ with known values on the set of disordered points (36), λ_h a Laplacian kernel satisfying (33) for some even integer $m \ge n$ and g_x given by (59) where f_5 is the piecewise Lagrange interpolation polynomial of degree 4 obtained from f by (37) .

Example 4.10. The Laplacian kernel $\lambda_h = k''_{h,6}$ yields, by way of (13),

$$\lambda_h^{(6-j)}(r) = \begin{cases} -1575/2h^7 & \text{if } j=2,\ |r|<h, \\ -1575r/2h^7 & \text{if } j=3,\ |r|<h, \\ 315\left(h^2-5r^2\right)/4h^7 & \text{if } j=4,\ |r|<h. \end{cases}$$

Thus

$$\left\|\lambda_h^{(6-j)}\right\|_\infty = \begin{cases} 1575/2h^7 & \text{if } j=2, \\ 1575/2h^6 & \text{if } j=3, \\ 315/h^5 & \text{if } j=4, \end{cases}$$

and so for all $f \in C^5(I)$, $x \in]a,b[\subset I = [a,b]$, and $h > 0$ with the property that $[x-h, x+h] \subset I$, we have

$$\left|f''(x) - B_{x-h}^{x+h}(g_x)\right| \leq \frac{7h^2}{64}\left\|f^{(iv)}\right\|_\infty + \frac{84}{25h^2}\sqrt{5}d^5\left\|f^{(v)}\right\|_\infty + \frac{25\Psi_u^v(7)}{4096h^7}\left\|f_5''\right\|_\infty + \frac{25h}{24}\left\|f_5'''\right\|_\infty + \frac{5h^2}{16}\left\|f_5^{iv}\right\|_\infty, \tag{63}$$

by virtue of (47) for $n = 4$, (51) for $n' = 5$ and (61) all applied to (62).

Example 4.11. The Laplacian kernel $\lambda_h = \delta_h^2$ yields $\lambda_h^{(6-j)} = 0$ almost everywhere for $j = 0, \ldots, 5$ and so for all $x \in]a,b[\subset I = [a,b]$ and $h > 0$ such that $[x-h, x+h] \subset I$, we have

$$f \in C^5(I) \Rightarrow \left|f''(x) - B_{x-h}^{x+h}(g_x)\right| \leq \frac{h^2}{15}\left\|f^{(iv)}\right\|_\infty + \frac{8d^5}{h^2}\left\|f^{(v)}\right\|_\infty \tag{64}$$

by virtue of (48), (52) for $n' = 5$ and (61) all applied to (62).

Example 4.12. The Laplacian kernel $\lambda_h = k_{h,D}^2$ given by (25) is piecewise a polynomial of degree two for which

$$\left\|\left(k_{h,D}^2\right)''\right\|_\infty = 192/h^5$$

and so, for all $x \in]a,b[\subset I = [a,b]$ and $h > 0$ such that $[x-h, x+h] \subset I$, we get

$$f \in C^5(I) \Rightarrow \left|f'(x) - B_{x-h}^{x+h}(g_x)\right| \leq \frac{h^2}{10}\left\|f^{(iv)}\right\|_\infty + \frac{8d^5}{h^2}\left\|f^{(v)}\right\|_\infty + \frac{4h^2}{21}\left\|f_5^{(iv)}\right\|_\infty \tag{65}$$

by virtue of (48), (52) for $n' = 5$, and (61) all applied to (62).

Example 4.13. For $\lambda_h = S_h$ we have $\lambda_h^{(6-j)} = 0$ almost everywhere for $j = 0, \ldots, 5$, and so for all $x \in]a,b[\subset I = [a,b]$ and $h > 0$ with the property that $[x-h, x+h] \subset I$, we have

$$f \in C^6(I) \Rightarrow \left|f''(x) - B_{x-h}^{x+h}(g_x)\right| \leq \frac{3}{320}h^4\left\|f^{(vi)}\right\|_\infty + \frac{63d^5}{2h^2}\left\|f^{(v)}\right\|_\infty \tag{66}$$

by virtue of (49) for $n = 6$, (53) for $n' = 5$ and (61) all applied to (62).

