



Error bounds for spline-based quadrature methods for strongly singular integrals

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Abstract

For the numerical evaluation of finite-part integrals with singularities of order $p \geq 1$, we give error bounds for quadrature methods based on spline approximation. These bounds behave in the same way as the optimal ones. The ideas of the proof are also useful for methods based on other approximation processes. © 1998 Elsevier Science B.V. All rights reserved.

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1. Finite-part integrals and their applications

We discuss the approximation of Hadamard finite-part integrals of the form

$$H_p[f](t) := \int_a^b |x-t|^{-p} f(x) dx, \quad p \in \mathbb{R}, \quad p \geq 1,$$

or

$$H_p^*[f](t) := \int_a^b (x-t)^{-p} f(x) dx, \quad p \in \mathbb{N}$$

where $a \leq t \leq b$. For $p=1$, the latter integral is the Cauchy principal value. Their main properties are described in [3, Section 1.6.1] (also in [9, 13]). Finite-part integrals are used to reformulate a boundary value problem for a partial differential equation in terms of a hypersingular integral equation (mainly leading to integrals with singularities of integer or half-integer order [9, 13]). Singularities of noninteger order also arise in fractional calculus: The Riemann–Liouville fractional derivative $d^p f(x)/d(x-a)^p$ of order $p \notin \mathbb{N}$ of the function f may be expressed as a

finite-part integral [10, Section 2]. Thus, quadrature formulas for these integrals can be used to approximate fractional derivatives. Moreover, any fractional differential equation is equivalent to a finite-part integral equation, and we may use quadrature rules to approximate its solution [7]. Fractional differential equations occur in the study of diffusion problems [14, Chapter 11] and other areas of chemistry, physics and engineering [14, pp. ix–x]. Note that, in fractional calculus, the operator H_p is also used with $p \in \mathbb{C}$. With small modifications, our results hold in that case too.

2. The quadrature methods and error bounds

For the numerical calculation of $H_p[f]$, we consider methods based on spline approximation for f . We give error bounds holding uniformly on $[a, b]$, assuming that $f^{(s)}$ is bounded. Such bounds can hold only if $p - 1 < s \leq d + 1$, where d is the degree of exactness of the approximation process, cf. [8]. We see that these formulas can compete with the optimal ones. The proofs rely on a general principle. More applications of this are given at the end of this paper.

The optimal quadrature formula Q_n^{opt} with n nodes for the integral H_p satisfies $H_p[f] - Q_n^{\text{opt}}[f] = O(n^{p-1-s}(1 + \delta_{p,1} \ln n))$ (where $\delta_{j,k}$ is Kronecker's symbol) if $f^{(s)}$ is bounded [17]. A comparison with Theorem 1 shows that our methods are of optimal order if $p \notin \mathbb{N}$. For $p \in \mathbb{N}$, we lose at most a factor $O(\ln n)$. All known better formulas require f' . Our formulas only use function values of f .

We start with the so-called nodal splines [4, 5]. We only mention some of their properties. We have a set of knots $\{x_j: 0 \leq j \leq dn\}$ with $a = x_0 < x_1 < \dots < x_{dn} = b$. The x_{di} , $0 \leq i \leq n$, are called the primary knots of the spline; the others are called secondary. The spline approximation operator interpolates at the primary knots, and it reproduces polynomials of degree d . For the integral H_1^* , the method based on this approximation is convergent [4]. Theorem 1 shows the rate of convergence for this method applied to H_p and H_p^* for arbitrary p .

We also look at interpolating splines for the function f with not-a-knot end condition, defined by being the (unique) splines of odd degree $d \geq p$ with knots $a + j(b - a)/(2n)$, $j = d + 1, d + 3, \dots, 2n - d - 1$, and interpolation points $a + j(b - a)/n$, $j = 0, 1, \dots, n$. In the case of Cauchy principal values (the operator H_1^*), they are known to give optimal order quadrature rules [6]. For H_p^* with $p = 2, 3, \dots$, they have been discussed in [16]. Our Theorem 1 generalizes these results to $p \notin \mathbb{N}$ and improves the bounds of [16].

