Calcolo (2022) 59:7
https://doi.org/10.1007/s10092-021-00446-1

PVTSI$^{(m)}$: A novel approach to computation of Hadamard finite parts of nonperiodic singular integrals

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Received: 15 August 2021 / Revised: 15 August 2021 / Accepted: 21 October 2021

Abstract
We consider the numerical computation of $I[f] = \;=\!\!\!\!\!\!\int_a^b f(x)\,dx$, the Hadamard finite part of the finite-range singular integral $\int_a^b f(x)\,dx$, $f(x) = g(x)/(x-t)^m$ with $a < t < b$ and $m \in \{1, 2, \ldots\}$, assuming that (i) $g \in C^\infty(a, b)$ and (ii) $g(x)$ is allowed to have arbitrary integrable singularities at the endpoints $x = a$ and $x = b$. We first prove that $=\!\!\!\!\!\!\int_a^b f(x)\,dx$ is invariant under any legitimate variable transformation $x = \psi(\xi)$, $\psi : [\alpha, \beta] \to [a, b]$, hence there holds $=\!\!\!\!\!\!\int_\alpha^\beta F(\xi)\,d\xi = \;=\!\!\!\!\!\!\int_a^b f(x)\,dx$, where $F(\xi) = f(\psi(\xi))\,\psi'(\xi)$. Based on this result, we next choose $\psi(\xi)$ such that $\mathcal{F}(\xi)$, the $\mathcal{T}$-periodic extension of $F(\xi)$, $\mathcal{T} = \beta - \alpha$, is sufficiently smooth, and prove, with the help of some recent extension/generalization of the Euler–Maclaurin expansion, that we can apply to $=\!\!\!\!\!\!\int_\alpha^\beta F(\xi)\,d\xi$ the quadrature formulas derived for periodic singular integrals developed in an earlier work of the author: [A. Sidi, "Unified compact numerical quadrature formulas for Hadamard finite parts of singular integrals of periodic functions." *Calcolo,* 58, 2021. Article number 22]. We give a whole family of numerical quadrature formulas for $=\!\!\!\!\!\!\int_\alpha^\beta F(\xi)\,d\xi$ for each m, which we denote $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$. Letting $G(\xi) = (\xi - \tau)^m F(\xi)$, with $\tau \in (\alpha, \beta)$ determined from $t = \psi(\tau)$, and letting $h = \mathcal{T}/n$, for $m = 3$, for example, we have the three formulas

$$\widehat{T}^{(0)}_{3,n}[\mathcal{F}] = h \sum_{j=1}^{n-1} \mathcal{F}(\tau + jh) - \frac{\pi^2}{3}\,G'(\tau)\,h^{-1} + \frac{1}{6}\,G'''(\tau)\,h,$$

$$\widehat{T}^{(1)}_{3,n}[\mathcal{F}] = h \sum_{j=1}^{n} \mathcal{F}(\tau + jh - h/2) - \pi^2\,G'(\tau)\,h^{-1},$$

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Published online: 18 December 2021

$$\widehat{T}^{(2)}_{3,n}[\mathcal{F}] = 2h\sum_{j=1}^{n}\mathcal{F}(\tau + jh - h/2) - \frac{h}{2}\sum_{j=1}^{2n}\mathcal{F}(\tau + jh/2 - h/4).$$

We show that all of the formulas $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ converge to $I[f]$ as $n \to \infty$; indeed, if $\psi(\xi)$ is chosen such that $\mathcal{F}^{(i)}(\alpha) = \mathcal{F}^{(i)}(\beta) = 0$, $i = 0, 1, \ldots, q-1$, and $\mathcal{F}^{(q)}(\xi)$ is absolutely integrable in every closed interval not containing $\xi = \tau$, then

$$\widehat{T}^{(s)}_{m,n}[\mathcal{F}] - I[f] = O(n^{-q}) \quad \text{as } n \to \infty,$$

where q is a positive integer determined by the behavior of $g(x)$ at $x = a$ and $x = b$ and also by $\psi(\xi)$. As such, q can be increased arbitrarily (even to $q = \infty$, thus inducing spectral convergence) by choosing $\psi(\xi)$ suitably. We provide several numerical examples involving nonperiodic integrands and confirm our theoretical results.

Keywords Hadamard finite part · Singular integrals · Hypersingular integrals · Supersingular integrals · Euler–Maclaurin expansions · Asymptotic expansions · Variable transformation · Numerical quadrature · Trapezoidal rule

Mathematics Subject Classification 41A55 · 41A60 · 45B05 · 45E05 · 65B05 · 65B15 · 65D30 · 65D32

1 Introduction and background

Singular integrals $\int_a^b f(x)\,dx$ that do not exist in the regular sense but are defined in the sense of *Hadamard Finite Part (HFP)* arise in different areas of science and engineering, and the numerical computation of their HFPs, denoted

$$I[f] = \,=\!\!\!\!\!\!\int_a^b f(x)\,dx, \tag{1.1}$$

has been of considerable interest. Of special interest are the integrals $\int_a^b f(x)\,dx$, whose integrands are of the general form

$$f(x) = \frac{g(x)}{(x-t)^m}, \quad a < t < b, \quad m \in \{1, 2, \ldots\}. \tag{1.2}$$

The cases with $m = 1, 2, 3$ occur in many applications and they are known as *Cauchy Principal Value* integrals, *hypersingular* integrals, and *supersingular* integrals, respectively.[1] For the definition and properties of Hadamard Finite Part integrals, see the books by Davis and Rabinowitz [3], Evans [7], Krommer and Ueberhuber [11], and

[1] We reserve the notation $\int_a^b f(x)\,dx$ for integrals that exist in the regular sense. The notation used for the Hadamard Finite Part of the integral $\int_a^b f(x)\,dx$ is $=\!\!\!\!\!\!\int_a^b f(x)\,dx$ in general, while the accepted notation for the Cauchy Principal Value of the integral $\int_a^b f(x)\,dx$ is $-\!\!\!\!\!\!\int_a^b f(x)\,dx$.

Kythe and Schäferkotter [12], for example. Many numerical quadrature formulas for computing these three types of singular integrals can be found in the literature.

In the papers Sidi and Israeli [34] and Sidi [28,31,32], we derived and studied some interesting generalizations of the Euler–Maclaurin (E–M) expansion for singular integrals of the form described in (1.1)–(1.2), and we treated the special cases of $m = 1, 2, 3, 4$ in detail. Based on these generalized E–M expansions, we developed numerical quadrature formulas for the case in which the T-periodic extension of $f(x)$—which, we denote also by $f(x)$—is infinitely differentiable for all $x \in \mathbb{R}_t$, that is, $f \in C^\infty(\mathbb{R}_t)$, with

$$T = b - a, \quad \mathbb{R}_t = \mathbb{R} \setminus \{t + kT\}_{k=-\infty}^{\infty}. \tag{1.3}$$

All these quadrature formulas are very effective and enjoy *spectral* accuracy. In view of this, one may ask as to whether they will continue to be effective when the T-periodic extension of $f(x)$ fails to be infinitely differentiable on $\mathbb{R}_t$. This is precisely the issue we address in this work by relaxing considerably the condition that $f \in C^\infty(\mathbb{R}_t)$.

We assume throughout this work that $f(x)$ in (1.1) is as in

$$\begin{aligned} f(x) = \frac{g(x)}{(x-t)^m}, \quad a < t < b, \quad m \in \{1, 2, \dots\}, \\ g \in C^\infty(a, b), \quad g(x) \text{ integrable at } x = a \text{ and } x = b. \end{aligned} \tag{1.4}$$

We note first that $g(x)$ being integrable at $x = a$ and $x = b$ is the same as $f(x)$ being integrable at $x = a$ and $x = b$. Next, we note that we are *not* imposing on $g(x)$ [equivalently, on $f(x)$] differentiability or even continuity conditions at $x = a$ and $x = b$. Summarizing, the functions $f(x)$ treated in this work satisfy the following conditions:

(i) They are in $C^\infty((a, t) \cup (t, b))$,
(ii) They have a *nonintegrable polar singularity* at $x = t$, and
(iii) They are allowed to have *arbitrary integrable singularities* at $x = a$ and $x = b$.

Our approach to the numerical treatment of the integrals $\fint_a^b f(x)\,dx$ under (1.4) proceeds in three steps: (i) First, we periodize the integrands $f(x)$ in (1.4) in some sense by using suitable variable transformations. (ii) Next, we develop a further generalization of the E–M expansion derived in [26] to accommodate the HFP integrals of this work. (iii) Finally, on the basis of the new generalized E–M expansion, we apply the appropriate quadrature formulas developed in [28,31,34] on the transformed integrals.

There are, however, three major questions related to this approach that need to be addressed:

1. We know that, if $\int_a^b u(x)\,dx$ exists as a regular integral, a legitimate variable transformation will not change its value. Can we guarantee that this will be the case also for the HFP integrals $\fint_a^b f(x)\,dx$ considered here, which do not exist in the regular sense? This question is relevant since HFP integrals have most, but not all, of the properties of regular integrals and some properties that are quite

unusual. For example, they are invariant with respect to translation of the variable of integration x, but they are not necessarily invariant under a nonlinear or even linear scaling of x. To see this, let us consider the HFP integral $⨎_0^1 dx/x = 0$ given in Davis and Rabinowitz [3, p. 13].

- Following the *nonlinear* scaling variable transformation $x = y^2/2$, the resulting HFP integral is $2⨎_0^{\sqrt{2}} dy/y = \log 2$.
- Following the *linear* scaling variable transformation $x = 2y$, the resulting HFP integral is $⨎_0^{1/2} dy/y = -\log 2$.

The variable transformations we will be using are *nonlinear* scalings of x.

2. Does the variable transformation change the nature of the singularity at $x = t$? If so, in what way?
3. The quadrature formulas of [28,31,34] have spectral accuracy when $g \in C^\infty[a, b]$ and $f(x)$ is T-periodic and $f \in C^\infty(\mathbb{R}_t)$. Can we guarantee that they will be effective when either (i) the periodic extension of $f(x)$ is not infinitely differentiable on $\mathbb{R}_t$, or (ii) $g(x)$ is not infinitely differentiable, or differentiable at all, at $x = a$ and/or $x = b$?

The answer to the first question is yes if $g(x)$ is in $C^m(a, b)$ and is integrable at $x = a$ and $x = b$. We give a detailed proof of this (for all $m = 1, 2, \dots$) in Theorem 3.1 in Sect. 3. So far, it has been known that the HFP integrals we consider here are invariant only under a linear change of the integration variable; see [11, Theorem 1.4.3], for example. The invariance of $I[f]$ with $m = 1$ under variable transformations has been shown by Gakhov [8]. Thus, our Theorem 3.1 seems to be new for $m = 2, 3, \dots$.

The answer to the second question is no, as we show again in Sect. 3; the singularity in the transformed integrand remains a pole of order m because $a < t < b$.

The answer to the third question is yes provided we use suitable variable transformations, and this is the subject of Theorem 5.2 in Sect. 5.

In Sect. 2, we give a brief description of the quadrature methods developed in [31] for the singular integrals in (1.1), in case $f(x)$ is T-periodic and infinitely differentiable for all x, except at $x = t + kT$, $k = 0, \pm1, \pm2, \dots$. In Sect. 3, we provide a detailed analysis of the singular integrals in (1.1) and (1.4) under legitimate variable transformations. In Sect. 4, we discuss the issue of periodization of the integrand $f(x)$ via suitable variable transformations and explore the analytical behavior of the transformed integrand in detail. In Sect. 5, we develop the quadrature formulas of this work for the nonperiodic singular integrals in (1.1), where the integrands $f(x)$ are as in (1.4). These formulas are based on a refined asymptotic analysis of the transformed integrand, followed by the application of Theorem A.2 in the appendix to this work that extends a generalized Euler–Maclaurin expansion due to the author given in [26]. We note that this appendix forms an integral part of this work. We will refer to the approach leading to the quadrature formulas thus developed as *Periodizing Variable Transformed Singular Integration* and will denote it *PVTSI*$^{(m)}$ for short. Finally, in Sect. 6, we provide numerical examples that illustrate the use of PVTSI$^{(m)}$ with $m = 1, 2, 3$ and confirm the theoretical results of this paper.

Before ending this section, we would like to recall that variable transformations have been used in the development of trapezoidal-like quadrature formulas for the Hadamard finite part integrals we consider here by Elliott [5] for the case $m = 1$, by Elliott and Venturino [6] and by Choi, Kim, and Yun [2] for the cases $m = 1, 2$. The quadrature formulas in these papers are then modeled after the work of Lyness [13] for Cauchy principal value integrals, namely, these papers apply the offset trapezoidal rule to the transformed integral with special correction terms to take care of the point of singularity when an abscissa in the trapezoidal sum coincides with the point of singularity. In this work, we take a completely different approach that avoids the point of singularity $x = t$ altogether. Our approach provides a rigorous unified treatment, both theoretical and numerical, for *all* $m = 1, 2, \ldots$.