5. Numerical results based on $k_{h,D}^2$ and S_h

For the three functions $f(x) = 1 + x^2 + x^3 + x^4 + x^5$, $f(x) = \exp x$ and $f(x) = 1/(x+5)$ we calculated the error in approximating f'' by $B_{x-h}^{x+h}(g_x)$ for $\lambda_h = k_{h,D}^2$ and g_x given by (59). More precisely, for $N = 250$ and $N = 500$ we chose an increasing sequence of points $\{x_i\}_{i=1}^N$ at random in $[-2,2]$. Then, for each N, we calculated for different values of h (*i.e.*, $h_j = 2^{-j}$, $j = 1, \ldots, 11$) and each $x_i \in [-1,1]$, the errors

$$e_{h_j,D}^2(f, x_i) = \left|f''(x_i) - B_{x_i-h_j}^{x_i+h_j}(g_x)\right|.$$

	$N=500$		$N=250$	
h_j	$E^2_{h_j,D}(f)$	$v_j=\log_2\frac{E^2_{h_j,D}}{E^2_{h_{j+1},D}}$	$E^2_{h_j,D}(f)$	$v_j=\log_2\frac{E^2_{h_j,D}}{E^2_{h_{j+1},D}}$
$h_1=2^{-1}$	9.16E-01	2.00E+00	9.17E-01	2.00E+00
$h_2=2^{-2}$	2.29E-01	2.00E+00	2.29E-01	2.00E+00
$h_3=2^{-3}$	5.73E-02	2.00E+00	5.73E-02	2.00E+00
$h_4=2^{-4}$	1.43E-02	2.00E+00	1.43E-02	2.00E+00
$h_5=2^{-5}$	3.58E-03	2.00E+00	3.58E-03	2.01E+00
$h_6=2^{-6}$	8.95E-04	2.00E+00	8.88E-04	1.90E+00
$h_7=2^{-7}$	2.24E-04	1.97E+00	2.38E-04	1.41E+00
$h_8=2^{-8}$	5.72E-05	1.76E+00	8.95E-05	6.26E-01
$h_9=2^{-9}$	1.69E-05	9.85E-01	5.80E-05	1.16E-01
$h_{10}=2^{-10}$	8.54E-06	1.88E-01	5.35E-05	-5.24E-03
$h_{11}=2^{-11}$	7.50E-06		5.37E-05	

TABLE 1. $E^2_{h,D}$ and v for $f(x)=1+x^2+x^3+x^4+x^5$

	$N=500$		$N=250$	
h_j	$E^2_{h_j,D}(f)$	$v_j=\log_2\frac{E^2_{h_j,D}}{E^2_{h_{j+1},D}}$	$E^2_{h_j,D}(f)$	$v_j=\log_2\frac{E^2_{h_j,D}}{E^2_{h_{j+1},D}}$
$h_1=2^{-1}$	1.71E-02	2.01E+00	1.69E-02	2.01E+00
$h_2=2^{-2}$	4.25E-03	2.00E+00	4.20E-03	2.00E+00
$h_3=2^{-3}$	1.06E-03	2.00E+00	1.05E-03	2.00E+00
$h_4=2^{-4}$	2.66E-04	2.00E+00	2.62E-04	2.00E+00
$h_5=2^{-5}$	6.64E-05	2.00E+00	6.55E-05	2.01E+00
$h_6=2^{-6}$	1.66E-05	2.00E+00	1.62E-05	1.99E+00
$h_7=2^{-7}$	4.14E-06	2.00E+00	4.08E-06	1.67E+00
$h_8=2^{-8}$	1.04E-06	1.92E+00	1.28E-06	9.23E-01
$h_9=2^{-9}$	2.74E-07	5.24E-01	6.77E-07	1.38E-01
$h_{10}=2^{-10}$	1.90E-07	-1.78E+00	6.15E-07	-5.45E-01
$h_{11}=2^{-11}$	6.54E-07		8.97E-07	