Finally, we consider quasi-interpolatory spline approximation operators [11]. Their use has been suggested for Cauchy principal values [2]. The results are as in the previous cases, completing the error analysis of [2].

Theorem 1. Assume $p - 1 < s \leq d + 1$. Let $f^{(s)}$ be bounded. Let (J_n) be

- a sequence of nodal spline approximation operators of degree d with $x_j = a + (b - a)j/(dn)$ ($j = 1, 2, \dots, dn$), or
- a sequence of not-a-knot spline interpolation operators of odd degree $d \geq p$ with uniform partitions, or
- a sequence of quasi-interpolatory spline approximation operators of degree $d \geq p$ with uniform partitions as described above.

Denote by $H_{p,n}[f] := H_p[J_n[f]]$ the quadrature rule for H_p based on J_n . Then,

$$\|H_p[f] - H_{p,n}[f]\|_\infty = \begin{cases} O(n^{p-1-s} \ln n) & \text{if } p \in \mathbb{N}, \\ O(n^{p-1-s}) & \text{if } p \notin \mathbb{N}. \end{cases}$$

In the case $p \in \mathbb{N}$, the same result holds if we replace H_p by H_p^* .

Theorem 2. Assume $p - 1 < s$. Let $J_n: [a, b] \rightarrow \mathcal{A}^s[a, b]$ satisfy

$$\sup\{\|(J_n[f] - f)^{(k)}\|_\infty : f \in C^s[a, b], \|f^{(s)}\|_\infty \leq 1\} = n^{k-s} \varepsilon_{k,n} \tag{1}$$

where $(\varepsilon_{k,n})_{n=1}^\infty$ are given for $k = 0, 1, \dots, s$. Then, for every $f \in C^s[a, b]$,

$$\|H_p[f] - H_p[J_n[f]]\|_\infty = \begin{cases} O(n^{p-1-s}) (\sum_{k=0}^p \varepsilon_{k,n} + \varepsilon_{p-1,n} \ln n) & \text{if } p \in \mathbb{N}, \\ O(n^{p-1-s}) \sum_{k=0}^{\lfloor p \rfloor} \varepsilon_{k,n} & \text{if } p \notin \mathbb{N}. \end{cases}$$

In the case $p \in \mathbb{N}$, the same result holds if we replace H_p by H_p^* .

Here, $\mathcal{A}^s[a, b]$ is the set of functions on $[a, b]$ whose $(s - 1)$ st derivative is absolutely continuous, and $\lfloor x \rfloor$ denotes the largest integer not exceeding x .

Proof of Theorem 2. We assume that $x \in (a + 1/n, b - 1/n)$. The other cases require only minor modifications. Then, defining $r_n := f - J_n[f]$, we write

$$H_p[f](x) - H_p[J_n[f]](x) = \left(\int_a^{x-1/n} + \int_{x-1/n}^x + \int_x^{x+1/n} + \int_{x+1/n}^b \right) \frac{r_n(t)}{|x-t|^p} dt$$

and deal with the four integrals separately. First, we see that

$$\begin{aligned} \left| \int_{|x-t| \geq 1/n} \frac{r_n(t)}{|x-t|^p} dt \right| &\leq \|r_n\|_\infty \int_{|x-t| \geq 1/n} |x-t|^{-p} dt \\ &\leq \begin{cases} 2(p-1)^{-1} n^{p-1-s} \varepsilon_{0,x} \|f^{(s)}\|_{1,\infty} & \text{if } p > 1, \\ 2n^{-s} (\ln n + \ln(b-a)) \varepsilon_{0,n} \|f^{(s)}\|_\infty & \text{if } p = 1, \end{cases} \end{aligned}$$

uniformly for all x . Furthermore, for $p \in \mathbb{N}$, we have by definition [3, Section 1.6.1]

