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José A. Adell
Carmen Sangüesa

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A probabilistic approach to divided difference expansions [1]

José A. Adell and C. Sangüesa

Departamento de Métodos Estadísticos. Facultad de Ciencias.

Universidad de Zaragoza. 50009 Zaragoza (Spain)

Abstract

In this paper, we improve some recent results by Floater [8] on divided difference expansions. Such improvements refer to the smoothness of the function under consideration, the leading coefficient of the main term of the approximation and, in some circumstances, the rate of convergence. We use a probabilistic approach in the spirit of Ignatov and Kaishev [9] and Karlin et al. [12] based on the representation of divided differences as mathematical expectations involving linear combinations of uniform order statistics.

Key words: Divided difference, Modulus of smoothness, Order statistics, Probabilistic Taylor's formula

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Email addresses: `adell@unizar.es`, `csangues@unizar.es` (José A. Adell and C. Sangüesa).

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1 Introduction

The starting point of this work is a recent paper by Floater [8] dealing with divided difference expansions (more general expansions can be found in de Boor [5] and Wang et al. [16]). Specifically, let n be a positive integer, which we fix from now on, and let $r = 1, \ldots, n$. Denote by $\mathbf{F}_r$ the set of all finite ordered sequences of real numbers $\mathbf{x} := (x_0, \ldots, x_n)$ having $r+1$ distinct knots among $x_0, \ldots, x_n$, that is,

$$(x_0, \ldots, x_n) = (\underbrace{\tilde{x}_0, \ldots, \tilde{x}_0}_{m_0}, \ldots, \underbrace{\tilde{x}_r, \ldots, \tilde{x}_r}_{m_r}). \tag{1}$$

If $\mathbf{x} \in \mathbf{F}_r$, we write $h_i := x_i - x_{i-1}$, $i = 1, \ldots, n$, $\tilde{h}_i := \tilde{x}_i - \tilde{x}_{i-1}$, $i = 1, \ldots, r$, $h := \max(h_1, \ldots, h_n)$ and $\tilde{h} := \min(\tilde{h}_1, \ldots, \tilde{h}_r)$. We define the sets

$$\mathbf{F} := \bigcup_{r=1}^{n} \mathbf{F}_r \qquad \text{and} \qquad \mathbf{F}_r(a) := \{\mathbf{x} \in \mathbf{F}_r : \frac{\tilde{h}}{h} \geq a\}, \quad 0 < a \leq 1.$$

Finally, if $\mathbf{x} \in \mathbf{F}$ we denote by $\|\cdot\|$ the sup-norm on the interval $I := [x_0, x_n]$ and by $C^m(I)$ the set of m times differentiable functions f defined on I such that $f^{(m)}$ is continuous, $m = 1, 2, \ldots$.

For any $\mathbf{x} \in \mathbf{F}$ and $f \in C^p(I)$, $p = n+1, n+2, \ldots$, Floater [8] has shown divided difference expansions of the form

$$[x_0, \ldots, x_n]f = \sum_{k=n}^{p-1} c_k \frac{f^{(k)}(x)}{k!} + R_p, \quad x \in I, \tag{2}$$

where each coefficient c_k is expresable in different ways, particularly in terms of the symmetric polynomial σ_{k-n} of degree $k-n$, as

$$c_k = [x_0, \ldots, x_n](\cdot - x)^k = \sigma_{k-n}(x_0 - x, \ldots, x_n - x)$$

$$:= \sum_{\tau_0 + \cdots + \tau_n = k-n} (x_0 - x)^{\tau_0} \ldots (x_n - x)^{\tau_n}, \tag{3}$$

and the remainder R_p is estimated in terms of the maximum grid spacing h as

$$|R_p| \leq \frac{n^{p-n}}{n!(p-n)!} h^{p-n} \|f^{(p)}\|. \tag{4}$$

Choosing x in (2) as the arithmetic mean of the knots $\bar{x} := (n+1)^{-1}(x_0 + \cdots + x_n)$, Floater [8] also shows that for any $f \in C^{n+2}(I)$ we have

$$|n![x_0, \ldots, x_n]f - f^{(n)}(\bar{x})| \leq \frac{\sigma_2(x_0 - \bar{x}, \ldots, x_n - \bar{x})}{(n+2)(n+1)} \|f^{(n+2)}\|$$

$$\leq \frac{n}{24} h^2 \|f^{(n+2)}\|, \tag{5}$$

where the constant $n/24$ is the best possible in the sense that it is attained in the case of equidistant simple knots.

In this paper, we improve Floater's results in various ways. First, we show in Theorem 3 that divided difference expansions still hold if we reduce in one unit the degree of differentiability of the functions we are working with (to this respect, see also the concluding remark at the end of the paper). Second, we consider separately the leading term implicitly contained in (5) and give sharp lower and upper bounds for its leading coefficient. Such bounds heavily depend on the number $r+1$ of distinct knots and their corresponding multiplicities m_i and therefore are given on each of the sets $\mathbf{F}_r$ and $\mathbf{F}_r(a)$ (see Corollary 4 in Section 3 and Propositions 7, 8 and 9 in Section 4). Finally, we show that if we choose x in formula (2) as a small perturbation of the arithmetic mean $\bar{x}$,

then the order of convergence in the approximation becomes h^3 (see Theorem 5 in Section 3) or even h^4 under the additional assumption of equidistant simple knots (see Theorem 6 in Section 3). This small perturbation, however, depends on the function f under consideration.

To prove the preceding results, we use a probabilistic approach (see Section 2) based on the representation

$$n![x_0, \ldots, x_n]f = Ef^{(n)}(Z(\mathbf{x})), \quad f \in C^n(I), \quad \mathbf{x} \in \mathbf{F}, \tag{6}$$

where E stands for mathematical expectation and $Z(\mathbf{x})$ is a linear combination of uniform order statistics. Formula (6) is nothing else but Hermite-Genocchi's formula written in probabilistic terms. Apparently, a multivariate version of (6) was discovered independently by Ignatov and Kaishev [9] and by Karlin et al. [12]. Although divided differences, specially B-splines, enjoy a wide applicability in diverse branches of probability and statistics (see, for instance, Redner [15], Ignatov and Kaishev [10] and Agarwal et al. [3]), it does not seem that the probabilistic interpretation contained in (6) has been exploited to investigate purely analytical properties of divided differences.