TABLE 2. $E^2_{h,D}$ and v for $f(x)=\exp x$

We then took the average $E^2_{h_j,D}(f)$ of all $e^2_{h_j,D}(f,x_i)$ for those $x_i\in[-1,1]$. To show numerically that $E^2_{h_j,D}(f)=O\left(h_j^v\right)$ for $v\geq 2$ (when the first term to the right of (65) dominates the other two), we also calculated the values

$$v_j=\log_2\left(\frac{E^2_{h_j,D}(f)}{E^2_{h_{j+1},D}(f)}\right)$$

for $j=1,\ldots,10$. The results are presented in Tables 1–3. We note that v becomes less than 2 once $E^2_{h_j,D}$ is of the same magnitude as the second right-hand term in (65).

	$N = 500$		$N = 250$	
h_j	$E^2_{h_j,D}(f)$	$v_j = \log_2 \frac{E^2_{h_j,D}}{E^2_{h_{j+1},D}}$	$E^2_{h_j,D}(f)$	$v_j = \log_2 \frac{E^2_{h_j,D}}{E^2_{h_{j+1},D}}$
$h_1 = 2^{-1}$	1.40E-04	2.01E+00	1.42E-04	2.01E+00
$h_2 = 2^{-2}$	3.47E-05	2.00E+00	3.52E-05	2.00E+00
$h_3 = 2^{-3}$	8.67E-06	2.00E+00	8.78E-06	2.00E+00
$h_4 = 2^{-4}$	2.17E-06	2.00E+00	2.19E-06	2.00E+00
$h_5 = 2^{-5}$	5.42E-07	2.00E+00	5.49E-07	2.00E+00
$h_6 = 2^{-6}$	1.35E-07	2.00E+00	1.37E-07	1.99E+00
$h_7 = 2^{-7}$	3.38E-08	1.99E+00	3.45E-08	1.82E+00
$h_8 = 2^{-8}$	8.51E-09	8.36E-01	9.80E-09	5.85E-01
$h_9 = 2^{-9}$	4.77E-09	-1.62E+00	6.53E-09	-1.56E+00
$h_{10} = 2^{-10}$	1.46E-08	-2.09E+00	1.92E-08	-2.19E+00
$h_{11} = 2^{-11}$	6.21E-08		8.79E-08	

TABLE 3. $E^2_{h,D}$ and v for $f(x) = 1/(x+5)$

	$N = 500$		$N = 250$	
h_j	$E_{h_j,S}(f)$	$v_j = \log_2 \frac{E_{h_j,S}}{E_{h_{j+1},S}}$	$E_{h_j,S}(f)$	$v_j = \log_2 \frac{E_{h_j,S}}{E_{h_{j+1},S}}$
$h_1 = 2^{-1}$	1.15E-07	-1.97E+00	3.43E-06	-2.00E+00
$h_2 = 2^{-2}$	4.50E-07	-1.46E+00	1.37E-05	-1.27E+00
$h_3 = 2^{-3}$	1.24E-06	-9.82E-01	3.31E-05	-7.79E-01
$h_4 = 2^{-4}$	2.45E-06	-1.01E+00	5.68E-05	7.67E-02
$h_5 = 2^{-5}$	4.93E-06	-3.02E-01	5.38E-05	-6.52E-03
$h_6 = 2^{-6}$	6.08E-06	4.43E-03	5.41E-05	3.91E-02
$h_7 = 2^{-7}$	6.06E-06	-5.21E-02	5.26E-05	8.99E-03
$h_8 = 2^{-8}$	6.28E-06	-1.33E-01	5.23E-05	-2.88E-02
$h_9 = 2^{-9}$	6.89E-06	-6.97E-01	5.34E-05	-4.27E-02
$h_{10} = 2^{-10}$	1.12E-05	-2.30E+00	5.50E-05	-6.59E-01
$h_{11} = 2^{-11}$	5.52E-05		8.67E-05	

TABLE 4. $E_{h,S}$ and v for $f(x) = 1 + x^2 + x^3 + x^4 + x^5$

We also measured numerically the average error $E_{h_j,S}(f)$ in approximating f'' by $B^{x+h}_{x-h}(g_x)$ for $\lambda_h = S_h$. When compared with Tables 1–3, the results in Tables 4–6 clearly show the superiority of S_h over $k^2_{h,D}$ when approximating a second derivative by our method. This time v becomes less than 4 once $E_{h_j,S}$ is of the same magnitude as the second right hand term in error bound (66). Table 4 shows that this is true from the start for $f(x) = 1 + x^2 + x^3 + x^4 + x^5$.