Finally, we note the following facts concerning the Riemann Zeta function $\zeta(z)$, which we will need later:

$$\zeta(-2k) = 0, \quad k = 1, 2, \ldots; \quad \zeta(2k) = (-1)^{k+1}\frac{(2\pi)^{2k}}{2(2k)!}B_{2k} > 0, \quad k = 0, 1, \ldots.$$

Here B_s are the Bernoulli numbers.

2 Review of numerical quadrature formulas for periodic singular integrals

2.1 Review of numerical quadrature formulas for arbitrary *m*

In [31], we developed the following numerical quadrature formulas for the HFP integrals $⨍_a^b f(x)\,dx$, where $f(x)$ are as in (1.2) with arbitrary integer m, are T-periodic and belong to $C^\infty(\mathbb{R}_t)$, with T and $\mathbb{R}_t$ as in (1.3):

- For even m, $m = 2r$, $r = 1, 2, \ldots$, and with $h = T/n$, we have

$$\widehat{T}^{(0)}_{2r,n}[f] = h\sum_{j=1}^{n-1} f(t + jh) - 2\sum_{i=0}^{r} \frac{g^{(2i)}(t)}{(2i)!}\,\zeta(2r-2i)\,h^{-2r+2i+1}. \tag{2.1}$$

- For odd m, $m = 2r + 1$, $r = 0, 1, \ldots$, and with $h = T/n$, we have

$$\widehat{T}^{(0)}_{2r+1,n}[f] = h\sum_{j=1}^{n-1} f(t + jh) - 2\sum_{i=0}^{r} \frac{g^{(2i+1)}(t)}{(2i+1)!}\,\zeta(2r-2i)\,h^{-2r+2i+1}. \tag{2.2}$$

We also proved that, as $n \to \infty$, $\widehat{T}^{(0)}_{m,n}[f] \to I[f]$ spectrally, that is,

$$\widehat{T}^{(0)}_{m,n}[f] - I[f] = o(n^{-\mu}) \quad \text{as } n \to \infty \quad \forall \mu > 0. \tag{2.3}$$

In addition, we showed that, with the $\widehat{T}^{(0)}_{m,n}[f]$ available, we can construct the numerical quadrature formulas $\widehat{T}^{(s)}_{m,n}[f]$, $s = 1, 2, \ldots, \lfloor\frac{m+2}{2}\rfloor$, by performing s steps of a

"Richardson-like extrapolation" process on the relevant sequences $\{\widehat{T}^{(0)}_{m,2^kn}[f]\}_{k=0}^{s}$, by which we eliminate the powers $h^1, h^{-1}, h^{-3}, \ldots,$ in this order, from $\widehat{T}^{(0)}_{m,n}[f]$. This also amounts to eliminating the $g^{(p)}(t)$ from $\widehat{T}^{(0)}_{m,n}[f]$ one by one, starting from the highest order derivative and down. Thus, we eliminate $g^{(m)}(t), g^{(m-2)}(t), \ldots, g^{(2)}(t), g^{(0)}(t)$, for even m and $g^{(m)}(t), g^{(m-2)}(t), \ldots, g^{(3)}(t), g^{(1)}(t)$ for odd m. For example, with $s = 1, 2, 3$, we have

$$\begin{aligned}
\widehat{T}^{(1)}_{m,n}[f] &= 2\widehat{T}^{(0)}_{m,2n}[f] - \widehat{T}^{(0)}_{m,n}[f],\\
\widehat{T}^{(2)}_{m,n}[f] &= 2\widehat{T}^{(1)}_{m,n}[f] - \widehat{T}^{(1)}_{m,2n}[f]\\
&= -2\widehat{T}^{(0)}_{m,n}[f] + 5\widehat{T}^{(0)}_{m,2n}[f] - 2\widehat{T}^{(0)}_{m,4n}[f],\\
\widehat{T}^{(3)}_{m,n}[f] &= \frac{8}{7}\widehat{T}^{(2)}_{m,n}[f] - \frac{1}{7}\widehat{T}^{(2)}_{m,2n}[f]\\
&= \frac{16}{7}\widehat{T}^{(1)}_{m,n}[f] - \frac{10}{7}\widehat{T}^{(1)}_{m,2n}[f] + \frac{2}{7}\widehat{T}^{(1)}_{m,4n}[f]\\
&= -\frac{16}{7}\widehat{T}^{(0)}_{m,n}[f] + 6\widehat{T}^{(0)}_{m,2n}[f] - 3\widehat{T}^{(0)}_{m,4n}[f] + \frac{2}{7}\widehat{T}^{(0)}_{m,8n}[f].
\end{aligned}$$

In general, eliminating only the powers $h^1, h^{-1}, h^{-3}, \ldots, h^{-2s+3}$, we have

$$\widehat{T}^{(s)}_{m,n}[f] = \sum_{k=0}^{s} \alpha^{(s)}_{m,k}\widehat{T}^{(0)}_{m,2^kn}[f], \quad \sum_{k=0}^{s}\alpha^{(s)}_{m,k} = 1; \quad \alpha^{(s)}_{m,k} \text{ independent of } n. \tag{2.4}$$

Concerning the formulas $\widehat{T}^{(s)}_{m,n}[f]$, we have the following general convergence theorem:

Theorem 2.1 *If $f(x)$ is as in (1.2), T-periodic, and infinitely differentiable for all $x \in \mathbb{R}_t$, then all the numerical quadrature formulas $\widehat{T}^{(s)}_{m,n}[f]$ in (2.4) converge to $I[f] = \oint_a^b f(x)\,dx$ with spectral accuracy, namely,*

$$\widehat{T}^{(s)}_{m,n} - I[f] = o(n^{-\mu}) \quad \text{as } n \to \infty \quad \forall\, \mu > 0. \tag{2.5}$$

In words, the errors $\widehat{T}^{(s)}_{m,n}[f] - I[f]$ tend to zero as $n \to \infty$ faster than every negative power of n.

2.2 Review of the cases $m = 1, 2, 3, 4$

For $m = 1, 2, 3, 4$ the formulas above assume the following specific forms:

1. The case $m = 1$:

$$\widehat{T}^{(0)}_{1,n}[f] = h\sum_{j=1}^{n-1} f(t + jh) + g'(t)h, \tag{2.6a}$$

$$\widehat{T}^{(1)}_{1,n}[f] = h\sum_{j=1}^{n} f(t + jh - h/2). \tag{2.6b}$$

2. The case $m = 2$:

$$\widehat{T}^{(0)}_{2,n}[f] = h\sum_{j=1}^{n-1} f(t + jh) - \frac{\pi^2}{3}g(t)h^{-1} + \frac{1}{2}g''(t)h, \tag{2.7a}$$

$$\widehat{T}^{(1)}_{2,n}[f] = h\sum_{j=1}^{n} f(t + jh - h/2) - \pi^2 g(t)h^{-1}, \tag{2.7b}$$

$$\widehat{T}^{(2)}_{2,n}[f] = 2h\sum_{j=1}^{n} f(t + jh - h/2) - \frac{h}{2}\sum_{j=1}^{2n} f(t + jh/2 - h/4). \tag{2.7c}$$

3. The case $m = 3$:

$$\widehat{T}^{(0)}_{3,n}[f] = h\sum_{j=1}^{n-1} f(t + jh) - \frac{\pi^2}{3}g'(t)h^{-1} + \frac{1}{6}g'''(t)h, \tag{2.8a}$$

$$\widehat{T}^{(1)}_{3,n}[f] = h\sum_{j=1}^{n} f(t + jh - h/2) - \pi^2 g'(t)h^{-1}, \tag{2.8b}$$

$$\widehat{T}^{(2)}_{3,n}[f] = 2h\sum_{j=1}^{n} f(t + jh - h/2) - \frac{h}{2}\sum_{j=1}^{2n} f(t + jh/2 - h/4). \tag{2.8c}$$

4. *The case* $m = 4$:

$$\widehat{T}^{(0)}_{4,n}[f] = h\sum_{j=1}^{n-1} f(t + jh) - \frac{\pi^4}{45}g(t)h^{-3} - \frac{\pi^2}{6}g''(t)h^{-1} + \frac{1}{24}g^{(4)}(t)h, \tag{2.9a}$$

$$\widehat{T}^{(1)}_{4,n}[f] = h\sum_{j=1}^{n} f(t + jh - h/2) - \frac{\pi^4}{3}g(t)h^{-3} - \frac{\pi^2}{2}g''(t)h^{-1}, \tag{2.9b}$$

$$\widehat{T}^{(2)}_{4,n}[f] = 2h\sum_{j=1}^{n} f(t + jh - h/2) - \frac{h}{2}\sum_{j=1}^{2n} f(t + jh/2 - h/4) + 2\pi^4 g(t)h^{-3}, \tag{2.9c}$$

$$\widehat{T}^{(3)}_{4,n}[f] = \frac{16h}{7}\sum_{j=1}^{n} f(t + jh - h/2) - \frac{5h}{7}\sum_{j=1}^{2n} f(t + jh/2 - h/4) + \frac{h}{28}\sum_{j=1}^{4n} f(t + jh/4 - h/8). \tag{2.9d}$$

These formulas are derived and studied in [34] (for $m = 1$), in [28,29] (for $m = 1, 2$), and in [31,32] (for $m = 3$). Concerning all the formulas with $m = 1, 2, 3, 4$, we have the following convergence theorem (see Sidi [33]) that strengthens Theorem 2.1:

Theorem 2.2 *If $f(z)$ is both T-periodic and analytic in a strip D_σ of the complex z-plane,*

$$D_\sigma = \{z \in \mathbb{C} : |\mathbf{Im} z| < \sigma\},$$

then, for $m = 1, 2, 3, 4$, we have

$$\widehat{T}^{(s)}_{m,n} - I[f] = O(e^{-2n\pi\rho/T}) \quad \text{as } n \to \infty, \quad \forall \rho < \sigma. \tag{2.10}$$

Thus, practically speaking, we have

$$\widehat{T}^{(s)}_{m,n} - I[f] = O(e^{-2n\pi\sigma/T}) \quad \text{as } n \to \infty.$$

3 Variable transformations and singular integrals

Theorem 3.1 that follows shows that the HFP integrals in (1.4) are invariant under a variable transformation $x = \psi(\xi)$ provided $g(x)$ and $\psi(\xi)$ have enough continuous derivatives.

Theorem 3.1 *Let m be a positive integer, and let*

$$f(x) = \frac{g(x)}{(x-t)^m}, \quad a < t < b, \quad g \in C^m(a,b), \quad g(x) \text{ integrable at } x = a \text{ and } x = b, \tag{3.1}$$

and let the variable transformation $x = \psi(\xi)$ be such that

$$\begin{aligned} &\psi : [\alpha, \beta] \to [a, b]; \quad \psi(\alpha) = a, \quad \psi(\beta) = b, \\ &\psi \in C^m[\alpha, \beta]; \quad \psi'(\xi) > 0 \ \text{ for } \alpha < \xi < \beta. \end{aligned} \tag{3.2}$$

Then

$$\neq\!\!\!\!\!\!\int_\alpha^\beta f(\psi(\xi))\, \psi'(\xi)\, d\xi = \neq\!\!\!\!\!\!\int_a^b f(x)\, dx \quad \text{independent of } \psi(\xi). \tag{3.3}$$

Remark 1. The differentiability conditions imposed on $g(x)$ and $\psi(\xi)$ seem to be minimal possible. Of course, the theorem is correct also when $g \in C^p(a,b)$ and $\psi \in C^q[\alpha,\beta]$, for all $p, q \geq m$. The result for $m = 1$ (Cauchy Principal Value) is not new; see Gakhov [8, p. 17]; we provide a proof of this case for completeness.

2. Let us denote the transformed integrand by $F(\xi)$, that is,

$$F(\xi) = f(\psi(\xi))\,\psi'(\xi). \tag{3.4}$$

It is easy to see that $F(\xi)$ has the same kind of singularity structure as $f(x)$; actually, $F(\xi)$ is of the form

$$F(\xi) = \frac{G(\xi)}{(\xi-\tau)^m}, \quad G(\xi) = \frac{g(\psi(\xi))}{(\psi[\xi,\tau])^m}\,\psi'(\xi),$$
$$\psi[\xi,\tau] = \frac{\psi(\xi)-\psi(\tau)}{\xi-\tau} \neq 0 \quad \text{for } \xi \neq \tau, \quad \psi[\tau,\tau] = \psi'(\tau) > 0, \tag{3.5}$$

$\tau \in (\alpha,\beta)$ being the unique solution of the equation $t = \psi(\xi)$ for ξ since $\psi'(\xi) > 0$ on (α,β).[2] Consequently, we also have

$$G(\tau) = \frac{g(\psi(\tau))}{[\psi'(\tau)]^{m-1}} = \frac{g(t)}{[\psi'(\tau)]^{m-1}}. \tag{3.6}$$

As for $G^{(i)}(\tau)$, $i \geq 1$, these can be obtained by differentiating $G(\xi)$ in (3.5) and letting $\xi \to \tau$. Thus,

$$G'(\tau) = \frac{g'(t)}{[\psi'(\tau)]^{m-2}} + \left(1 - \frac{m}{2}\right)\frac{g(t)\psi''(\tau)}{[\psi'(\tau)]^m}, \tag{3.7}$$

for example. It is clear that $G^{(i)}(\tau)$ involves $g^{(r)}(t)$, $r = 0, 1, \ldots, i$.