Starting from (6), we give a probabilistic Taylor's formula in (11)-(12) below which allows us to write the remainder R_p in (2) in closed form (a slightly different closed form for R_p when $p - n$ is even has also been obtained by Floater [8, Theorem 2]). Formulae (11)-(12), together with the estimates of the variance of $Z(\mathbf{x})$ given in Propositions 8 and 9, are the key points to provide a unified approach to divided difference expansions from a probabilistic perspective. We refer the reader to Conte and de Boor [4] or DeVore and Lorentz [6] for the necessary properties of divided differences.

2 The probabilistic representation

Let $(U_k)_{k=1}^n$ be a sequence of independent identically distributed random variables having the uniform distribution on $[0,1]$. Denote by $(U_{(k)})_{k=1}^n$ its associated sequence of order statistics, i.e., $U_{(k)}$ is the k-th smallest random variable among $U_1, \ldots, U_n,\ k = 1, \ldots, n$. We define the random variable

$$Z(\mathbf{x}) := x_0 + h_1 U_{(n)} + \cdots + h_n U_{(1)}, \quad \mathbf{x} \in \mathbf{F}. \tag{7}$$

It is well-known (cf. [11, p. 280]) that the joint probability density of the random vector $(U_{(1)}, \ldots, U_{(n)})$ is given by

$$\rho(u_1, \ldots, u_n) = n!, \quad 0 \le u_1 \le \cdots \le u_n \le 1.$$

Therefore, Hermite-Genocchi's formula for divided differences can be written as

$$\begin{aligned} n![x_0, \ldots, x_n]f &= \int_0^1 du_1 \int_0^{u_1} du_2 \ldots \int_0^{u_{n-1}} f^{(n)}(x_0 + h_1 u_n + \cdots + h_n u_1) du_n \\ &= E f^{(n)}(Z(\mathbf{x})), \quad f \in C^n(I), \quad \mathbf{x} \in \mathbf{F}. \end{aligned}$$

If $\mathbf{x} \in \mathbf{F}_r$ for some $r = 1, \ldots, n$, we see from (1) and (7) that $Z(\mathbf{x})$ takes on the form

$$Z(\mathbf{x}) := \tilde{x}_0 + \sum_{i=1}^{r} \tilde{h}_i U_{(n+1-s_i)}, \quad s_i := m_0 + \cdots + m_{i-1}, \quad i = 1, \ldots, r. \tag{8}$$

In the case of equidistant simple knots, i.e., if $h = h_i > 0$, $i = 1, \ldots, n$, we have

$$Z(\mathbf{x}) = x_0 + h(U_{(n)} + \cdots + U_{(1)}) = x_0 + h(U_1 + \cdots + U_n) \tag{9}$$

and, therefore, for any $f \in C^n(I)$, we can write

$$n![x_0, \ldots, x_n]f = \frac{1}{h^n}\Delta_h^n f(\bar{x}) = Ef^{(n)}(x_0 + h(U_1 + \cdots + U_n)), \qquad (10)$$

where $\Delta_h^n f$ stands for the n-th symmetric difference of f with step h.

Let $\mathbf{x} \in \mathbf{F}$. For any $m = 1, 2, \ldots$, denote by β_m a random variable independent of $Z(\mathbf{x})$ having the beta density $\rho_m(u) := m(1-u)^{m-1},\ u \in [0,1]$ ($\beta_0 := 1$). For any $f \in C^{p-1}(I)$, $x \in I$ and $p = n+1, n+2, \ldots$, we claim that

$$Ef^{(n)}(Z(\mathbf{x})) = \sum_{k=n}^{p-1} \frac{f^{(k)}(x)}{(k-n)!} E(Z(\mathbf{x}) - x)^{k-n} + R_p(x), \qquad (11)$$

where

$$R_p(x) := \frac{E(Z(\mathbf{x}) - x)^{p-1-n}\left(f^{(p-1)}\left(x + (Z(\mathbf{x}) - x)\beta_{p-1-n}\right) - f^{(p-1)}(x)\right)}{(p-1-n)!}. \qquad (12)$$

Indeed, if $Z(\mathbf{x}) = z \in I$, formulae (11) and (12) are the classical Taylor's formula with remainder in integral form written with the help of the random variable β_{p-1-n}. Thus, (11) and (12) follow by replacing z by $Z(\mathbf{x})$ and then taking expectations. Similar probabilistic Taylor's formulae for nonnegative random variables X with remainders written in terms of the p-th equilibrium distribution of X can be found in Massey and Whitt [14] and Lin [13].

Comparing (11) and (12) with (2) and (3), we see that

$$c_k = \sigma_{k-n}(x_0 - x, \ldots, x_n - x) = \binom{k}{n} E(Z(\mathbf{x}) - x)^{k-n}, \qquad (13)$$

where $n \le k \le p-1$ and $x \in I$. This formula can also be checked by direct computation of the expectation on the right-hand side in (13). On the other hand, (12) gives us a closed form expression for the remainder R_p in (2).

To bound the remainder term in (12), we shall need the following.