	$N = 500$		$N = 250$	
h_j	$E_{h_j,S}(f)$	$v_j = \log_2 \frac{E_{h_j,S}}{E_{h_{j+1},S}}$	$E_{h_j,S}(f)$	$v_j = \log_2 \frac{E_{h_j,S}}{E_{h_{j+1},S}}$
$h_1 = 2^{-1}$	5.27E-05	4.01E+00	5.20E-05	3.96E+00
$h_2 = 2^{-2}$	3.28E-06	4.02E+00	3.34E-06	2.79E+00
$h_3 = 2^{-3}$	2.02E-07	2.64E+00	4.84E-07	-4.64E-01
$h_4 = 2^{-4}$	3.25E-08	-7.40E-01	6.67E-07	1.71E-01
$h_5 = 2^{-5}$	5.43E-08	-2.34E-01	5.93E-07	3.31E-02
$h_6 = 2^{-6}$	6.39E-08	-6.11E-02	5.79E-07	7.46E-02
$h_7 = 2^{-7}$	6.66E-08	-7.65E-01	5.50E-07	-5.80E-02
$h_8 = 2^{-8}$	1.13E-07	-2.42E+00	5.73E-07	-7.20E-01
$h_9 = 2^{-9}$	6.05E-07	-2.96E+00	9.43E-07	-2.36E+00
$h_{10} = 2^{-10}$	4.71E-06	-3.00E+00	4.85E-06	-2.93E+00
$h_{11} = 2^{-11}$	3.77E-05		3.69E-05	

TABLE 5. $E_{h,S}$ and v for $f(x) = \exp x$

	$N = 500$		$N = 250$	
h_j	$E_{h_j,S}(f)$	$v_j = \log_2 \frac{E_{h_j,S}}{E_{h_{j+1},S}}$	$E_{h_j,S}(f)$	$v_j = \log_2 \frac{E_{h_j,S}}{E_{h_{j+1},S}}$
$h_1 = 2^{-1}$	6.19E-07	4.02E+00	6.30E-07	4.02E+00
$h_2 = 2^{-2}$	3.83E-08	4.00E+00	3.87E-08	3.53E+00
$h_3 = 2^{-3}$	2.39E-09	3.12E+00	3.35E-09	-1.26E-01
$h_4 = 2^{-4}$	2.75E-10	-4.38E-01	3.65E-09	-1.81E-02
$h_5 = 2^{-5}$	3.73E-10	-7.04E-01	3.70E-09	-1.00E-01
$h_6 = 2^{-6}$	6.07E-10	-1.55E+00	3.97E-09	-2.73E-01
$h_7 = 2^{-7}$	1.78E-09	-2.78E+00	4.79E-09	-1.48E+00
$h_8 = 2^{-8}$	1.22E-08	-3.01E+00	1.33E-08	-2.90E+00
$h_9 = 2^{-9}$	9.81E-08	-3.00E+00	9.95E-08	-2.99E+00
$h_{10} = 2^{-10}$	7.85E-07	-3.00E+00	7.91E-07	-3.00E+00
$h_{11} = 2^{-11}$	6.28E-06		6.34E-06	

TABLE 6. $E_{h,S}$ and v for $f(x) = 1/(x+5)$

6. Comparison with classic SPH based on $k''_{h,6}$

In classic SPH, one restricts λ_h to the case $\lambda_h = k''_h$ for some twice differentiable kernel k_h. For this to work, k_h must satisfy (8) for all twice continuously differentiable f. An example of such a kernel is $k_{h,6}$ given by (6). By contrast, δ_h, $k_{h,D}$ and S_h given by (5), (7) and (28) respectively do not satisfy (8) and so are of no use in classic SPH. We repeated the above numerical procedure for $\lambda_h = k''_{h,6}$ and obtained the results given in Tables 7–9.