3. We recall that if $u(x)$ has a nonintegrable singularity at $x = t$ for $t \in (a,b)$ but is integrable on any subinterval of (a,b) that does not contain $x = t$, then $\,=\!\!\!\!\!\!\int_a^b u(x)\,dx$ is obtained by expanding

$$\phi(\epsilon) = \int_a^{t-\epsilon} u(x)\,dx + \int_{t+\epsilon}^b u(x)\,dx, \quad \epsilon > 0,$$

asymptotically as $\epsilon \to 0$, discarding those terms that go to infinity, and retaining the limit of the remaining terms, as $\epsilon \to 0$. (See Monegato [15], for example.)

Proof Let us express $f(x)$ in the form

$$f(x) = w(x) + \sum_{i=0}^{m-1} \frac{g^{(i)}(t)}{i!}\,\frac{1}{(x-t)^{m-i}},$$

[2] Given $t \in (a,b)$, we can determine τ as the solution to the equation $\theta(\xi) = 0$ with $\theta(\xi) = \psi(\xi) - t$, which can be achieved by using the Newton–Raphson method, for example. For some of the variable transformations we present later in Sect. 4.3, given t, τ is readily available, however.

where

$$w(x) = \frac{g(x) - \sum_{i=0}^{m-1} \frac{g^{(i)}(t)}{i!}(x-t)^i}{(x-t)^m} \quad \text{when } x \neq t, \quad w(t) = \frac{g^{(m)}(t)}{m!}.$$

Clearly, $w(x)$ is continuous on (a, b) and integrable at $x = a$ and $x = b$.

Now, for each $t \in (a, b)$, there is a unique $\tau \in (\alpha, \beta)$ such that $t = \psi(\tau)$, as already explained above. Therefore,

$$\begin{aligned} \neq\!\!\!\!\!\!\int_{\alpha}^{\beta} f(\psi(\xi))\, \psi'(\xi)\, d\xi &= \neq\!\!\!\!\!\!\int_{\alpha}^{\beta} w(\psi(\xi))\, \psi'(\xi)\, d\xi \\ &\quad + \sum_{i=0}^{m-1} \frac{g^{(i)}(t)}{i!} \neq\!\!\!\!\!\!\int_{\alpha}^{\beta} \frac{\psi'(\xi)}{(\psi(\xi) - \psi(\tau))^{m-i}}\, d\xi. \end{aligned} \tag{3.8}$$

First, because $w(x)$ is continuous on (a, b) and integrable at $x = a$ and $x = b$, we have that $w(\psi(\xi))\psi'(\xi)$ is continuous on (α, β) and integrable at $\xi = \alpha$ and $\xi = \beta$. Consequently,

$$\neq\!\!\!\!\!\!\int_{\alpha}^{\beta} w(\psi(\xi))\, \psi'(\xi)\, d\xi = \int_{\alpha}^{\beta} w(\psi(\xi))\, \psi'(\xi)\, d\xi = \int_{a}^{b} w(x)\, dx. \tag{3.9}$$

Next, for $k = 1, 2, \ldots, m$, let us consider

$$\phi_k(\epsilon) = \int_{\alpha}^{\tau-\epsilon} \frac{\psi'(\xi)}{(\psi(\xi) - \psi(\tau))^k}\, d\xi + \int_{\tau+\epsilon}^{\beta} \frac{\psi'(\xi)}{(\psi(\xi) - \psi(\tau))^k}\, d\xi. \tag{3.10}$$

In what follows, we make repeated use of the facts that $\psi(\alpha) = a$, $\psi(\beta) = b$, and $\psi(\tau) = t$.

For $k = 1$, we have

$$\phi_1(\epsilon) = \log\left|\frac{\psi(\tau - \epsilon) - \psi(\tau)}{\psi(\alpha) - \psi(\tau)}\right| + \log\left|\frac{\psi(\beta) - \psi(\tau)}{\psi(\tau + \epsilon) - \psi(\tau)}\right|,$$

hence

$$\phi_1(\epsilon) = \log\left|\frac{b - t}{a - t}\right| + \Lambda_1(\epsilon),$$

where

$$\Lambda_1(\epsilon) = \log\left|\frac{\psi(\tau - \epsilon) - \psi(\tau)}{\psi(\tau + \epsilon) - \psi(\tau)}\right|.$$

Application of L'Hôpital's rule results in $\lim_{\epsilon\to 0+}\Lambda_1(\epsilon)=0$. Thus,

$$\ne\!\!\!\!\!\!\int_{\alpha}^{\beta}\frac{\psi'(\xi)}{\psi(\xi)-\psi(\tau)}\,d\xi=\log\left|\frac{b-t}{a-t}\right|, \tag{3.11}$$

independent of $\psi(\xi)$.

For $k=2,3,\ldots,m$, we have

$$\begin{aligned}\phi_k(\epsilon)=-\frac{1}{k-1}\Bigg\{&\left[\frac{1}{(\psi(\tau-\epsilon)-\psi(\tau))^{k-1}}-\frac{1}{(\psi(\alpha)-\psi(\tau))^{k-1}}\right]\\&+\left[\frac{1}{(\psi(\beta)-\psi(\tau))^{k-1}}-\frac{1}{(\psi(\tau+\epsilon)-\psi(\tau))^{k-1}}\right]\Bigg\},\end{aligned}$$

hence

$$\phi_k(\epsilon)=\frac{1}{k-1}\left[\frac{1}{(a-t)^{k-1}}-\frac{1}{(b-t)^{k-1}}\right]+\Lambda_k(\epsilon),$$

where

$$\Lambda_k(\epsilon)=\frac{1}{k-1}\left[\frac{1}{(\psi(\tau+\epsilon)-\psi(\tau))^{k-1}}-\frac{1}{(\psi(\tau-\epsilon)-\psi(\tau))^{k-1}}\right].$$

Since $2\le k\le m$, $\psi\in C^k[\alpha,\beta]$. By the fact that $\psi'(\tau)>0$, there exists a function $\theta(\eta)\in C^{k-1}(I)$, where $I=(-\rho,\rho)$ with $\rho\le\min\{\beta-\tau,\tau-\alpha\}$, such that

$$\psi(\tau+\eta)-\psi(\tau)\equiv\eta\,\theta(\eta),\quad \theta(0)=\psi'(\tau)>0.$$

Consequently,

$$\Lambda_k(\epsilon)=\epsilon^{-k+1}[M_k(\epsilon)+(-1)^kM_k(-\epsilon)];\quad M_k(\eta)=\frac{1}{k-1}\frac{1}{[\theta(\eta)]^{k-1}}\in C^{k-1}(I).$$

Expanding in a Taylor series about $\epsilon=0$, we obtain

$$\begin{aligned}\Lambda_k(\epsilon)&=\epsilon^{-k+1}\left\{\left[\sum_{i=0}^{k-2}c_i\epsilon^i+c_{k-1}^{+}\epsilon^{k-1}\right]+(-1)^k\left[\sum_{i=0}^{k-2}(-1)^ic_i\epsilon^i+(-1)^{k-1}c_{k-1}^{-}\epsilon^{k-1}\right]\right\}\\&=\sum_{i=0}^{k-2}[1+(-1)^{k+i}]c_i\epsilon^{-k+i+1}+(c_{k-1}^{+}-c_{k-1}^{-})\epsilon^0,\end{aligned}$$

where

$$c_i=\frac{M_k^{(i)}(0)}{i!};\quad c_{k-1}^{\pm}=\frac{M_k^{(k-1)}(\eta^{\pm})}{(k-1)!},\quad \eta^{\pm}\text{ between 0 and }\pm\epsilon.$$

The sum $\sum_{i=0}^{k-2}[1+(-1)^{k+i}]c_i\epsilon^{-k+i+1}$ gives a linear combination of the following (odd) powers of ϵ:

$$\epsilon^{-\hat{k}}, \epsilon^{-\hat{k}+2}, \epsilon^{-\hat{k}+4}, \ldots, \epsilon^{-3}, \epsilon^{-1}; \quad \hat{k} = \begin{cases} k-2 & \text{if } k \text{ odd} \\ k-1 & \text{if } k \text{ even} \end{cases}.$$

Since each of these powers tends to infinity as $\epsilon \to 0+$, we discard them all. The remaining term, namely,

$$(c_{k-1}^{+} - c_{k-1}^{-})\epsilon^0 = \left[\frac{M_k^{(k-1)}(\eta^+)}{(k-1)!} - \frac{M_k^{(k-1)}(\eta^-)}{(k-1)!}\right]\epsilon^0,$$

tends to zero as $\epsilon \to 0$ because $\lim_{\epsilon\to 0}\eta^{\pm} = 0$ and $M_k^{(k-1)}(\eta)$ is continuous in I. Thus, we have shown that $\Lambda_k(\epsilon)$ has zero contribution to $\oint_\alpha^\beta \frac{\psi'(\xi)}{(\psi(\xi)-\psi(\tau))^k}\,d\xi$. Therefore, we have

$$\oint_\alpha^\beta \frac{\psi'(\xi)}{(\psi(\xi)-\psi(\tau))^k}\,d\xi = \frac{1}{k-1}\left[\frac{1}{(a-t)^{k-1}} - \frac{1}{(b-t)^{k-1}}\right], \quad k = 2, 3, \ldots, m, \tag{3.12}$$

independent of $\psi(\xi)$.

Substituting (3.9), (3.11), and (3.12) in (3.8), we obtain

$$\begin{aligned}\oint_\alpha^\beta f(\psi(\xi))\,\psi'(\xi)\,d\xi = \int_a^b w(x)\,dx + \frac{g^{(m-1)}(t)}{(m-1)!}\log\left|\frac{b-t}{a-t}\right| \\ + \sum_{i=0}^{m-2}\frac{g^{(i)}(t)}{i!}\frac{1}{m-i-1}\left[\frac{1}{(a-t)^{m-i-1}} - \frac{1}{(b-t)^{m-i-1}}\right],\end{aligned}$$

independent of $\psi(\xi)$. This completes the proof. □

Theorem 3.1 continues to hold when $f(x) = g(x)/|x-t|^s$, if $s \geq 1$ and s is not an integer. It also holds when s is an even integer since $|x-t|^s = (x-t)^s$ in this case, which we have already covered in Theorem 3.1. It does *not* hold when $s \geq 1$ and s is an odd integer, however. These facts are the subject of the next two theorems, which we include for completeness. These theorems can be proved using the technique employed in proving Theorem 3.1.

Theorem 3.2 *Let $s > 1$ such that s is not an integer, let $m = \lceil s \rceil$, and let*

$$f(x) = \frac{g(x)}{|x-t|^s}, \quad a < t < b, \quad g \in C^m(a,b), \quad g(x) \text{ integrable at } x = a \text{ and } x = b, \tag{3.13}$$

and let the variable transformation $x = \psi(\xi)$ *be as in Theorem 3.1. Then*

$$\fint_{\alpha}^{\beta} f(\psi(\xi))\,\psi'(\xi)\,d\xi = \fint_{a}^{b} f(x)\,dx \quad \textit{independent of } \psi(\xi). \tag{3.14}$$

Theorem 3.3 *Let* $m \geq 1$ *be an odd integer and*

$$f(x) = \frac{g(x)}{|x-t|^m}, \quad a < t < b, \quad g \in C^m(a,b), \quad g(x) \textit{ integrable at } x = a \textit{ and } x = b, \tag{3.15}$$

and let the variable transformation $x = \psi(\xi)$ *be as in Theorem 3.1. Then, in general,*

$$\fint_{\alpha}^{\beta} f(\psi(\xi))\,\psi'(\xi)\,d\xi \neq \fint_{a}^{b} f(x)\,dx. \tag{3.16}$$

For example, when $m = 1$*, we have*

$$\fint_{\alpha}^{\beta} f(\psi(\xi))\,\psi'(\xi)\,d\xi = \fint_{a}^{b} f(x)\,dx - 2g(t)\log\psi'(\tau), \tag{3.17}$$

where

$$\fint_{a}^{b} f(x)\,dx = \int_{a}^{b} \frac{g(x)-g(t)}{|x-t|}\,dx + g(t)\log\big|(a-t)(b-t)\big|. \tag{3.18}$$

4 Periodization of $F(\xi)$ via variable transformations

4.1 Preliminaries

In view of Theorem 3.1, with $\psi(\xi)$ as in (3.2), we have

$$I[f] = \fint_{a}^{b} f(x)\,dx = \fint_{\alpha}^{\beta} F(\xi)\,d\xi = I[F], \quad F(\xi) = f(\psi(\xi))\,\psi'(\xi). \tag{4.1}$$

We now aim to choose $\psi(\xi)$ so as to periodize the transformed integrand $F(\xi)$ in the sense that

$$F^{(i)}(\alpha) = F^{(i)}(\beta), \quad i = 0, 1, \ldots, q-1, \quad \text{for some integer } q.$$

The easiest way of achieving this goal is by choosing $\psi(\xi)$ such that

$$\psi^{(i)}(\alpha) = \psi^{(i)}(\beta) = 0, \quad i = 1, 2, \ldots, r, \quad \text{for some integer } r. \tag{4.2}$$

Provided r is sufficiently large, this will periodize $F(\xi)$ in the sense that

$$F^{(i)}(\alpha) = 0 = F^{(i)}(\beta), \quad i = 0, 1, \ldots, q-1, \quad \text{for some integer } q. \tag{4.3}$$

To demonstrate this point, let us look at the following examples.