Proposition 1 *For any real $p \geq 1$, we have*

$$\sup\left\{E\left|\frac{Z(\mathbf{x})-x}{h}\right|^p : \ \mathbf{x}\in\mathbf{F},\ x\in I\right\} \leq E(U_1+\cdots+U_n)^p \leq n^p.$$

PROOF. Let $\mathbf{x}\in\mathbf{F}$. For any $p\geq 1$, the function $g_p(x) := E|Z(\mathbf{x})-x|^p,\ x\in I$, is non-negative and convex, and therefore attains its maximum at one of the endpoints x_0 or x_n. By (7) and (9), we have

$$|Z(\mathbf{x})-x_0| \leq h(U_1+\cdots+U_n), \quad |Z(\mathbf{x})-x_n| \leq h((1-U_1)+\cdots+(1-U_n)). \quad (14)$$

Since $1-U_i$ has the uniform distribution on $[0,1]$, $i=1,\ldots,n$, Proposition 1 follows from (14). $\square$

Remark 2 *It follows from Proposition 1 that, for any positive integer p, the order of convergence of $E(Z(\mathbf{x})-x)^p$ is h^p at least. This order of convergence is actually attained. Consider, for instance, the case of equidistant simple knots and choose $x := x_0+bh$, where $0\leq b\leq n$ and $b\neq n/2$. Denote by E_p the set of even integers among $\{0,1,\ldots,p\}$. We see from (9) that $Z(\mathbf{x})-x = h(U_1+\cdots+U_n-b)$. Hence,*

$$\begin{aligned} h^{-p}E(Z(\mathbf{x})-x)^p &= E\left(U_1+\cdots+U_n-b\right)^p \\ &= \sum_{i\in E_p}\binom{p}{i}E\left(U_1+\cdots+U_n-\frac{n}{2}\right)^i\left(\frac{n}{2}-b\right)^{p-i} \neq 0, \end{aligned}$$

because $U_1+\cdots+U_n-n/2$ has a symmetric probability density and therefore its odd moments vanish.

3 Main results

Recall that for $i = 1, 2, \ldots$, the usual i-th modulus of smoothness of a function f defined on I is given by

$$\omega_i(f;\epsilon) := \sup\left\{ |\Delta_\delta^i f(x)| : \ [x - \frac{i\delta}{2}, x + \frac{i\delta}{2}] \subseteq I, \ 0 \le \delta \le \epsilon \right\}, \quad \epsilon \ge 0. \tag{15}$$

It is known (cf. [7, p.37]) that

$$\omega_i(f; b\epsilon) \le (1+b)^i \omega_i(f;\epsilon), \qquad b \ge 0, \quad \epsilon \ge 0, \quad i = 1, 2, \ldots \tag{16}$$

We state the following.

Theorem 3 *Let $f \in C^{p-1}(I)$ for some $p = n+1, n+2, \ldots$ For any $x \in I$, we have*

$$n![x_0, \ldots, x_n]f = \sum_{k=n}^{p-1} \frac{f^{(k)}(x)}{(k-n)!} E(Z(\mathbf{x}) - x)^{k-n} + R_p(x), \tag{17}$$

where

$$\sup_{x \in I} |R_p(x)| \le \frac{pn^{p-1-n}}{(p-n)!} h^{p-1-n} \omega_1\left(f^{(p-1)}; h\right). \tag{18}$$

PROOF. Formula (17) readily follows from (6) and (11), where $R_p(x)$ is defined in (12). On the other hand, let $x \in I$. It follows from (12), (16) and Proposition 1 that

$$\begin{aligned}
|R_p(x)| &\le \frac{1}{(p-1-n)!} E|Z(\mathbf{x}) - x|^{p-1-n} \omega_1\left(f^{(p-1)}; |Z(\mathbf{x}) - x|\beta_{p-1-n}\right) \\
&\le \frac{1}{(p-1-n)!} E|Z(\mathbf{x}) - x|^{p-1-n} \left(1 + \frac{|Z(\mathbf{x}) - x|\beta_{p-1-n}}{h}\right) \omega_1\left(f^{(p-1)}; h\right) \\
&\le \left(\frac{n^{p-1-n}}{(p-1-n)!} + \frac{n^{p-n}}{(p-n)!}\right) h^{p-1-n} \omega_1\left(f^{(p-1)}; h\right),
\end{aligned}$$

where we have used the fact that $E\beta_m = 1/(m+1),\ m = 0, 1, \ldots$ This shows (18) and completes the proof of Theorem 3 $\square$

As follows from Proposition 1 and Remark 2, the order of convergence of the expectation $E(Z(\mathbf{x}) - x)^{k-n}$ appearing in the main term of (17) is, in general, h^{k-n}. Also, observe that the smoothness requirements on f in Theorem 3 are weaker than those in (2).

Denote by $\sigma^2(\mathbf{x}) := E(Z(\mathbf{x}) - \bar{x})^2$ the variance of the random variable $Z(\mathbf{x})$. Setting $x = \bar{x}$ and $p = n + 3$ in (17), we obtain the following immediate consequence.

Corollary 4 *For any $f \in \mathcal{C}^{n+2}(I)$, we have*

$$\left| n![x_0, \ldots, x_n]f - f^{(n)}(\bar{x}) - \frac{\sigma^2(\mathbf{x})}{2} f^{(n+2)}(\bar{x}) \right| \leq \frac{(n+3)n^2}{6} h^2 \omega_1 \left(f^{(n+2)}; h \right).$$

Comparing Corollary 4 with (5) we observe the following. Although both results are stated under the same smoothness assumptions on f, the leading term of the approximation is considered separately in Corollary 4. As follows from Propositions 8 and 9 below, the order of convergence of this leading term is h^2, while its leading coefficient is

$$\frac{\sigma^2(\mathbf{x})}{2h^2} f^{(n+2)}(\bar{x}).$$

Exact values of $h^{-2}\sigma^2(\mathbf{x})$ are provided in Proposition 7. Whenever $\mathbf{x} \in \mathbf{F}_r$, sharp upper and lower bounds for $h^{-2}\sigma^2(\mathbf{x})$ are given in Propositions 8 and 9. All these results are postponed to Section 4 because their proofs are rather

technical. Finally, we observe from (28) below that

$$\left|\frac{\sigma^2(\mathbf{x})}{2h^2} f^{(n+2)}(\bar{x})\right| \leq \frac{n}{24}|f^{(n+2)}(\bar{x})|, \quad \mathbf{x} \in \mathbf{F},$$

$n/24$ being the best possible constant on $\mathbf{F}$. This last statement has already been shown by Floater [8].