$$\begin{aligned} \left| \int_{x-1/n}^{x+1/n} \frac{r_n(t)}{|x-t|^p} dt \right| &\leq 2 \sum_{k=0}^{p-2} \frac{|r_n^{(k)}(x)|}{|k+1-p|k!n^{k+1-p}} + 2 \frac{|r_n^{(p-1)}(x)|}{(p-1)!} \ln n \\ &\quad + \frac{2}{(p-1)!} \int_0^{1/n} t^{-p} \int_x^{x+t} (t+x-u)^{p-1} r_n^{(p)}(u) du dt \\ &\leq 2 \|f^{(s)}\|_\infty n^{p-1-s} \left(\sum_{\substack{k=0 \\ k \neq p-1}}^p \frac{\varepsilon_{k,n}}{|k+1-p|k!} + \frac{\varepsilon_{p-1,n} \ln n}{(p-1)!} \right) \end{aligned}$$

uniformly for all x . A similar calculation for $p \notin \mathbb{N}$ yields uniformly

$$\left| \int_{x-1/n}^{x+1/n} \frac{r_n(t)}{|x-t|^p} dt \right| \leq 2 \|f^{(s)}\|_{\infty} n^{p-1-s} \sum_{k=0}^{\lfloor p \rfloor} \frac{\varepsilon_{k,n}}{|k+1-p|k!}.$$

Adding up these estimates, we obtain

$$\|H_p[f] - H_p[J_n[f]]\|_{\infty} \leq \|f^{(s)}\|_{\infty} n^{p-1-s} \gamma_{p,n}, \quad (2)$$

$$\gamma_{p,n} = \begin{cases} 4\varepsilon_{0,n}/(p-1) + 2 \sum_{k=1}^{\lfloor p \rfloor} \frac{\varepsilon_{k,n}}{|k+1-p|k!} & \text{if } p \notin \mathbb{N}, \\ 4\varepsilon_{0,n} \ln n + 2(\varepsilon_{1,n} + \varepsilon_{0,n} \ln(b-a)) & \text{if } p = 1, \\ 4\varepsilon_{0,n}/(p-1) + 2 \sum_{k=1, k \neq p-1}^p \frac{\varepsilon_{k,n}}{|k+1-p|k!} + \frac{2\varepsilon_{p-1,n}}{(p-1)!} \ln n & \text{if } p \in \mathbb{N} \setminus \{1\}, \end{cases} \quad (3)$$

and the claim for H_p follows. With respect to H_p^* , we proceed similarly. \square

Proof of Theorem 1. For our nodal spline operators, relation (1) holds with $\varepsilon_{k,n} = O(1)$ for all $k \leq s$ [5, Corollary 3.1], so the claim follows from Theorem 2.

For not-a-knot splines, (1) holds with $\varepsilon_{k,n} = O(1)$ for $k \leq s = d+1$ [15, Lemma 1]. Using the idea of [2, Proof of Lemma 3.3], we see that this also holds for $s = 0, 1, 2, \dots, d$. So, applying Theorem 2, we derive this case too.

For the quasi-interpolatory splines, property (1) with $\varepsilon_{k,n} = O(1)$ is also known [2, Lemma 3.2], and Theorem 2 again yields the desired result. \square

Remark 3. We have only considered splines with uniform partitions. This condition can be relaxed to allow, e.g., for more nodes in certain subintervals. This may lead to larger $\varepsilon_{k,n}$, but Theorem 2 is still applicable, thus giving error bounds for the quadrature problem. Typically [2, 4], we have $\varepsilon_{k,n} = O((n\Delta_n)^{s-k})$ where Δ_n is the maximum distance of consecutive knots.

Remark 4. If precise values or sharp bounds for $\varepsilon_{k,n}$ are known, we can use (2) and (3) to determine upper bounds for the asymptotic constants implicitly contained in the O -terms of Theorem 1. Then, by comparing these constants, one may decide which formula to use. However, all rules based on spline interpolation have very similar error constants [1], and they are all close to the (often unknown) optimal method. We may thus expect only small differences in the quality of the various spline-based algorithms.

Remark 5. Theorem 2 can be used for methods not relying on splines too. For polynomial interpolation, we can find nodes satisfying (1) with $\varepsilon_{k,n} = O(\ln n)$ [12] to get quadrature rules for H_p with error bounds being close to optimal. They compare favourably with known polynomial-based methods [9, 13].

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