Example 4.1 In case $f(x)$ is sufficiently differentiable on $[a, b] \setminus \{t\}$, (4.2) will force (4.3) to be valid with $q = r$. Let us illustrate this for $r = 1, 2, 3$: We start with

$$F = f(\psi)\psi', \tag{4.4}$$

$$F' = f(\psi)\psi'' + f'(\psi)(\psi')^2, \tag{4.5}$$

$$F'' = f(\psi)\psi''' + 3f'(\psi)\psi'\psi'' + f''(\psi)(\psi')^3. \tag{4.6}$$

- For $r = 1$, that $F(\alpha) = F(\beta) = 0$ is obvious by (4.4) and by $\psi'(\alpha) = \psi'(\beta) = 0$ in (4.2).
- For $r = 2$, that $F^{(i)}(\alpha) = F^{(i)}(\beta) = 0$, $i = 0, 1$, is obvious by (4.4)–(4.5) and by $\psi^{(i)}(\alpha) = \psi^{(i)}(\beta) = 0$, $i = 1, 2$, in (4.2).
- For $r = 3$, that $F^{(i)}(\alpha) = F^{(i)}(\beta) = 0$, $i = 0, 1, 2$, is obvious by (4.4)–(4.6) and by $\psi^{(i)}(\alpha) = \psi^{(i)}(\beta) = 0$, $i = 1, 2, 3$, in (4.2).

It is now easy to see that, if $\psi(\xi)$ satisfies (4.2) with some r, we have that (4.3) is valid with $q = r$.
Clearly, $q = \infty$ when $r = \infty$. □

Example 4.2 In case $f(x)$ is not continuous or differentiable at $x = a$ and/or $x = b$ but is integrable there, we can still use the variable transformation $x = \psi(\xi)$ satisfying (4.2) and achieve (4.3), but with some $q < r$. To illustrate this point, let us consider $f(x) = (x-a)^c u_a(x) = (b-x)^c u_b(x)$, where $-1 < c < 0$ and $u_a(x)$ and $u_b(x)$ are such that $u_a(a) \neq 0$ and $u_b(b) \neq 0$ and are sufficiently differentiable on $[a, b) \setminus \{t\}$ and $(a, b] \setminus \{t\}$, respectively. [The fact that $c > -1$ guarantees that $f(x)$ is integrable at $x = a$ and $x = b$, as required in (1.4), even though $f(x)$ and all its derivatives are unbounded at $x = a$ and $x = b$ when $c < 0$.] Now, assuming that $\psi^{(r+1)}(\alpha) \neq 0$ and $\psi^{(r+1)}(\beta) \neq 0$,

$$\psi(\xi) - \psi(\alpha) \sim \frac{\psi^{(r+1)}(\alpha)}{(r+1)!}(\xi-\alpha)^{r+1}, \quad \psi'(\xi) \sim \frac{\psi^{(r+1)}(\alpha)}{r!}(\xi-\alpha)^r \quad \text{as } \xi \to \alpha+,$$

and

$$\psi(\xi) - \psi(\beta) \sim \frac{\psi^{(r+1)}(\beta)}{(r+1)!}(\xi-\beta)^{r+1}, \quad \psi'(\xi) \sim \frac{\psi^{(r+1)}(\beta)}{r!}(\xi-\beta)^r \quad \text{as } \xi \to \beta- .$$

Therefore, $F(\xi)$ satisfies the asymptotic equalities

$$F(\xi) \sim \begin{cases} M(\xi-\alpha)^\rho & \text{as } \xi \to \alpha+ \\ N(\beta-\xi)^\rho & \text{as } \xi \to \beta- \end{cases}, \quad \text{for some } M, N \neq 0, \quad \rho = c(r+1) + r.$$

Thus, $F(\xi)$ satisfies (4.3) with $q = \lceil \rho \rceil$, and $q \geq 1$ provided $r \geq (1-c)/(1+c)$, which can be accomplished by choosing $\psi(\xi)$ appropriately. When $c = -1/2$, for example, (4.3) holds with $q = \lceil \frac{r-1}{2} \rceil$.
Clearly, $q = \infty$ when $r = \infty$ in this example too. □

Remark Before going on, we would like to emphasize that variable transformations as described here will be useful only if $f(x)$ is *integrable* at the endpoints $x = a$ and $x = b$. If $f(x)$ has *nonintegrable* singularities at $x = a$ or $x = b$, then the transformed integrand $F(\xi)$ has *worse* singularities at $\xi = \alpha$ or $\xi = \beta$. We can verify this by letting $c < -1$ in Example 4.2, which causes $\rho < c$; for example, with $c = -3/2$, we have $\rho = c - r/2$.

In Sect. 4.3, we give examples of $\psi(\xi)$ with both r finite and $r = \infty$.

4.2 Consequences of periodization

The periodization of $F(\xi)$ as in (4.3) has important consequences, which we discuss next. With $\mathcal{T} = \beta - \alpha$, let us denote the $\mathcal{T}$-periodic extension of $F(\xi)$ by $\mathcal{F}(\xi)$. Thus,

$$\mathcal{F}(\xi) = F(\xi) \quad \text{if } \xi \in (\alpha, \beta) \quad \text{and} \quad \mathcal{F}(\xi + k\mathcal{T}) = \mathcal{F}(\xi), \quad k = 0, \pm 1, \pm 2, \dots. \tag{4.7}$$

As a result, for arbitrary $i = 0, 1, \dots,$

$$\mathcal{F}^{(i)}(\xi) = \begin{cases} F^{(i)}(\xi) & \text{if } \xi \in (\alpha, \beta), \\ F^{(i)}(\xi - \mathcal{T}) & \text{if } \xi \in (\beta, \beta + \mathcal{T}). \end{cases} \tag{4.8}$$

Therefore, with $\epsilon > 0$ and small,

$$\mathcal{F}^{(i)}(\beta - \epsilon) = F^{(i)}(\beta - \epsilon), \quad \mathcal{F}^{(i)}(\beta + \epsilon) = F^{(i)}(\alpha + \epsilon), \tag{4.9}$$

which, upon letting $\epsilon \to 0$, gives

$$\mathcal{F}^{(i)}(\beta-) = F^{(i)}(\beta), \quad \mathcal{F}^{(i)}(\beta+) = F^{(i)}(\alpha), \quad i = 0, 1, \dots, q-1, \tag{4.10}$$

which, by (4.3), leads to

$$\mathcal{F}^{(i)}(\beta-) = \mathcal{F}^{(i)}(\beta+) = 0, \;\; i = 0, 1, \dots, q-1 \;\; \Rightarrow \;\; \mathcal{F} \in C^{q-1} \text{ in a neighborhood of } \beta. \tag{4.11}$$

Thus, $\mathcal{F}(\xi)$, the $\mathcal{T}$-periodic extension of $F(\xi)$ that is defined for $\xi \in [\alpha, \beta]$ is in $C^{q-1}(\mathbb{R}_\tau)$, where, analogous to (1.3),

$$\mathcal{T} = \beta - \alpha, \quad \mathbb{R}_\tau = \mathbb{R} \setminus \{\tau + k\mathcal{T}\}_{k=-\infty}^{\infty}. \tag{4.12}$$

Remark It is clear from the examples we have given above that q increases with r. Because r is at our disposal, we may choose $\psi(\xi)$ such that (4.2) is satisfied with r

as large as we wish, including $r = \infty$. Thus, we can also make q as large as we wish, including $q = \infty$, forcing $\mathcal{F}(\xi)$ to be as smooth as we wish.

4.3 Examples of periodizing variable transformations

Variable transformations were originally developed and used for enhancing the accuracy of the trapezoidal rule approximations to finite-range integrals $\int_a^b \phi(x)\,dx$ defined in the regular sense.[3] There are different types of variable transformations; for surveys of these and their applications in numerical integration, see Beckers and Haegemans [1], Elliott [4], Monegato and Scuderi [16], and Sidi [21,23–25], Yun [37], and Yun and Kim [38], for example. Because we only wish to achieve (4.2) in this work, here we will mention, without going into much detail, only a few of those that have simple representations.

For all the transformations we mention next, we use the standard intervals $(a, b) = (0, 1)$ and $(\alpha, \beta) = (0, 1)$, and we will denote these by $\hat{\psi}(\xi)$ to emphasize this fact.[4]

Korobov [10]: $$\hat{\psi}(\xi) = \frac{\theta(\xi)}{\theta(1)}, \quad \theta(\xi) = \int_0^\xi [u(1-u)]^{p-1}\,du. \tag{4.13}$$

Sidi [21], [25]: $$\hat{\psi}(\xi) = \frac{\theta(\xi)}{\theta(1)}, \quad \theta(\xi) = \int_0^\xi (\sin \pi u)^{p-1}\,du. \tag{4.14}$$

Prösdorf and Rathsfeld [18]: $$\hat{\psi}(\xi) = \frac{\xi^p}{\xi^p + (1-\xi)^p}. \tag{4.15}$$

Sidi [24]: $$\hat{\psi}(\xi) = \frac{\left(\sin\frac{\pi\xi}{2}\right)^p}{\left(\sin\frac{\pi\xi}{2}\right)^p + \left(\cos\frac{\pi\xi}{2}\right)^p}. \tag{4.16}$$

Sag and Szekeres [20]: $$\hat{\psi}(\xi) = \frac{1}{2}\tanh\left(c\left(\frac{1}{1-\xi} - \frac{1}{\xi}\right)\right) + \frac{1}{2}, \quad c > 0. \tag{4.17}$$

Of course, by Theorem 3.1, with each of the transformations in (4.13)–(4.17), we have

$$\,\text{⨎}\!\!\int_0^1 f(x)\,dx = \text{⨎}\!\!\int_0^1 f(\hat{\psi}(\xi))\,\hat{\psi}'(\xi)\,d\xi, \quad f(x) = \frac{g(x)}{(x-t)^m}\,dx, \quad 0 < t < 1.$$

[3] Here we must emphasize that, in this work, we are using variable transformations for the sole purpose of achieving (4.3).

[4] In case $(a, b) \neq (0, 1)$, the variable transformation $\psi : [0, 1] \to [a, b]$ is simply $\psi(\xi) = a + (b-a)\hat{\psi}(\xi)$, hence $\text{⨎}\!\!\int_a^b f(x)\,dx = \text{⨎}\!\!\int_0^1 F(\xi)\,d\xi$, with $F(\xi) = f(\psi(\xi))\psi'(\xi) = (b-a)f(a + (b-a)\hat{\psi}(\xi))\hat{\psi}'(\xi)$.

For all the transformations in (4.13)–(4.17), we have

$$\hat{\psi}^{(i)}(0) = \hat{\psi}^{(i)}(1) = 0, \quad i = 1, \dots, r,$$

with (i) $r = p - 1$ in (4.13)–(4.16), p an integer, and (ii) $r = \infty$ in (4.17).

Remark 1. Note that p in (4.13)–(4.16) does not have to be chosen as an integer. It can be chosen as an integer or otherwise so as to optimize the quality of the quadrature approximations for regular integrals.