According to Corollary 4, the approximation of $f^{(n)}(\bar{x})$ by $n![x_0, \ldots, x_n]f$ takes place at the rate h^2. However, such a rate may be increased up to h^3 if we consider a small perturbation of the arithmetic mean $\bar{x}$ depending on the values $f^{(n+1)}(\bar{x})$ and $f^{(n+2)}(\bar{x})$, as stated in the following.

Theorem 5 *For any $f \in \mathcal{C}^{n+3}(I)$, we have*

(a) If $f^{(n+1)}(\bar{x}) \neq 0$ and $\bar{x} + c\sigma^2(\mathbf{x}) \in I$, where

$$c := \frac{1}{2}\frac{f^{(n+2)}(\bar{x})}{f^{(n+1)}(\bar{x})}, \tag{19}$$

then

$$\begin{aligned} &\left|n![x_0, \ldots, x_n]f - f^{(n)}(\bar{x} + c\sigma^2(\mathbf{x})) - \frac{1}{6}f^{(n+3)}(\bar{x})E(Z(\mathbf{x}) - \bar{x})^3\right| \\ &\leq \frac{n^3}{6}\left(1 + \frac{n}{4}\right)h^3\omega_1\left(f^{(n+3)}; h\right) + \frac{(cn)^2}{288}\|f^{(n+2)}\|h^4. \end{aligned} \tag{20}$$

(b) If $f^{(n+1)}(\bar{x}) = 0$ and $\bar{x} \pm \sigma(\mathbf{x}) \in I$, then

$$\begin{aligned} &\left|n![x_0, \ldots, x_n]f - f^{(n)}(\bar{x} \pm \sigma(\mathbf{x})) - \frac{1}{6}f^{(n+3)}(\bar{x})\left(E(Z(\mathbf{x}) - \bar{x})^3 - (\pm\sigma(\mathbf{x}))^3\right)\right| \\ &\leq \left(n^3\left(1 + \frac{n}{4}\right) + \frac{n}{24}\left(\sqrt{\frac{n}{3}} + \frac{n}{24}\right)\right)\frac{h^3}{6}\omega_1\left(f^{(n+3)}; h\right). \end{aligned} \tag{21}$$

PROOF. Let c be as in (19) and denote by $Z := Z(\mathbf{x})$ and by $\sigma := \sigma(\mathbf{x})$. Expanding $Ef^{(n)}(Z)$ and $f^{(n)}(\bar{x} + c\sigma^2)$ in a Taylor series around $\bar{x}$, we have

by virtue of (6), (11) and (12) that

$$n![x_0,\ldots,x_n]f - f^{(n)}(\bar{x}+c\sigma^2) = \frac{1}{6}f^{(n+3)}(\bar{x})E(Z-\bar{x})^3 + r_1, \qquad (22)$$

where

$$r_1 := \frac{1}{6}E(Z-\bar{x})^3\left(f^{(n+3)}(\bar{x}+(Z-\bar{x})\beta_3) - f^{(n+3)}(\bar{x})\right)$$
$$-\frac{(c\sigma^2)^2}{2}Ef^{(n+2)}(\bar{x}+c\sigma^2\beta_2). \qquad (23)$$

Proceeding as in the proof of Theorem 3, (20) follows from (22), (23) and the fact that $\sigma^2 \le nh^2/12$, as follows from (28).

The proof of (21) is similar by taking into account that

$$n![x_0,\ldots,x_n]f - f^{(n)}(\bar{x}\pm\sigma^2) = \frac{1}{6}f^{(n+3)}(\bar{x})\left(E(Z-\bar{x})^3 - (\pm\sigma)^3\right) + r_2,$$

where

$$r_2 := \frac{1}{6}E(Z-\bar{x})^3\left(f^{(n+3)}(\bar{x}+(Z-\bar{x})\beta_3) - f^{(n+3)}(\bar{x})\right)$$
$$-\frac{1}{6}(\pm\sigma^3)\left(Ef^{(n+3)}(\bar{x}\pm\sigma\beta_3) - f^{(n+3)}(\bar{x})\right).$$

The proof of Theorem 5 is complete. □

Note that, by Propositions 1 and 8, the order of convergence of the leading terms in (20) and (21) is, in general, h^3. Nevertheless, in the case of equidistant simple knots, Theorem 5(a) may be improved as follows.

Theorem 6 *Let $f \in \mathcal{C}^{n+4}(I)$. Assume that $f^{(n+1)}(\bar{x}) \neq 0$ and let c be as in*

(19). *Then,*

$$\left|\frac{1}{h^n}\Delta_h^n f(\bar{x}) - f^{(n)}\left(\bar{x}+\frac{cn}{12}h^2\right) + \frac{f^{(n+2)}(\bar{x})}{2}\left(\frac{cn}{12}\right)^2 h^4\right.$$

$$\left. - \frac{f^{(n+4)}(\bar{x})}{4!}\left(\frac{n(n-1)}{48}+\frac{n}{80}\right)h^4\right|$$

$$\leq \frac{n^4}{4!}\left(1+\frac{n}{5}\right)h^4\omega_1\left(f^{(n+4)};h\right) + \frac{\|f^{(n+3)}\|}{3!}\left(\frac{|c|n}{12}\right)^3 h^6.$$

PROOF. Let $\mathbf{x} \in \mathbf{F}_n$ be such that $x_i := x_0 + hi$, $i = 0, \ldots, n$, where $h > 0$ and $x_0 \in \mathbb{R}$. By (9), we have that $Z := Z(\mathbf{x}) = x_0 + h(U_1 + \cdots + U_n)$. It follows by calculus (see also (28) below) that

$$\sigma^2 := E(Z-\bar{x})^2 = \frac{nh^2}{12} \quad \text{and} \quad E(Z-\bar{x})^4 = \left(\frac{n(n-1)}{48}+\frac{n}{80}\right)h^4. \tag{24}$$