Compared with Tables 1–6, the superiority of $k^2_{h,D}$ and $k_{h,S}$ over $k''_{h,6}$ when estimating a second derivative by our method is evident when intervals of length $2h$ contain

	$N = 500$		$N = 250$	
h_j	$E''_{h_j,6}(f)$	$v_j = \log_2 \frac{E''_{h_j,6}}{E''_{h_{j+1},6}}$	$E''_{h_j,6}(f)$	$v_j = \log_2 \frac{E''_{h_j,6}}{E''_{h_{j+1},6}}$
$h_1 = 2^{-1}$	8.73E-01	2.00E+00	8.74E-01	2.00E+00
$h_2 = 2^{-2}$	2.18E-01	2.00E+00	2.18E-01	2.01E+00
$h_3 = 2^{-3}$	5.45E-02	2.02E+00	5.44E-02	2.04E+00
$h_4 = 2^{-4}$	1.35E-02	2.16E+00	1.32E-02	3.35E+00
$h_5 = 2^{-5}$	3.00E-03	2.42E+00	2.59E-03	2.24E+00
$h_6 = 2^{-6}$	5.61E-04	-6.78E-01	5.50E-04	-9.40E-01
$h_7 = 2^{-7}$	8.97E-04	-4.56E-01	1.05E-03	-3.22E-01
$h_8 = 2^{-8}$	1.23E-03	-1.73E-01	1.32E-03	-9.68E-02
$h_9 = 2^{-9}$	1.39E-03	-9.77E-02	1.41E-03	-8.25E-02
$h_{10} = 2^{-10}$	1.48E-03	-4.44E-02	1.49E-03	-2.76E-02
$h_{11} = 2^{-11}$	1.53E-03		1.52E-03	

TABLE 7. $E''_{h,6}$ and v for $f(x) = 1 + x^2 + x^3 + x^4 + x^5$

	$N = 500$		$N = 250$	
h_j	$E''_{h_j,6}(f)$	$v_j = \log_2 \frac{E''_{h_j,6}}{E''_{h_{j+1},6}}$	$E''_{h_j,6}(f)$	$v_j = \log_2 \frac{E''_{h_j,6}}{E''_{h_{j+1},6}}$
$h_1 = 2^{-1}$	1.63E-02	2.01E+00	1.61E-02	2.01E+00
$h_2 = 2^{-2}$	4.05E-03	2.00E+00	4.00E-03	2.04E+00
$h_3 = 2^{-3}$	1.01E-03	2.11E+00	9.73E-04	2.35E+00
$h_4 = 2^{-4}$	2.35E-04	2.65E+00	1.91E-04	1.86E+00
$h_5 = 2^{-5}$	3.73E-05	-1.28E+00	5.25E-05	-1.31E+00
$h_6 = 2^{-6}$	9.05E-05	-7.40E-01	1.30E-04	-4.29E-01
$h_7 = 2^{-7}$	1.51E-04	-2.56E-01	1.75E-04	-1.50E-01
$h_8 = 2^{-8}$	1.80E-04	-1.48E-01	1.95E-04	-7.53E-02
$h_9 = 2^{-9}$	2.00E-04	-7.54E-02	2.05E-04	-5.96E-02
$h_{10} = 2^{-10}$	2.11E-04	-3.61E-02	2.14E-04	-1.56E-02
$h_{11} = 2^{-11}$	2.16E-04		2.16E-04	

TABLE 8. $E''_{h,6}$ and v for $f(x) = \exp x$

sufficiently many of the disordered points. As was the case for $k^2_{h,D}$, v becomes less than 2 once the average error $E_{h_j,6}$ is of the same magnitude as the second or third right-hand term in error bound (63).