2. All five variable transformations we just mentioned satisfy

$$\hat{\psi}(1-\xi) = 1 - \hat{\psi}(\xi) \quad \text{and} \quad \hat{\psi}'(1-\xi) = \hat{\psi}'(\xi), \quad \xi \in [0, 1].$$

Clearly, $\hat{\psi}'(\xi)$ are symmetric with respect to $\xi = 1/2$, that is,

$$\hat{\psi}(\tfrac{1}{2}) = \tfrac{1}{2}; \quad \hat{\psi}'(\tfrac{1}{2}) = 0, \quad \hat{\psi}'(\tfrac{1}{2} + \epsilon) = \hat{\psi}'(\tfrac{1}{2} - \epsilon).$$

3. For $\hat{\psi}(\xi)$ in (4.15)–(4.17), we can obtain τ from $\psi(\tau) = t$ analytically. In all three cases, τ is the solution to the equation

$$\frac{\rho(\tau)}{\rho(\tau)+1} = t \quad \Rightarrow \quad \rho(\tau) = \frac{t}{1-t},$$

where

$$\text{for (4.15)}: \quad \rho(\tau) = \left(\frac{\tau}{1-\tau}\right)^p, \tag{4.18}$$

$$\text{for (4.16)}: \quad \rho(\tau) = \left(\tan\frac{\pi\tau}{2}\right)^p, \tag{4.19}$$

$$\text{for (4.17)}: \quad \rho(\tau) = \exp\left[2c\left(\frac{1}{1-\tau} - \frac{1}{\tau}\right)\right]. \tag{4.20}$$

Then we have the following:

$$\text{For (4.15)}: \quad \tau = \frac{t^{1/p}}{t^{1/p} + (1-t)^{1/p}}. \tag{4.21}$$

$$\text{For (4.16)}: \quad \tau = \frac{2}{\pi}\tan^{-1}\lambda; \quad \lambda = \left(\frac{t}{1-t}\right)^{1/p}. \tag{4.22}$$

$$\text{For (4.17)}: \quad \tau = \begin{cases} \dfrac{\sqrt{\lambda^2+4}+\lambda-2}{2\lambda} & \text{if } \lambda > 0 \\ \dfrac{2}{\sqrt{\lambda^2+4}-\lambda+2} & \text{if } \lambda \le 0 \end{cases}; \quad \lambda = \frac{1}{2c}\log\left(\frac{t}{1-t}\right). \tag{4.23}$$

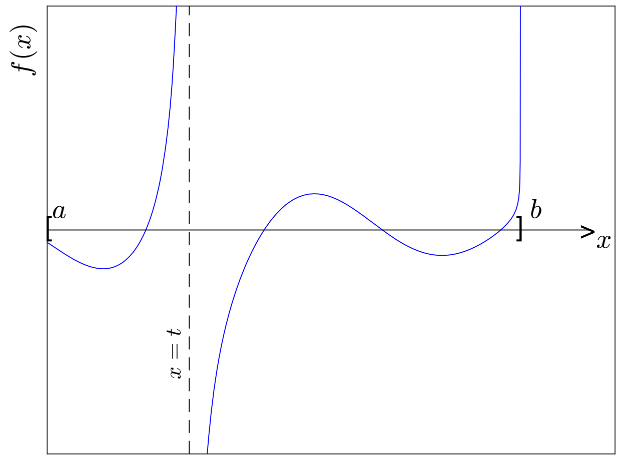

Fig. 1 Graph of the function $f(x) = \sin(4\pi x + \pi/6)(1 - x)^{-1/3}/(x - t)$ on $[a, b] = [0, 1]$, with $t = 0.3$

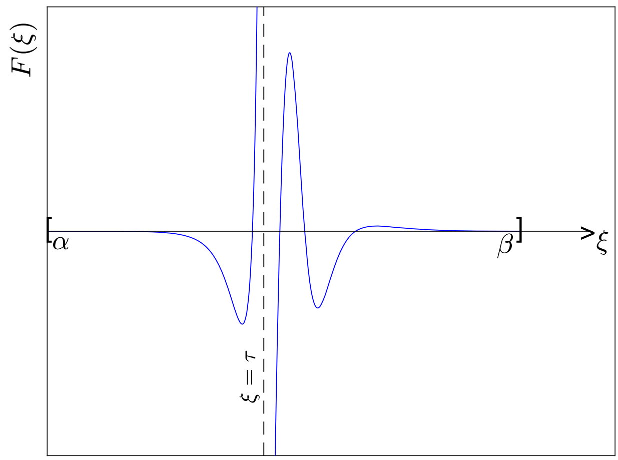

Fig. 2 Graph of the function $F(\xi) = f(\hat{\psi}(\xi))\hat{\psi}'(\xi)$ on $[\alpha, \beta] = [0, 1]$. Here $f(x)$ is the function in Fig. 1, $\hat{\psi}(\xi)$ is as in (4.15) with $p = 5$, and τ is given by (4.21) with $p = 5$ and $t = 0.3$ there

5 PVTSI$^{(m)}$: development of numerical quadrature formulas via periodization

We go back to the HFP integrals $⨎_a^b f(x)\,dx$ described in Sect. 1, assuming that $f(x)$ is as in (1.4); therefore, $f \in C^\infty((a, b) \setminus \{t\})$ since $g \in C^\infty(a, b)$. Let us periodize $f(x)$ via a suitable variable transformation $x = \psi(\xi)$, where

$$\psi \in C[\alpha, \beta],\ \psi \in C^\infty(\alpha, \beta);\ \ \psi(\alpha) = a,\ \psi(\beta) = b;\ \ \psi'(\xi) > 0 \text{ for } \xi \in (\alpha, \beta), \tag{5.1}$$

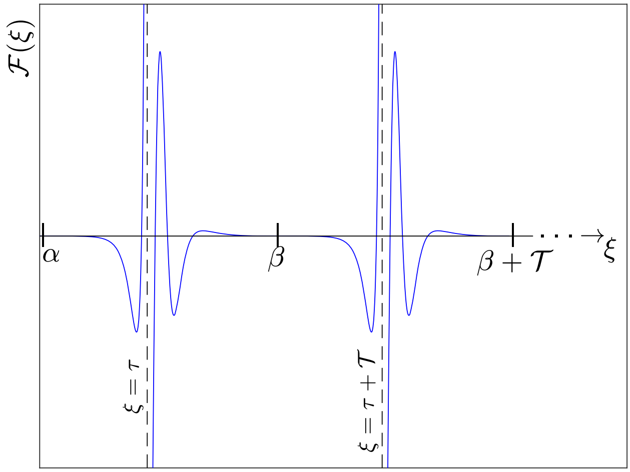

Fig. 3 Graph of the function $\mathcal{T}(\xi)$, the $\mathcal{T}$-periodic extension of the function $F(\xi) = f(\hat{\psi}(\xi))\hat{\psi}'(\xi)$ in Fig. 2, with $\mathcal{T} = \beta - \alpha = 1$

as described in the preceding section, such that the transformed integrand $F(\xi) = f(\psi(\xi))\,\psi'(\xi)$ satisfies (4.3), which is possible by a judicious choice of $\psi(\xi)$, as we have already seen. Then we have $I[f] = I[F]$ by Theorem 3.1, and

$$I[F] = \text{⨎}_{\alpha}^{\beta} F(\xi)\,d\xi = \text{⨎}_{\tau}^{\tau+\mathcal{T}} \mathcal{F}(\xi)\,d\xi, \quad \mathcal{T} = \beta - \alpha, \tag{5.2}$$

the function $\mathcal{F}(\xi)$ being the $\mathcal{T}$-periodic extension of $F(\xi)$ introduced in Sect. 4.2. Our aim is to develop numerical quadrature formulas specifically for the integral $\text{⨎}_{\tau}^{\tau+\mathcal{T}} \mathcal{F}(\xi)\,d\xi$ to compute $I[F]$ as given in (5.2). We will achieve this via Theorem A.2 that is proved in the appendix. For this, we need to study in detail the analytical properties of $\mathcal{F}(\xi)$ in the interval $(\tau, \tau + \mathcal{T})$.

1. First, note that both endpoints $\xi = \tau$ and $\xi = \tau + \mathcal{T}$ of the integration interval $J = (\tau, \tau + \mathcal{T})$ are points of singularity of $\mathcal{F}(\xi)$ and $\mathcal{F} \in C^{\infty}(J \setminus \{\beta\})$. Next, at $\xi = \beta$, which is in the interior of J, the function $\mathcal{F}(\xi)$ is continuous and has $q-1$ continuous derivatives, and $\mathcal{F}^{(i)}(\beta) = 0$, $i = 0, 1, \ldots, q-1$, by (4.11). We now assume, without loss of generality, that $\mathcal{F}^{(q)}(\xi)$ is absolutely integrable through $\xi = \beta$, which can be achieved by choosing $\psi(\xi)$ appropriately. To have a visual idea about what we have just explained, see the Figs. 1, 2, and 3.
2. Let us choose σ and ρ such that

$$\tau < \sigma < \beta < \rho < \tau + \mathcal{T},$$

and let

$$J_1 = (\tau, \sigma) \cup (\rho, \tau + \mathcal{T}), \quad J_2 = [\sigma, \rho].$$

Then $\mathcal{F} \in C^{\infty}(J_1)$ and $\mathcal{F} \in C^{q-1}(J_2)$, $\mathcal{F}^{(q)}(\xi)$ being absolutely integrable in J_2.

3. We are now interested in determining the asymptotic expansions of $\mathcal{F}(\xi)$ as $\xi \to \tau+$ and as $\xi \to (\tau + \mathcal{T})-$, recalling from (3.5) that $F(\xi)$ can be expressed as $F(\xi) = G(\xi)/(\xi - \tau)^m$ with $G \in C^\infty(\alpha, \beta)$.

   - First, we have that

$$\mathcal{F}(\xi) = F(\xi) = \frac{G(\xi)}{(\xi - \tau)^m} \quad \text{if } \xi \in (\alpha, \beta).$$

     Since $\tau \in (\alpha, \beta)$, expanding $G(\xi)$ in a Taylor series about $\xi = \tau$, we have that

$$\mathcal{F}(\xi) \sim \sum_{i=0}^{\infty} \frac{G^{(i)}(\tau)}{i!} (\xi - \tau)^{i-m} \quad \text{as } \xi \to \tau,$$

     which we write in the form

$$\mathcal{F}(\xi) \sim \frac{G^{(m-1)}(\tau)}{(m-1)!} (\xi - \tau)^{-1} + \sum_{\substack{i=0 \\ i \neq m-1}}^{\infty} \frac{G^{(i)}(\tau)}{i!} (\xi - \tau)^{i-m} \quad \text{as } \xi \to \tau. \tag{5.3}$$

   - Next, by $\mathcal{T}$-periodicity of $\mathcal{F}(\xi)$, we have that

$$\mathcal{F}(\xi) = F(\xi - \mathcal{T}) = \frac{G(\xi - \mathcal{T})}{(\xi - \mathcal{T} - \tau)^m} \quad \text{if } \xi \in (\beta, \beta + \mathcal{T}).$$

     Expanding $G(\xi - \mathcal{T})$ in a Taylor series about $\xi = \tau + \mathcal{T}$, which is in $(\beta, \beta + \mathcal{T})$, we have the asymptotic expansion

$$\mathcal{F}(\xi) \sim \sum_{i=0}^{\infty} \frac{G^{(i)}(\tau)}{i!} (\xi - \tau - \mathcal{T})^{i-m} \quad \text{as } \xi \to \tau + \mathcal{T},$$

     which we write in the form

$$\begin{aligned} \mathcal{F}(\xi) \sim & -\frac{G^{(m-1)}(\tau)}{(m-1)!} (\tau + \mathcal{T} - \xi)^{-1} \\ & + \sum_{\substack{i=0 \\ i \neq m-1}}^{\infty} (-1)^{i-m} \frac{G^{(i)}(\tau)}{i!} (\tau + \mathcal{T} - \xi)^{i-m} \quad \text{as } \xi \to \tau + \mathcal{T}. \end{aligned} \tag{5.4}$$

4. Thus, Theorem A.2 applies to $⨍_{\tau}^{\tau+\mathcal{T}} \mathcal{F}(\xi)\,d\xi$ with $h = \mathcal{T}/n$, and we have, as $h \to 0$,

$$h \sum_{j=1}^{n-1} \mathcal{F}(\tau + jh) \sim I[F] + R_q(h) + \sum_{\substack{i=0 \\ i \neq m-1}}^{\infty} [1 + (-1)^{i-m}] \frac{G^{(i)}(\tau)}{i!} \zeta(-i + m) h^{i-m+1}, \tag{5.5}$$

where $\zeta(z)$ is the Riemann Zeta function and

$$R_q(h) = O(h^q) \quad \text{as } h \to 0. \tag{5.6}$$

Observe that the contributions of the terms involving $(\xi - \tau)^{-1}$ and $(\tau + \mathcal{T} - \xi)^{-1}$ that appear in (5.3) and (5.4) cancel each other.

Now the infinite sum in (5.5) contains only those terms with $i - m$ an even integer, which involve the zeta function $\zeta(2s)$, s being an integer, positive, negative, or zero. Invoking the fact that $\zeta(-2k) = 0$ for $k = 1, 2, \ldots,$ we see that this (infinite) sum reduces further to a *finite* sum. We summarize the end result in the following theorem:

Theorem 5.1 *Depending on whether m is even or odd, (5.5) assumes the following forms:*
1. For $m = 2r$, $r = 1, 2, \ldots,$

$$h \sum_{j=1}^{n-1} \mathcal{F}(\tau + jh) = I[F] + 2 \sum_{i=0}^{r} \frac{G^{(2i)}(\tau)}{(2i)!} \zeta(2r - 2i)\, h^{-2r+2i+1} + O(h^q) \quad \text{as } h \to 0. \tag{5.7}$$

2. For $m = 2r + 1$, $r = 0, 1, \ldots,$

$$h \sum_{j=1}^{n-1} \mathcal{F}(\tau + jh) = I[F] + 2 \sum_{i=0}^{r} \frac{G^{(2i+1)}(\tau)}{(2i+1)!} \zeta(2r - 2i)\, h^{-2r+2i+1} + O(h^q) \quad \text{as } h \to 0. \tag{5.8}$$

Clearly, q depends only on (i) $g(x)$ at $x = a$ and $x = b$ and (ii) $\psi(\xi)$, and is independent of m.