Proceeding as in the proof of Theorem 5(a) and taking into account that the odd moments of Z vanish, as we have seen in Remark 2, we have

$$\left|Ef^{(n)}(Z) - f^{(n)}\left(\bar{x}+c\sigma^2\right) + \frac{1}{2}f^{(n+2)}(\bar{x})(c\sigma^2)^2 - \frac{1}{4!}f^{(n+4)}(\bar{x})E(Z-\bar{x})^4\right|$$

$$\leq \frac{1}{4!}\left|E(Z-\bar{x})^4\left(f^{(n+4)}(\bar{x}+(Z-\bar{x})\beta_4) - f^{(n+4)}(\bar{x})\right)\right| + \frac{\|f^{(n+3)}\|}{3!}|c|^3\sigma^6$$

$$\leq \frac{n^4}{4!}\left(1+\frac{n}{5}\right)h^4\omega_1\left(f^{(n+4)};h\right) + \frac{\|f^{(n+3)}\|}{3!}\left(\frac{|c|n}{12}\right)^3 h^6.$$

This, in conjuction with (10) and (24), completes the proof of Theorem 6. □

4 Sharp bounds for the leading coefficient

For any $\mathbf{x} \in \mathbf{F}$, we consider the 'standardized' random variable $h^{-1}(Z(\mathbf{x}) - \bar{x})$, whose variance $h^{-2}\sigma^2(\mathbf{x})$ appears in the leading coefficient of the main term

of the approximation in Corollary 4. It turns out that both exact values and upper and lower bounds for $h^{-2}\sigma^2(\mathbf{x})$ heavily depend on the number $r+1$ of distinct knots of $\mathbf{x}$ and their corresponding multiplicities $m_i,\ i=0,\dots,r$.

From now on, we fix $r=1,\dots,n$, and denote by $\lfloor x \rfloor$ the integer part of x and by 1_A the indicator function of the set A. Let i and j be two positive integers with $1 \le i \le j \le n$. The first and second moments of the order statistics are given, respectively (cf. [11, p.280]), by

$$EU_{(i)} = \frac{i}{n+1} \tag{25}$$

and

$$Cov(U_{(i)}, U_{(j)}) := E(U_{(i)} - EU_{(i)})(U_{(j)} - EU_{(j)}) = \frac{i(n+1-j)}{(n+2)(n+1)^2}. \tag{26}$$

Exact values of $h^{-2}\sigma^2(\mathbf{x})$ are given in the following.

Proposition 7 *For any $\mathbf{x} \in \mathbf{F}_r$, we have*

$$(n+2)(n+1)^2\sigma^2(\mathbf{x}) = \sum_{i=1}^{r} \tilde{h}_i^2 s_i(n+1-s_i) + 2\sum_{i=1}^{r}\sum_{j=i+1}^{r} \tilde{h}_i\tilde{h}_j s_i(n+1-s_j), \tag{27}$$

where s_i is defined in (8)*. Moreover, we have*

$$\sup\{h^{-2}\sigma^2(\mathbf{x}) :\ \mathbf{x} \in \mathbf{F}\} = \frac{n}{12} \tag{28}$$

and this supremum is attained in the case of equidistant simple knots, that is, at $\mathbf{x}^* \in \mathbf{F}_n$ such that $x_i^* = x_0^* + hi$, $i=0,\dots,n$, where $x_0^* \in \mathbb{R}$ is arbitrary.

PROOF. If $\mathbf{x} \in \mathbf{F}_r$, we have from (8) and (26) that

$$\sigma^2(\mathbf{x}) = Var\left(\sum_{i=1}^{r} \tilde{h}_i U_{(n+1-s_i)}\right)$$

$$= \sum_{i=1}^{r} \tilde{h}_i^2 Var(U_{(n+1-s_i)}) + 2\sum_{i=1}^{r}\sum_{j=i+1}^{r} \tilde{h}_i\tilde{h}_j Cov(U_{(n+1-s_i)}, U_{(n+1-s_j)})$$

$$= \frac{1}{(n+2)(n+1)^2}\left(\sum_{i=1}^{r} \tilde{h}_i^2 s_i(n+1-s_i) + 2\sum_{i=1}^{r}\sum_{j=i+1}^{r} \tilde{h}_i\tilde{h}_j s_i(n+1-s_j)\right), \quad (29)$$

thus showing (27). On the other hand, let $\mathbf{x} \in \mathbf{F}$. Proceeding as in (29), we have from (7) and (9) that

$$h^{-2}\sigma^2(\mathbf{x}) = h^{-2}Var\left(\sum_{i=1}^{n} h_i U_{(n+1-i)}\right) \leq Var\left(\sum_{i=1}^{n} U_{(n+1-i)}\right) = Var\left(\sum_{i=1}^{n} U_i\right)$$

$$= \sum_{i=1}^{n} Var(U_i) = \frac{n}{12}. \quad (30)$$

Similarly, $h^{-2}\sigma^2(\mathbf{x}^*) = n/12$, where $\mathbf{x}^* \in \mathbf{F}_n$ is defined in Proposition 7. This, together with (30), shows (28) and completes the proof of Proposition 7. $\square$

As follows from (29), $h^{-2}\sigma^2(\mathbf{x})$ is a positive linear combination of the covariances $Cov(U_{(n+1-s_i)}, U_{(n+1-s_j)})$, which, according to (26), increase as $n+1-s_i$ and $n+1-s_j$ approach to $\lfloor (n+1)/2 \rfloor$. Therefore, the maximum of $h^{-2}\sigma^2(\mathbf{x})$ over the set $\mathbf{F}_r$ must be attained when the order statistics $U_{(n+1-s_i)}$ are close to $U_{(\lfloor (n+1)/2 \rfloor)}$. Translating this into multiplicities, observe from (1) that if $\mathbf{x} \in \mathbf{F}_r$ then $m_0 + \cdots + m_r = n+1$. Therefore, the maximum of $h^{-2}\sigma^2(\mathbf{x})$ over $\mathbf{F}_r$ must be attained when the intermediate multiplicities are as low as possible (all of them equal to 1) and the extreme multiplicities are as high as possible. The opposite holds concerning the minimum of $h^{-2}\sigma^2(\mathbf{x})$ over the set $\mathbf{F}_r(a)$. More precise statements are given in the following two propositions.