	$N = 500$		$N = 250$	
h_j	$E''_{h_j,6}(f)$	$v_j = \log_2 \frac{E''_{h_j,6}}{E''_{h_{j+1},6}}$	$E''_{h_j,6}(f)$	$v_j = \log_2 \frac{E''_{h_j,6}}{E''_{h_{j+1},6}}$
$h_1 = 2^{-1}$	1.33E-04	2.01E+00	1.35E-04	2.01E+00
$h_2 = 2^{-2}$	3.31E-05	2.01E+00	3.35E-05	2.05E+00
$h_3 = 2^{-3}$	8.23E-06	2.14E+00	8.06E-06	2.68E+00
$h_4 = 2^{-4}$	1.86E-06	1.87E+00	1.26E-06	1.64E-01
$h_5 = 2^{-5}$	5.09E-07	-1.49E+00	1.12E-06	-9.50E-01
$h_6 = 2^{-6}$	1.43E-06	-6.95E-01	2.17E-06	-3.20E-01
$h_7 = 2^{-7}$	2.31E-06	-2.25E-01	2.71E-06	-1.52E-01
$h_8 = 2^{-8}$	2.70E-06	-1.57E-01	3.01E-06	-6.41E-02
$h_9 = 2^{-9}$	3.01E-06	-7.53E-02	3.15E-06	-3.43E-02
$h_{10} = 2^{-10}$	3.17E-06	-3.49E-02	3.23E-06	-2.16E-02
$h_{11} = 2^{-11}$	3.25E-06		3.27E-06	

TABLE 9. $E''_{h,6}$ and v for $f(x) = 1/(x+5)$

7. Interpreting the results

One finds in the literature numerous examples of (classic) Laplacian kernels, each with its own strengths and weaknesses [16]. Good results in calculating the second derivative of a piecewise smooth function by our new method can be obtained by choosing appropriate Laplacian kernels λ_h, be they continuous or not. The Laplacian kernels $\lambda_h = \delta_h$ introduced in [3] and $\lambda_h = S_h$ introduced here are discontinuous on $\mathbb{R}$. Moreover, $\lambda_h = k_h^2$ and $\lambda_h = k''_h$ for $k_h = k_{h,D}$ and $k_h = k_{h,6}$ (respectively) also provide results, some better than others as a comparison of Tables 1–3 with Tables 7–9 shows. In all cases, $\|\lambda_h\|_1$ and the essential supremum of λ_h and of its first six derivatives influence the approximation as $h \downarrow 0$ since, the smaller they are, the less is the error bound due to (50) and (61). For example, $\lambda_h = \delta_h^2$ and $\lambda_h = k_{h,D}^2$ yield (64) and (65) respectively, which are of similar magnitude, so leading us to expect similar numerical results for these two kernels. Furthermore, $\lambda_h = k_{h,D}^2$ can be expected to give better results than $\lambda_h = k''_{h,6}$ if one compares (65) with (63). Finally, (66) explains the superiority of S_h over all other kernels studied here since the error bound is $O\left(h^4\right)$ when intervals of length $2h$ contain sufficiently many of the disordered points.

8. Conclusion

We developed a new method to estimate numerically the derivative of a twice differentiable real function f on $\mathbb{R}$ from scattered data $\{x_i, f(x_i)\}_{i=1}^N \subset \mathbb{R}^2$. It is based on the convolution $f * \lambda_h$ of f with a Laplacian kernel which, by our definition, consists of a family λ_h (indexed by $h > 0$) of real piecewise smooth even functions of mean zero on $\mathbb{R}$ with support in $[-h, h]$ and satisfying (10) and (11). Such a convolution is then approximated by first substituting for f its piecewise Lagrange polynomial interpolation f_5 based on the scattered data and given by (37), followed by an approximation of

$f_5 * \lambda_h$ by Boole's rule. Error bounds such as (63)–(66) establish the theoretical validity of our method which in turn is corroborated by numerical results found in Tables 1–9. The magnitude of such error bounds is dominated by the first term to the right until h is so small that the subsequent terms start to dominate over the first. A comparison of Tables 1–9 corroborates the superiority of our method based on S_h over the classic SPH method based on the Laplacian kernel (13) and the divided difference approach (20) based on kernel (7). Finally, any classic Laplacian kernel (like (13)) must satisfy (8) to be of use in classic SPH. There is no corresponding restriction on the Laplacian kernel for our method to work.

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