In view of (5.7)–(5.8), we define our PVTSI$^{(m)}$ numerical quadrature formulas $\widehat{T}_{m,n}^{(s)}[\mathcal{F}]$ for $I[F]$ precisely as those in [31], which we have summarized in Sect. 2:
1. For $m = 2r$, $r = 1, 2, \ldots,$

$$\widehat{T}_{2r,n}^{(0)}[\mathcal{F}] = h \sum_{j=1}^{n-1} \mathcal{F}(\tau + jh) - 2 \sum_{i=0}^{r} \frac{G^{(2i)}(\tau)}{(2i)!} \zeta(2r - 2i)\, h^{-2r+2i+1}. \tag{5.9}$$

2. For $m = 2r + 1$, $r = 0, 1, \dots,$

$$\widehat{T}^{(0)}_{2r+1,n}[\mathfrak{F}] = h \sum_{j=1}^{n-1} \mathfrak{F}(\tau + jh) - 2 \sum_{i=0}^{r} \frac{G^{(2i+1)}(\tau)}{(2i+1)!}\, \zeta(2r - 2i)\, h^{-2r+2i+1}. \tag{5.10}$$

From these, we obtain the rest of the formulas $\widehat{T}^{(s)}_{m,n}[\mathfrak{F}]$ with $s = 1, 2, \dots$ precisely as the $\widehat{T}^{(s)}_{m,n}[f]$ described in Sect. 2. For example, with $h = \mathfrak{T}/n$, for $m = 1, 2, 3, 4$, we have the following numerical quadrature formulas:

1. The case $m = 1$:

$$\widehat{T}^{(0)}_{1,n}[\mathfrak{F}] = h \sum_{j=1}^{n-1} \mathfrak{F}(\tau + jh) + G'(\tau)\, h, \tag{5.11a}$$

$$\widehat{T}^{(1)}_{1,n}[\mathfrak{F}] = h \sum_{j=1}^{n} \mathfrak{F}(\tau + jh - h/2). \tag{5.11b}$$

2. The case $m = 2$:

$$\widehat{T}^{(0)}_{2,n}[\mathfrak{F}] = h \sum_{j=1}^{n-1} \mathfrak{F}(\tau + jh) - \frac{\pi^2}{3}\, G(\tau)\, h^{-1} + \frac{1}{2}\, G''(\tau)\, h, \tag{5.12a}$$

$$\widehat{T}^{(1)}_{2,n}[\mathfrak{F}] = h \sum_{j=1}^{n} \mathfrak{F}(\tau + jh - h/2) - \pi^2 G(\tau) h^{-1}, \tag{5.12b}$$

$$\widehat{T}^{(2)}_{2,n}[\mathfrak{F}] = 2h \sum_{j=1}^{n} \mathfrak{F}(\tau + jh - h/2) - \frac{h}{2} \sum_{j=1}^{2n} \mathfrak{F}(\tau + jh/2 - h/4). \tag{5.12c}$$

3. The case $m = 3$:

$$\widehat{T}^{(0)}_{3,n}[\mathfrak{F}] = h \sum_{j=1}^{n-1} \mathfrak{F}(\tau + jh) - \frac{\pi^2}{3}\, G'(\tau)\, h^{-1} + \frac{1}{6}\, G'''(\tau)\, h, \tag{5.13a}$$

$$\widehat{T}^{(1)}_{3,n}[\mathfrak{F}] = h \sum_{j=1}^{n} \mathfrak{F}(\tau + jh - h/2) - \pi^2\, G'(\tau)\, h^{-1}, \tag{5.13b}$$

$$\widehat{T}^{(2)}_{3,n}[\mathfrak{F}] = 2h \sum_{j=1}^{n} \mathfrak{F}(\tau + jh - h/2) - \frac{h}{2} \sum_{j=1}^{2n} \mathfrak{F}(\tau + jh/2 - h/4). \tag{5.13c}$$

4. *The case $m = 4$:*

$$\widehat{T}^{(0)}_{4,n}[\mathcal{F}] = h\sum_{j=1}^{n-1}\mathcal{F}(\tau + jh) - \frac{\pi^4}{45}G(\tau)h^{-3} - \frac{\pi^2}{6}G''(\tau)h^{-1} + \frac{1}{24}G^{(4)}(\tau)h \tag{5.14a}$$

$$\widehat{T}^{(1)}_{4,n}[\mathcal{F}] = h\sum_{j=1}^{n}\mathcal{F}(\tau + jh - h/2) - \frac{\pi^4}{3}G(\tau)h^{-3} - \frac{\pi^2}{2}G''(\tau)h^{-1} \tag{5.14b}$$

$$\widehat{T}^{(2)}_{4,n}[\mathcal{F}] = 2h\sum_{j=1}^{n}\mathcal{F}(\tau + jh - h/2) - \frac{h}{2}\sum_{j=1}^{2n}\mathcal{F}(\tau + jh/2 - h/4) + 2\pi^4 G(\tau)h^{-3} \tag{5.14c}$$

$$\widehat{T}^{(3)}_{4,n}[\mathcal{F}] = \frac{16h}{7}\sum_{j=1}^{n}\mathcal{F}(\tau + jh - h/2) - \frac{5h}{7}\sum_{j=1}^{2n}\mathcal{F}(\tau + jh/2 - h/4) + \frac{h}{28}\sum_{j=1}^{4n}\mathcal{F}(\tau + jh/4 - h/8) \tag{5.14d}$$

Before, we go on, we wish to emphasize that no limitations are put on $\tau \in (\alpha, \beta)$ in these formulas. Therefore, no limitations are put on $t \in (a, b)$, either.

Concerning all of these formulas, we have the following convergence theorem that is analogous to Theorem 2.1:

Theorem 5.2 *Under the conditions imposed on $f(x)$, $F(\xi)$, and $\mathcal{F}(\xi)$, there holds $\lim_{n\to\infty}\widehat{T}^{(s)}_{m,n}[\mathcal{F}] = I[F]$ for all m and s. Actually, for each m, we have the following:*

1. *If q is finite, then, independent of s,*

$$\widehat{T}^{(s)}_{m,n}[\mathcal{F}] - I[F] = O(n^{-q}) \quad \text{as } n \to \infty. \tag{5.15}$$

[Recall that, if finite, q depends only (i) on the behavior of $g(x)$ at $x = a$ and $x = b$ and (ii) on $\psi(\xi)$, and is independent of m.]

2. *If $q = \infty$, then, independent of s,*

$$\widehat{T}^{(s)}_{m,n}[\mathcal{F}] - I[F] = o(n^{-\mu}) \quad \text{as } n \to \infty \quad \forall\, \mu > 0, \tag{5.16}$$

that is, the quadrature formulas $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ achieve spectral accuracy. [Recall that $q = \infty$ depends only on $\psi(\xi)$ and is independent of $g(x)$.]

Remark 1. Let us recall the first remark at the end of Sect. 4.2 that says that we can make q in (4.3) as large as we wish by choosing $\psi(\xi)$ appropriately. From this and from Theorem 5.2, it is clear that we can improve the accuracy of the $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ at will by choosing $\psi(\xi)$ such that r in (4.2) is sufficiently large to make q as large as we wish.

2. Note that, because $\alpha < \tau < \beta$, some of the abscissas in each of the quadrature formulas above are in (α, β), while others are necessarily in $(\beta, \beta + \mathcal{T})$. We can invoke the $\mathcal{T}$-periodicity of $\mathcal{F}(\xi)$ for those abscissas in $(\beta, \beta + \mathcal{T})$. Thus, in all the formulas $\widehat{T}^{(0)}_{m,n}[\mathcal{F}]$, (i) if $\tau + jh \le \beta$, then $\mathcal{F}(\tau + jh) = F(\tau + jh)$, while (ii) if $\tau + jh > \beta$, then $\mathcal{F}(\tau + jh) = F(\tau + jh - \mathcal{T}) = F(\tau - (n - j)h)$ since $\tau - (n - j)h \in [\alpha, \tau)$.
3. Clearly, we need $G^{(i)}(\tau)$, $i = 0, 1, 2, \ldots,$ in the quadrature formulas $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$. We recall that $G(\tau)$ and $G'(\tau)$ are given in (3.6)–(3.7). All of the $G^{(i)}(\tau)$ can be obtained by differentiating $G(\xi)$ in (3.5) and letting $\xi \to \tau$. For this, it is clear that we also need the derivatives with respect to ξ of $Q(\xi) = \psi[\xi, \tau]$, evaluated at $\xi = \tau$. Expanding $\psi(\xi)$ in a Taylor series about $\xi = \tau$, it is readily seen that

$$Q^{(k)}(\tau) = \frac{\psi^{(k+1)}(\tau)}{k+1}, \quad k = 0, 1, \ldots.$$

4. In case the function $f(x)$, in addition to being in $C^{\infty}((a, b) \setminus \{t\})$, already satisfies

$$f^{(i)}(a) = f^{(i)}(b), \quad i = 0, 1, \ldots, q - 1,$$

   $f^{(q)}(x)$ being absolutely integrable through $x = a$ and $x = b$, Theorem 5.2 applies directly to the $(b-a)$-periodic extension of $f(x)$, which we denote by $f(x)$ again. Thus, $\lim_{n\to\infty} \widehat{T}^{(s)}_{m,n}[f] = I[f]$, such that

$$\widehat{T}^{(s)}_{m,n}[f] - I[f] = O(n^{-q}) \quad \text{as } n \to \infty, \qquad \text{for each } m \text{ and } s.$$

6 Numerical examples with PVTSI$^{(m)}$ quadrature formulas

We have applied the PVTSI$^{(m)}$ formulas, with the variable transformations in (4.15)–(4.17), to several HFP integrals with $m = 1, 2, 3$. The numerical results obtained lead us to conclude that they achieve high accuracies in all cases.

In all these examples, $[a, b] = [0, 1]$ and $[\alpha, \beta] = [0, 1]$ and we present those results obtained by using the variable transformation $\hat{\psi}(\xi) = \xi^p/[\xi^p + (1 - \xi)^p]$ with $p = 5$, $p = 10$, and $p = 15$. (All three transformations in (4.15)–(4.17) seem to produce very similar numerical results.) We have carried out all our computations in quadruple-precision arithmetic (approximately 34 decimal digits).

Below, we use the notation

$$I_m(t) = \,=\!\!\!\!\!\!\int_a^b \frac{g(x)}{(x-t)^m}\,dx, \quad m = 1, 2 \ldots.$$

We first treat three HFP integrals, taken from Kaya and Erdogan [9], involving the Chebyshev polynomials of the first and second kinds, namely, $T_k(z)$ and $U_k(z)$, respectively, as examples. The integrands have square-root singularities at the endpoints in all cases. In all the three examples $g(x)$ is finite at the endpoints $x = a$ and $x = b$,

Table 1 Relative errors in the approximations $\widehat{T}^{(0)}_{1,n}[\mathcal{F}]$ and $\widehat{T}^{(1)}_{1,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.1

r	$E^{(0)}_{1,2^r}, p=5$	$E^{(1)}_{1,2^r}, p=5$	$E^{(0)}_{1,2^r}, p=10$	$E^{(1)}_{1,2^r}, p=10$	$E^{(0)}_{1,2^r}, p=15$	$E^{(1)}_{1,2^r}, p=15$
1	6.021D+00	9.420D–01	1.295D+01	1.000D+00	1.989D+01	1.000D+00
2	2.539D+00	1.586D+00	5.973D+00	9.413D–01	9.445D+00	9.974D–01
3	4.769D–01	4.916D–01	2.516D+00	1.587D+00	4.224D+00	9.209D–01
4	7.352D–03	7.352D–03	4.641D–01	4.807D–01	1.652D+00	1.654D+00
5	1.505D–08	1.505D–08	8.315D–03	8.315D–03	1.401D–03	1.237D–03
6	6.128D–15	6.137D–15	2.398D–08	2.398D–08	8.164D–05	8.164D–05
7	4.636D–18	4.920D–18	1.529D–20	1.529D–20	3.535D–12	3.535D–12
8	1.420D–19	1.397D–19	4.162D–34	1.387D–34	3.760D–29	3.758D–29
9	1.131D–21	1.142D–21	2.774D–34	2.358D–33	1.110D–32	3.510D–32
10	5.575D–24	5.624D–24	1.249D–33	5.965D–33	2.303D–32	7.047D–32

Here $E^{(s)}_{1,n} = |\widehat{T}^{(s)}_{1,n}[\mathcal{F}] - I_1(0.3)|/|I_1(0.3)|$

but all its derivatives are unbounded there. (Note that the first two examples were also treated by Choi et al. [2].)

Example 6.1 With $m = 1$:

$$I_1(t) = \int_0^1 \sqrt{x(1-x)}\,\frac{U_k(2x-1)}{x-t}\,dx = -\frac{\pi}{2}\,T_{k+1}(2t-1).$$

We have computed $I_1(t)$ with $k = 4$ and for $t = 0.3$.
We now have $I_1(0.3) = 1.38833262547440142794141136393888$. The results of the computation are given in Table 1.