Proposition 8 *We have*

$$\sup\{h^{-2}\sigma^2(\mathbf{x}) : \ \mathbf{x} \in \mathbf{F}_r\}$$

$$= \frac{r(r+1)\Big((r+1)(r+2) + 2(2r+1)(n-r)\Big) + 12\theta r^2(n-r-\theta)}{12(n+2)(n+1)^2}, \qquad (31)$$

where

$$\theta := \lfloor (n+1-r)/2 \rfloor. \qquad (32)$$

The supremum in (31) *is attained at* $\mathbf{x}^* \in \mathbf{F}_r$ *such that* $x_i^* = x_0^* + hi, \ i = 1, \ldots, r$, *where* $x_0^* \in \mathbb{R}$ *is arbitrary and* $m_0 = \theta + 1$, $m_1 = \cdots = m_{r-1} = 1$ *and* $m_r = n + 1 - r - \theta$.

Proposition 9 *For any* $0 < a \leq 1$, *we have*

$$\inf\{h^{-2}\sigma^2(\mathbf{x}) : \ \mathbf{x} \in \mathbf{F}_r(a)\} \geq a^2 \inf\{\tilde{h}^{-2}\sigma^2(\mathbf{x}) : \ \mathbf{x} \in \mathbf{F}_r\}$$

$$= \frac{a^2}{(n+2)(n+1)} \left(\frac{\nu(\nu+1)(2\nu+1)}{3} + \frac{n(\nu+1)^2}{(n+1)} 1_O(r) \right), \qquad (33)$$

where O *is the set of odd positive integers and*

$$\nu := \lfloor r/2 \rfloor. \qquad (34)$$

The second infimum in (33) *is attained at* $\mathbf{x}' \in \mathbf{F}_r$ *such that* $x_i' = x_0' + \tilde{h}i, \ i = 1, \ldots, r$, *where* $x_0' \in \mathbb{R}$ *is arbitrary and* $m_{r-\nu} = n + 1 - r$, $m_i = 1, \ i \neq r - \nu$.

It should be observed that if $r = n$ the upper bounds in (28) and (31) coincide. Such bounds also coincide with the lower bound in (33) whenever $a = 1$, that is, in the case of equally spaced simple knots.

The proof of the preceding propositions will be split in various lemmas. By

(26), we see that

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) = Var\left(\sum_{i=1}^{r} U_{(n+1-s_i)}\right). \tag{35}$$

Denote by

$$l := \#\left\{s_i : \ s_i \leq \lfloor (n+1)/2 \rfloor\right\}. \tag{36}$$

Taking into account (35), no generality is lost if we assume that $l \geq \lfloor (r+1)/2 \rfloor$.

Lemma 10 *Let l be as in* (36)*. Then,*

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) \leq Var\left(\sum_{i=\lfloor (n+1)/2 \rfloor - l+1}^{\lfloor (n+1)/2 \rfloor - l+r} U_{(i)}\right).$$

PROOF. We first claim that

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) \leq Var\left(\sum_{i=\lfloor (n+1)/2 \rfloor - l+1}^{\lfloor (n+1)/2 \rfloor} U_{(i)} + \sum_{i=l+1}^{r} U_{(s_i)}\right). \tag{37}$$

In fact, assume that $(s_1, \ldots, s_l) \neq (\lfloor (n+1)/2 \rfloor - l + 1, \ldots, \lfloor (n+1)/2 \rfloor)$, since otherwise (37) is trivial. Denote by

$$\bar{t} := \min\{1 \leq i \leq l : \ s_{i+1} - s_i > 1\} \quad (s_{r+1} := n+1),$$

and define the sequence $(\bar{s}_1, \ldots, \bar{s}_r)$ as

$$\bar{s}_i := \begin{cases} s_i + 1 & \text{if } i \leq \bar{t} \\ s_i & \text{if } i > \bar{t}, \end{cases} \qquad i = 1, \ldots, r.$$

Using (26) it can be checked that

$$Var\left(U_{(s_i)}\right) \leq Var\left(U_{(\bar{s}_i)}\right), \quad i = 1, \ldots, r,$$

as well as

$$Cov\left(U_{(s_i)}, U_{(s_j)}\right) \leq Cov\left(U_{(\bar{s}_i)}, U_{(\bar{s}_j)}\right), \quad 1 \leq i \leq j \leq r,$$

thus implying that

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) \leq Var\left(\sum_{i=1}^{r} U_{(\bar{s}_i)}\right). \tag{38}$$

Therefore, (37) follows from (38) by repeating the previous procedure a finite number of steps. To complete the proof, it suffices to apply similar techniques to the right-hand side in (37), that is, to define

$$\underline{t} := \max\{l+1 \leq i \leq r : \ s_i - s_{i-1} > 1\},$$

and

$$\underline{s}_i := \begin{cases} s_i - 1, & \text{if } i \geq \underline{t} \\ s_i, & \text{if } i < \underline{t}\,, \end{cases} \qquad i = 1, \ldots, r.$$

The proof of Lemma 10 is complete. □

Lemma 11 *Let θ and l be as in* (32) *and* (36)*, respectively. Then,*

$$Var\left(\sum_{i=\lfloor(n+1)/2\rfloor-l+1}^{\lfloor(n+1)/2\rfloor-l+r} U_{(i)}\right) \leq Var\left(\sum_{i=\theta+1}^{\theta+r} U_{(i)}\right).$$

PROOF. Since $l \geq \lfloor(r+1)/2\rfloor$, we have

$$\lfloor(n+1)/2\rfloor - l \leq \lfloor(n+1)/2\rfloor - \lfloor(r+1)/2\rfloor \leq \lfloor(n+1-r)/2\rfloor =: \theta,$$

as follows by calculus. Therefore, Lemma 11 will follow as soon as we show that

$$Var\left(\sum_{i=p}^{p+r-1} U_{(i)}\right) \leq Var\left(\sum_{i=p+1}^{p+r} U_{(i)}\right), \quad p = 1, \ldots, \theta. \tag{39}$$

Since $p \leq \theta$, it can be checked using (26) that

$$Var\left(U_{(p)}\right) \leq Var\left(U_{(p+r)}\right) \tag{40}$$

and

$$\sum_{j=p+1}^{p+r-1} Cov\left(U_{(p)}, U_{(j)}\right) \leq \sum_{j=p+1}^{p+r-1} Cov\left(U_{(j)}, U_{(p+r)}\right). \tag{41}$$

Clearly, (39) follows from (40) and (41), thus completing the proof of Lemma 11. □

The following lemma readily follows from (26).

Lemma 12 *Denote by* $S := s_1 + \cdots + s_r$. *Then,*

$$(n+2)(n+1)^2 Var(\sum_{i=1}^{r} U_{(s_i)}) = (n+1)(2r+1)S - S^2 - 2(n+1)\sum_{i=1}^{r} i s_i.$$

Proof of Proposition 8. Let $\mathbf{x} \in \mathbf{F}_r$ and let θ be as in (32). Using succesively (29), (35) and Lemmas 10 and 11, we have

$$\begin{aligned} h^{-2}\sigma^2(\mathbf{x}) &\leq Var\left(\sum_{i=1}^{r} U_{(n+1-s_i)}\right) \leq Var\left(\sum_{i=\theta+1}^{\theta+r} U_{(i)}\right) \\ &= \frac{r(r+1)\Big((r+1)(r+2) + 2(2r+1)(n-r)\Big) + 12\theta r^2(n-r-\theta)}{12(n+2)(n+1)^2}, \end{aligned} \tag{42}$$

where the last equality follows from Lemma 12 by setting $s_i = \theta + i,\ i = 1, \ldots, r$, and the well-known identity

$$\sum_{i=1}^{r} i^2 = \frac{r(r+1)(2r+1)}{6}.$$

On the other hand, let $\mathbf{x}^* \in \mathbf{F}_r$ be as in Proposition 8. It follows from (8) and (35) that

$$h^{-2}\sigma^2(\mathbf{x}^*) = Var\left(\sum_{i=1}^{r} U_{(n+1-\theta-i)}\right) = Var\left(\sum_{i=1}^{r} U_{(\theta+i)}\right) = Var\left(\sum_{i=\theta+1}^{\theta+r} U_{(i)}\right).$$

This, together with (42), shows the last statement in Proposition 8, thus completing its proof. □

To prove Proposition 9, we shall need the following two auxiliary results.

Lemma 13 *Let ν be as in* (34)*. Then,*

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) \geq Var\left(\sum_{i=1}^{\nu} U_{(i)} + \sum_{i=1}^{r-\nu} U_{(n+1-i)}\right). \tag{43}$$

PROOF. Starting from the sequence $(s_i,\ i = 1, \ldots, r)$, we give a procedure to construct a new sequence $(\bar{s}_i,\ i = 1, \ldots, r)$ such that $1 \leq \bar{s}_1 < \cdots < \bar{s}_r \leq n$ and

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) \geq Var\left(\sum_{i=1}^{r} U_{(\bar{s}_i)}\right).$$

To this end, we define

$$c := \max\{1 \leq i \leq \nu :\ s_j = j,\ j = 1, \ldots, i\}$$

and

$$d := \max\{1 \leq i \leq r - \nu :\ s_{r+1-j} = n + 1 - j,\ j = 1, \ldots, i\},$$

where it is understood that $\max \varnothing = 0$. If $c = \nu$ and $d = r - \nu$, Lemma 13 is trivial. Otherwise, we distinguish the cases $c < d$ and $c \geq d$.

Case $c < d$. We define $(\bar{s}_i,\ i = 1, \ldots, r)$ by setting $\bar{s}_{c+1} := c + 1$ and $\bar{s}_i = s_i$, $i \neq c + 1$. Observe that, by construction, we have

$$c + 1 < s_{c+1} \leq n - c. \tag{44}$$

We claim that

$$\begin{aligned} Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) &= Var\left(\sum_{i=1}^{c}(U_{(i)} + U_{(n+1-i)}) + U_{(s_{c+1})} + \sum_{i=c+2}^{r-c} U_{(s_i)}\right) \\ &\geq Var\left(\sum_{i=1}^{c}(U_{(i)} + U_{(n+1-i)}) + U_{(c+1)} + \sum_{i=c+2}^{r-c} U_{(s_i)}\right) = Var\left(\sum_{i=1}^{r} U_{(\bar{s}_i)}\right). \end{aligned} \tag{45}$$

Actually, the equalities in (45) follow by definition. On the other hand, it can be checked from (26) and (44) that

$$Var(U_{(s_{c+1})}) \geq Var(U_{(c+1)}), \tag{46}$$

$$Cov(U_{(s_{c+1})}, U_{(s_i)}) \geq Cov(U_{(c+1)}, U_{(s_i)}), \quad c+2 \leq i \leq r-c, \tag{47}$$

and, for $1 \leq i \leq c$, that

$$Cov(U_{(i)}+U_{(n+1-i)}, U_{(s_{c+1})}) = \frac{i}{(n+2)(n+1)} = Cov(U_{(i)}+U_{(n+1-i)}, U_{(c+1)}). \tag{48}$$

Therefore, the inequality in (45) follows from (46)-(48), thus showing claim (45).