Example 6.2 With $m = 2$:

$$I_2(t) = \int_0^1 \sqrt{x(1-x)}\,\frac{U_k(2x-1)}{(x-t)^2}\,dx = -\pi(k+1)U_k(2t-1).$$

We have computed $I_2(t)$ with $k = 4$ and for $t = 0.3$.
The exact value of the integral is $I_2(0.3) = 8.01734445196115234455666591412929$. The results of the computation are given in Table 2.

Example 6.3 With $m = 3$:

$$I_3(t) = \int_0^1 \sqrt{x(1-x)}\,\frac{U_k(2x-1)}{(x-t)^3}\,dx = -\pi(k+1)U_k'(2t-1).$$

Here $U_k'(z) = \frac{d}{dz}U_k(z)$. We have computed $I_3(t)$ with $k = 4$ and for $t = 0.3$.
The exact value of the integral is $I_3(0.3) = -86.4566298267911099224919459078519$. The results of the computation are given in Table 3.

Table 2 Relative errors in the approximations $\widehat{T}^{(1)}_{2,n}[\mathcal{F}]$ and $\widehat{T}^{(2)}_{2,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.2

r	$E^{(1)}_{2,2^r}, p=5$	$E^{(2)}_{2,2^r}, p=5$	$E^{(1)}_{2,2^r}, p=10$	$E^{(2)}_{2,2^r}, p=10$	$E^{(1)}_{2,2^r}, p=15$	$E^{(2)}_{2,2^r}, p=15$
1	8.428D-01	9.769D-01	9.316D–01	1.027D+00	9.543D-01	1.001D+00
2	7.087D-01	1.137D+00	8.357D–01	9.643D–01	9.076D–01	1.084D+00
3	2.807D-01	5.613D–01	7.072D–01	1.126D+00	7.310D–01	7.883D–01
4	2.132D–04	4.263D–04	2.879D–01	5.756D–01	6.737D–01	1.284D+00
5	1.155D–09	2.311D–09	2.176D–04	4.352D–04	6.352D–02	1.271D–01
6	2.748D–15	5.486D–15	2.040D–09	4.080D–09	2.245D–05	4.491D–05
7	9.955D–18	1.990D–17	1.149D–22	2.298D–22	1.148D–13	2.296D–13
8	1.494D–20	2.925D–20	5.765D–34	1.286D–31	1.192D–30	2.469D–30
9	6.307D–22	1.263D–21	8.244D–32	9.280D–31	8.360D–32	6.822D–32
10	1.485D–24	2.990D–24	8.552D–32	2.994D–30	9.897D–32	6.726D–33

Here $E^{(s)}_{2,n} = |\widehat{T}^{(s)}_{2,n}[\mathcal{F}] - I_2(0.3)|/|I_2(0.3)|$

Table 3 Relative errors in the approximations $\widehat{T}^{(1)}_{3,n}[\mathcal{F}]$ and $\widehat{T}^{(2)}_{3,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.3

r	$E^{(1)}_{3,2^r}, p=5$	$E^{(2)}_{3,2^r}, p=5$	$E^{(1)}_{3,2^r}, p=10$	$E^{(2)}_{3,2^r}, p=10$	$E^{(1)}_{3,2^r}, p=15$	$E^{(2)}_{3,2^r}, p=15$
1	7.291D–01	1.069D+00	8.632D–01	1.000D+00	9.087D–01	1.000D+00
2	3.889D–01	7.611D–01	7.262D–01	1.068D+00	8.174D–01	1.009D+00
3	1.665D–02	3.339D–02	3.840D–01	7.517D–01	6.263D–01	1.078D+00
4	8.650D–05	1.730D–04	1.631D–02	3.272D–02	1.748D–01	3.510D–01
5	3.819D–11	7.638D–11	1.076D–04	2.152D–04	1.410D–03	2.820D–03
6	9.547D–16	1.908D–15	6.819D–11	1.364D–10	4.450D–07	8.901D–07
7	1.382D–18	2.751D–18	1.172D–23	2.345D–23	6.046D–15	1.209D–14
8	1.332D–20	2.645D–20	8.009D–31	1.031D–30	1.123D–30	6.811D–30
9	1.988D–22	3.982D–22	5.260D–30	1.194D–29	9.029D–30	5.592D–29
10	6.917D–25	1.394D–24	3.938D–29	1.119D–28	7.368D–29	4.094D–28

Here $E^{(s)}_{3,n} = |\widehat{T}^{(s)}_{3,n}[\mathcal{F}] - I_3(0.3)|/|I_3(0.3)|$

In the next three examples, we have obtained the $I_m(t)$ via iteration of the known relation (see Kaya and Erdogan [9], for example)

$$\Xint=_a^b \frac{g(x)}{(x-t)^{k+1}}\,dx = \frac{1}{k}\frac{d}{dt}\Xint=_a^b \frac{g(x)}{(x-t)^k}\,dx, \quad k = 1, 2, \ldots.$$

Thus, starting with

$$I_1(t) = M(t) + g(t)H(t); \quad M(t) = \int_a^b \frac{g(x)-g(t)}{x-t}\,dx, \quad H(t) = \log\frac{b-t}{t-a},$$

Table 4 Relative errors in the approximations $\widehat{T}^{(0)}_{1,n}[\mathcal{F}]$ and $\widehat{T}^{(1)}_{1,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.4

r	$E^{(0)}_{1,2^r}, p=5$	$E^{(1)}_{1,2^r}, p=5$	$E^{(0)}_{1,2^r}, p=10$	$E^{(1)}_{1,2^r}, p=10$	$E^{(0)}_{1,2^r}, p=15$	$E^{(1)}_{1,2^r}, p=15$
1	1.596D+00	8.813D–01	4.289D+00	9.989D–01	6.961D+00	1.000D+00
2	3.573D–01	3.343D–01	1.645D+00	8.913D–01	2.980D+00	9.871D–01
3	1.148D–02	1.151D–02	3.769D–01	3.515D–01	9.966D–01	7.188D–01
4	1.269D–05	1.269D–05	1.269D–02	1.273D–02	1.389D–01	1.381D–01
5	2.058D–09	2.226D–09	1.674D–05	1.674D–05	3.762D–04	3.764D–04
6	8.396D–11	8.672D–11	6.311D–12	6.311D–12	8.610D–08	8.610D–08
7	1.384D–12	1.544D–12	7.592D–24	7.778D–24	3.897D–16	3.897D–16
8	8.010D–14	7.609D–14	9.289D–26	9.300D–26	3.348D–32	1.030D–31
9	2.005D–15	2.169D–15	5.720D–29	5.728D–29	6.319D–32	2.020D–31
10	8.210D–17	8.384D–17	4.841D–32	2.358D–33	1.383D–31	4.139D–31

Here $E^{(s)}_{1,n} = |\widehat{T}^{(s)}_{1,n}[\mathcal{F}] - I_1(0.3)|/|I_1(0.3)|$

we have

$$I_2(t) = M'(t) + g(t)H'(t) + g'(t)H(t),$$
$$I_3(t) = \frac{1}{2}\big[M''(t) + g(t)H''(t) + 2g'(t)H'(t) + g''(t)H(t)\big],$$

and so on.

Example 6.4 With $m = 1$:

$$I_1(t) = \int_0^1 \frac{1+x-x^2}{x-t}\,dx = \frac{1}{2} - t + (1+t-t^2)\log\frac{1-t}{t}.$$

We have computed $I_1(t)$ for $t = 0.3$.
The exact value of the integral is $I_1(0.3) = 1.2252304110685163725892300828899$.
The results of the computation are given in Table 4.

Example 6.5 With $m = 2$:

$$I_2(t) = \int_0^1 \frac{1+x-x^2}{(x-t)^2}\,dx = -1 - \frac{1+t-t^2}{t(1-t)} + (1-2t)\log\frac{1-t}{t}.$$

We have computed $I_2(t)$ for $t = 0.3$.
The exact value of the integral is $I_2(0.3) = -6.4229856177498804592778617592965O$.
The results of the computation are given in Table 5.

Example 6.6 With $m = 3$:

$$I_3(t) = \int_0^1 \frac{1+x-x^2}{(x-t)^3}\,dx = \frac{(1+t-t^2)(1-2t)}{2[t(1-t)]^2} - \frac{1-2t}{t(1-t)} - \log\frac{1-t}{t}.$$

Table 5 Relative errors in the approximations $\widehat{T}^{(1)}_{2,n}[\mathcal{F}]$ and $\widehat{T}^{(2)}_{2,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.5

r	$E^{(1)}_{2,2^k}, p=5$	$E^{(2)}_{2,2^r}, p=5$	$E^{(1)}_{2,2^r}, p=10$	$E^{(2)}_{2,2^r}, p=10$	$E^{(1)}_{2,2^r}, p=15$	$E^{(2)}_{2,2^r}, p=15$
1	2.009D–01	3.877D–01	5.588D–01	9.044D–01	7.051D–01	9.889D–01
2	1.406D–02	2.911D–02	2.131D–01	4.106D–01	4.213D–01	7.419D–01
3	1.000D–03	2.000D–03	1.565D–02	3.245D–02	1.008D–01	2.024D–01
4	3.704D–07	7.416D–07	1.158D–03	2.316D–03	7.653D–04	1.362D–03
5	7.123D–10	1.457D–09	4.543D–07	9.086D–07	1.691D–04	3.381D–04
6	3.218D–11	6.489D–11	1.917D–13	3.833D–13	7.533D–09	1.507D–08
7	5.275D–13	1.082D–12	2.045D–23	4.079D–23	4.429D–18	8.859D–18
8	2.738D–14	5.397D–14	1.148D–25	2.297D–25	1.295D–32	3.094D–31
9	7.942D–16	1.619D–15	6.963D–29	1.437D–28	2.893D–31	4.553D–31
10	3.044D–17	6.124D–17	9.111D–31	1.930D–29	1.049D–30	5.133D–32

Here $E^{(s)}_{2,n} = |\widehat{T}^{(s)}_{2,n}[\mathcal{F}] - I_2(0.3)|/|I_2(0.3)|$

Table 6 Relative errors in the approximations $\widehat{T}^{(1)}_{3,n}[\mathcal{F}]$ and $\widehat{T}^{(2)}_{3,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.6

r	$E^{(1)}_{3,2^r}, p=5$	$E^{(2)}_{3,2^r}, p=5$	$E^{(1)}_{3,2^r}, p=10$	$E^{(2)}_{3,2^r}, p=10$	$E^{(1)}_{3,2^r}, p=15$	$E^{(2)}_{3,2^r}, p=15$
1	1.034D–01	1.359D–01	3.659D–01	8.073D–01	5.726D–01	9.778D–01
2	7.095D–02	1.408D–01	7.539D–02	8.150D–02	1.674D–01	4.613D–01
3	1.115D–03	2.229D–03	6.928D–02	1.372D–01	1.266D–01	2.306D–01
4	4.647D–10	6.997D–09	1.363D–03	2.727D–03	2.254D–02	4.505D–02
5	7.926D–09	1.618D–08	5.015D–07	1.003D–06	3.534D–05	7.069D–05
6	3.289D–10	6.634D–10	5.371D–14	1.074D–13	1.738D–09	3.476D–09
7	5.653D–12	1.159D–11	7.388D–23	1.470D–22	1.898D–18	3.795D–18
8	2.848D–13	5.614D–13	7.120D–25	1.424D–24	1.820D–28	1.134D–27
9	8.178D–15	1.667D–14	4.612D–28	1.352D–27	1.490D–27	9.074D–27
10	3.150D–16	6.336D–16	6.468D–27	1.888D–26	1.211D–26	6.680D–26

Here $E^{(s)}_{3,n} = |\widehat{T}^{(s)}_{3,n}[\mathcal{F}] - I_3(0.3)|/|I_3(0.3)|$

We have computed $I_3(t)$ for $t = 0.3$.
The exact value of the integral is $I_3(0.3) = 2.73546857952209343844408750481721$.
The results of the computation are given in Table 6.

Remark 1. Note that, in Tables 1, 2, 3, 4, 5, 6, we have recorded the *relative* errors in the approximations $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$. The reason for this is that relative errors in the $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ indicate the number of correct significant figures that can be trusted in these approximations.

2. Judging from Tables 1, 2, 3, 4, 5, 6, we may conclude that, for each m, and fixed $\hat{\psi}(\xi)$, the quadrature formulas $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ with different $s \geq 0$ produce approximately the same accuracies. This is consistent with Theorem 5.2 that says that $\widehat{T}^{(s)}_{m,n}[\mathcal{F}] -$

$I[f] = O(n^{-q})$ as $n \to \infty$ simultaneously for $s = 0, 1, \ldots$; that is, both formulas converge at the same rate as $n \to \infty$.