Case $c \geq d$. We define $(\bar{s}_i,\ i = 1, \ldots, r)$ as $\bar{s}_{r-d} := r-d$ and $\bar{s}_i = s_i$, $i \neq r-d$. In this case, it can be shown in a similar way that

$$Var\left(\sum_{i=1}^{r} U_{(s_i)}\right) = Var\left(\sum_{i=1}^{d}(U_{(i)} + U_{(n+1-i)}) + U_{(s_{r-d})} + \sum_{i=d+1}^{r-(d+1)} U_{(s_i)}\right)$$
$$\geq Var\left(\sum_{i=1}^{d}(U_{(i)} + U_{(n+1-i)}) + U_{(r-d)} + \sum_{i=d+1}^{r-(d+1)} U_{(s_i)}\right) = Var\left(\sum_{i=1}^{r} U_{(\bar{s}_i)}\right).$$

Applying the previous procedure to the new sequence $(\bar{s}_i,\ i = 1, \ldots, r)$, we arrive at (43) after a finite number of steps. The proof of Lemma 13 is complete. □

Lemma 14 *Let* ν *be as in* (34). *Then,*

$$Var\left(\sum_{i=1}^{\nu} U_{(i)} + \sum_{i=1}^{r-\nu} U_{(n+1-i)})\right) = \frac{\nu(\nu+1)(2\nu+1)}{3(n+2)(n+1)} + \frac{n(\nu+1)^2}{(n+2)(n+1)^2} 1_o(r).$$

PROOF. Assume first that r is even. Since $r - \nu = \nu$, we have from (26),

(35) and Lemma 12 that

$$Var\left(\sum_{i=1}^{\nu} U_{(i)} + \sum_{i=1}^{\nu} U_{(n+1-i)}\right) = 2Var\left(\sum_{i=1}^{\nu} U_{(i)}\right) + 2Cov\left(\sum_{i=1}^{\nu} U_{(i)}, \sum_{i=1}^{\nu} U_{(n+1-i)}\right)$$

$$= 2Var\left(\sum_{i=1}^{\nu} U_{(i)}\right) + \frac{2}{(n+2)(n+1)^2}\left(\sum_{i=1}^{\nu} i\right)^2 = \frac{\nu(\nu+1)(2\nu+1)}{3(n+2)(n+1)}. \tag{49}$$

If r is odd, then $r - \nu = \nu + 1$. Therefore, we have from (26), (48) and (49) that

$$Var\left(\sum_{i=1}^{\nu} U_{(i)} + \sum_{i=1}^{\nu+1} U_{(n+1-i)}\right) = Var\left(\sum_{i=1}^{\nu}(U_{(i)} + U_{(n+1-i)})\right) + Var(U_{(n-\nu)})$$

$$+ 2Cov\left(\sum_{i=1}^{\nu}(U_{(i)} + U_{(n+1-i)}), U_{(n-\nu)}\right) = \frac{\nu(\nu+1)(2\nu+1)}{3(n+2)(n+1)} + \frac{n(\nu+1)^2}{(n+2)(n+1)^2}.$$

This, together with (49), completes the proof of Lemma 14. □

Proof of Proposition 9 Let $\mathbf{x} \in \mathbf{F}_r(a)$. Applying successively (29), (35) and Lemmas 13 and 14, we obtain

$$h^{-2}\sigma^2(\mathbf{x}) \geq a^2\tilde{h}^{-2}\sigma^2(\mathbf{x}) \geq a^2 Var\left(\sum_{i=1}^{r} U_{(n+1-s_i)}\right) \geq a^2 Var\left(\sum_{i=1}^{\nu} U_{(i)} + \sum_{i=1}^{r-\nu} U_{(n+1-i)})\right)$$

$$= \frac{a^2}{(n+2)(n+1)}\left(\frac{\nu(\nu+1)(2\nu+1)}{3} + \frac{n(\nu+1)^2}{(n+1)} 1_{\mathrm{O}}(r)\right). \tag{50}$$

Finally, let $\mathbf{x}' \in \mathbf{F}_r(a)$ be as in Proposition 9. Recalling (8), it is readily seen that

$$\tilde{h}^{-2}\sigma^2(\mathbf{x}') = Var\left(\sum_{i=1}^{\nu} U_{(i)} + \sum_{i=1}^{r-\nu} U_{(n+1-i)}\right),$$

which, in conjunction with (50), shows Proposition 9. □

5 Concluding remark

Divided difference expansions still hold if the function under consideration satisfies weaker smoothness assumptions than those considered in Section 3. Indeed, let $\mathbf{x} \in \mathbf{F}$ and denote by $J := [x_0 - \sigma(\mathbf{x}), x_n + \sigma(\mathbf{x})]$. Then, for any $f \in C^n(J)$, we have

$$|n![x_0, \ldots, x_n]f - f^{(n)}(\bar{x})| \leq \frac{3}{2}\omega_2\left(f^{(n)}; \sigma(\mathbf{x})\right) \leq \frac{3}{2}\omega_2\left(f^{(n)}; h\sqrt{\frac{n}{12}}\right). \quad (51)$$

In estimate (51), $\omega_2\left(f^{(n)}; \cdot\right)$ is the usual second modulus of smoothness of $f^{(n)}$, as defined in (15), where the interval I is replaced by J. In particular, in the case of equidistant simple knots, we have by virtue of (10) that

$$\left|\frac{1}{h^n}\Delta_h^n f(\bar{x}) - f^{(n)}(\bar{x})\right| \leq \frac{3}{2}\omega_2\left(f^{(n)}; h\sqrt{\frac{n}{12}}\right). \quad (52)$$

A proof of inequalities (51) and (52) can be found in Adell and Sangüesa [1], where, in addition, a strong converse inequality for (52) is given. Alternatively, such estimates may be derived from Adell and Sangüesa [2, Theorem 3.1 and Corollary 3.1].

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