3. The floating-point computation of HFP integrals is accompanied by roundoff errors that increase with n. Thus, if we denote the computed $\widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ by $\bar{T}^{(s)}_{m,n}[\mathcal{F}]$, then the actual floating-point numerical error is $(\bar{T}^{(s)}_{m,n}[\mathcal{F}] - I[f])$, which we express as

$$\bar{T}^{(s)}_{m,n}[\mathcal{F}] - I[f] = (\bar{T}^{(s)}_{m,n}[\mathcal{F}] - \widehat{T}^{(s)}_{m,n}[\mathcal{F}]) + (\widehat{T}^{(s)}_{m,n}[\mathcal{F}] - I[f]).$$

Since $\lim_{n\to\infty}(\widehat{T}^{(s)}_{m,n}[\mathcal{F}] - I[f]) = 0$, we have

$$\bar{T}^{(s)}_{m,n}[\mathcal{F}] - I[f] \approx \bar{T}^{(s)}_{m,n}[\mathcal{F}] - \widehat{T}^{(s)}_{m,n}[\mathcal{F}] \quad \text{for all large } n.$$

As discussed in Sidi [30,31], for some constants $C^{(s)}_m$, the computational errors $\bar{T}^{(s)}_{m,n}[\mathcal{F}] - \widehat{T}^{(s)}_{m,n}[\mathcal{F}]$ grow like (i) $C^{(s)}_1 \mathbf{u} \log n$ when $m = 1$, (ii) $C^{(s)}_2 \mathbf{u} n$ when $m = 2$, and (iii) $C^{(s)}_3 \mathbf{u} n^2$ when $m = 3$, where $\mathbf{u}$ is the roundoff unit of the floating-point arithmetic being used.[5] The numbers at the bottom of Tables Tables 1, 2, 3, 4, 5, 6 (especially those corresponding to $n = 2^8, 2^9, 2^{10}$ with $p = 10$ and $p = 15$) exhibit this behavior since $\mathbf{u} = 1.93 \times 10^{-34}$ for quadruple-precision arithmetic. (Clearly, they should be much smaller than what they are in this table, and they will be if the floating-point arithmetic being used has a smaller roundoff unit than in quadruple-precision arithmetic.) Because the methods we have developed here converge quickly due to the fact that q can be made as large as we wish, sufficiently high accuracy is achieved before roundoff errors start to be felt. This is one important feature of our methods.

Additional considerations

1. In the examples above, we applied our quadrature formulas when t, the point of singularity of $f(x)$, is far from the endpoints a and b, and obtained high accuracies easily. The question as to whether these formulas can maintain their good performance also when t is close to the endpoints a or b is certainly intriguing. Our computations have shown that they do maintain their good performance in such cases too.

We have chosen to report our results for the integral treated in Example 6.6, since $f(x)$ in this example has a (strong) $(x - t)^{-3}$ singularity in $(0, 1)$. In addition, $\lim_{t\to 0+} I(t) = \infty$. All this makes Example 6.6 a good test case. In Table 7, we provide the results obtained by applying $\widehat{T}^{(s)}_{3,n}[\mathcal{F}]$ to the integral $I_3(t)$ treated in Example 6.6, now with $t = 0.001$, thus very close to the endpoint $a = 0$. The variable transformation used is again $\hat{\psi}(\xi) = \xi^p/[\xi^p + (1 - \xi)^p]$ with $p = 5$, $p = 10$, and $p = 15$. We now have $I_3(0.001) = 499493.0927442198494439784426646137 17$.

[5] Following [30,31], it can be shown that, for $s = 0$, we have $C^{(0)}_1 \approx 2\|G\|$, $C^{(0)}_2 \approx 2\zeta(2)\|G\|/T$, and $C^{(0)}_3 \approx 2\zeta(3)\|G\|/T^2$, where $\|G\| = \max_{\alpha\le\xi\le\beta} |G(\xi)|$.

Table 7 Relative errors in the approximations $\widehat{T}^{(1)}_{3,n}[\mathcal{F}]$ and $\widehat{T}^{(2)}_{3,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.001$ in Example 6.6

r	$E^{(1)}_{3,2^r}, p=5$	$E^{(2)}_{3,2^r}, p=5$	$E^{(1)}_{3,2^r}, p=10$	$E^{(2)}_{3,2^r}, p=10$	$E^{(1)}_{3,2^r}, p=15$	$E^{(2)}_{3,2^r}, p=15$
1	4.423D–01	8.850D–01	5.756D–01	9.506D–01	6.926D–01	9.931D–01
2	2.765D–04	1.787D–03	2.006D–01	3.964D–01	3.920D–01	7.225D–01
3	2.340D–03	4.642D–03	4.894D–03	9.823D–03	6.152D–02	1.227D–01
4	3.887D–05	7.684D–05	3.476D–05	6.951D–05	3.654D–04	7.309D–04
5	8.900D–07	1.817D–06	6.776D–11	1.355D–10	1.159D–07	2.319D–07
6	3.745D–08	7.353D–08	5.893D–17	1.178D–16	1.820D–14	3.640D–14
7	1.366D–09	2.760D–09	2.763D–20	5.514D–20	1.426D–24	2.853D–24
8	2.778D–11	5.685D–11	1.220D–22	2.442D–22	3.098D–29	1.170D–28
9	1.285D–12	2.541D–12	1.141D–25	2.294D–25	2.455D–28	9.376D–28
10	2.936D–14	6.004D–14	2.428D–27	6.014D–27	2.063D–27	7.308D–27

Here $E^{(s)}_{3,n} = |\widehat{T}^{(s)}_{3,n}[\mathcal{F}] - I_3(0.001)|/|I_3(0.001)|$

Table 8 Relative errors in the approximations $\widehat{T}^{(1)}_{3,n}[\mathcal{F}]$ and $\widehat{T}^{(2)}_{3,n}[\mathcal{F}]$, with $n = 2^r$, for $t = 0.3$ in Example 6.6

r	$E^{(1)}_{3,2^r}, p=5$	$E^{(2)}_{3,2^r}, p=5$	$E^{(1)}_{3,2^r}, p=10$	$E^{(2)}_{3,2^r}, p=10$	$E^{(1)}_{3,2^r}, p=15$	$E^{(2)}_{3,2^r}, p=15$
1	1.034D–01	1.359D–01	3.659D–01	8.073D–01	5.726D–01	9.778D–01
2	7.095D–02	1.408D–01	7.539D–02	8.150D–02	1.674D–01	4.613D–01
3	1.115D–03	2.229D–03	6.928D–02	1.372D–01	1.266D–01	2.306D–01
4	4.660D–10	7.002D–09	1.363D–03	2.727D–03	2.254D–02	4.505D–02
5	7.936D–09	1.613D–08	5.015D–07	1.003D–06	3.534D–05	7.069D–05
6	2.603D–10	1.089D–09	3.054D–12	2.034D–11	1.741D–09	3.466D–09
7	6.229D–10	3.002D–09	2.712D–11	1.454D–10	2.552D–11	9.893D–11
8	4.899D–09	2.682D–08	2.013D–10	1.129D–09	1.995D–10	7.536D–10
9	3.927D–08	2.040D–07	1.540D–09	6.349D–09	1.474D–09	6.692D–09
10	3.073D–07	1.493D–06	9.434D–09	6.507D–08	1.309D–08	4.870D–08

Here $E^{(s)}_{3,n} = |\widehat{T}^{(s)}_{3,n}[\mathcal{F}] - I_3(0.3)|/|I_3(0.3)|$. Computations carried out in double-precision arithmetic

2. To demonstrate/verify that the $\widehat{T}^{(s)}_{m,n}[\mathcal{F}] \to I[f]$ fast as $n \to \infty$, as suggested by Theorem 5.2, we applied these formulas in quadruple-precision arithmetic. The question arises as to whether we can observe fast convergence in double-precision arithmetic too. To check this point, we have done all our computations in the examples above in double-precision arithmetic (approximately 15 decimal digits). The conclusion from these computations is that fast convergence is indeed observed in double-precision arithmetic too.

In Table 8, we produce the results obtained again for the integral in Example 6.6, which is the most problematic again due to the (strong) $(x - t)^{-3}$ singularity of its integrand. As in Example 6.6, we took $t = 0.3$ in our computations.

Acknowledgements The author would like to thank Mr. Eitan Kaminski for producing the graphs included in this paper.

Appendix: Further generalization of the Euler–Maclaurin expansion

Lemma A.1 *Let $w \in C^{p-1}[a,b]$, $w^{(p)}(x)$ being absolutely integrable on $[a,b]$, and let*

$$w^{(i)}(a) = w^{(i)}(b) = 0, \quad i = 0, 1, \ldots, p-1. \tag{A.1}$$

Let also $h = (b-a)/n$, $n = 1, 2, \ldots$. Then,

$$h \sum_{j=1}^{n-1} w(a + jh) = \int_a^b w(x)\, dx + R_p(h), \tag{A.2}$$

with $R_p(h) = O(h^p)$ as $h \to 0$. Actually,

$$R_p(h) = -h^p \int_a^b w^{(p)}(x) \frac{\bar{B}_p(n\frac{a-x}{b-a})}{p!}\, dx, \tag{A.3}$$

$$\big|R_p(h)\big| \leq C_p\, h^p, \quad C_p = \frac{1}{p!} \Big(\max_{0 \leq z \leq 1} \big|B_p(z)\big|\Big)\bigg(\int_a^b \big|w^{(p)}(x)\big|\, dx \bigg) < \infty. \tag{A.4}$$

Here $B_p(x)$ is the p^{th} Bernoulli polynomial and $\bar{B}_p(x)$ is the p^{th} periodic Bernoulli function.[6]

Proof First, the classical E–M expansion with remainder[7] applies to the trapezoidal rule for $\int_a^b w(x)\, dx$ and we have

[6] $\bar{B}_p(x)$ is the 1-periodic extension of $B_p(x)$ defined as

$$\bar{B}_p(x) = B_p(x) \quad \text{if } 0 \leq x \leq 1 \quad \text{and} \quad \bar{B}_p(x) = B_p(x-k) \quad \text{if } k \leq x \leq k+1, \quad k = \pm 1, \pm 2, \ldots.$$

[7] For the classical E–M expansion with remainder, see Steffensen [35], Ralston and Rabinowitz [19, pp. 136–138], Stoer and Bulirsch [36, pp. 156–159], and Sidi [22, Appendix D], for example.

$$h\sum_{j=0}^{n}{}'' w(a+jh) = \int_a^b w(x)\,dx + \sum_{k=2}^{p} \frac{B_k}{k!}[w^{(k-1)}(b) - w^{(k-1)}(a)]h^k + R_p(h), \tag{A.5}$$

with

$$\sum_{j=0}^{n}{}'' \epsilon_j = \frac{1}{2}\epsilon_0 + \sum_{j=1}^{n-1} \epsilon_j + \frac{1}{2}\epsilon_n.$$

By (A.1), we have

$$h\sum_{j=0}^{n}{}'' w(a+jh) = h\sum_{j=1}^{n-1} w(a+jh) \quad \text{and} \quad \sum_{k=2}^{p} \frac{B_k}{k!}[w^{(k-1)}(b) - w^{(k-1)}(a)]h^k = 0.$$

Thus, (A.5) reduces to (A.2). Next, (A.4) follows by taking absolute values in (A.3). □

Theorem A.2 below, which we use in this work, is an extension of Theorem 2.3 in [26] that concerns HFP integrals $\oint_a^b f(x)\,dx$ with arbitrary algebraic endpoint singularities.

Theorem A.2 *Let $u \in C^{p-1}(a,b)$ such that $u \in C^{\infty}(I_1)$ and $u \in C^{p-1}(I_2)$, $u^{(p)}(x)$ being absolutely integrable in I_2, where*

$$I_1 = (a, a'') \cup (b'', b), \quad I_2 = [a'', b''], \quad a < a'' < b'' < b,$$

and assume that $u(x)$ has the asymptotic expansions

$$\begin{aligned} u(x) &\sim K(x-a)^{-1} + \sum_{s=0}^{\infty} c_s\,(x-a)^{\gamma_s} \quad \text{as } x \to a+, \\ u(x) &\sim L(b-x)^{-1} + \sum_{s=0}^{\infty} d_s\,(b-x)^{\delta_s} \quad \text{as } x \to b-, \end{aligned} \tag{A.6}$$

where the γ_s and δ_s are distinct complex numbers that satisfy

$$\begin{aligned} &\gamma_s \neq -1 \quad \forall s; \quad \mathbf{Re}\gamma_0 \leq \mathbf{Re}\gamma_1 \leq \mathbf{Re}\gamma_2 \leq \cdots; \lim_{s\to\infty} \mathbf{Re}\gamma_s = +\infty, \\ &\delta_s \neq -1 \quad \forall s; \quad \mathbf{Re}\delta_0 \leq \mathbf{Re}\delta_1 \leq \mathbf{Re}\delta_2 \leq \cdots; \lim_{s\to\infty} \mathbf{Re}\delta_s = +\infty. \end{aligned} \tag{A.7}$$

Assume furthermore that, for each positive integer k, $u^{(k)}(x)$ has asymptotic expansions as $x \to a+$ and $x \to b-$ that are obtained by differentiating those of $u(x)$ term by term k times.[8] *Let also $h = (b-a)/n$ for $n = 1, 2, \ldots$. Then, as $h \to 0$,*

[8] We express this briefly by saying that "the asymptotic expansions in (A.6) can be differentiated infinitely many times."

$$h\sum_{j=1}^{n-1}u(a+jh)\sim \oint_a^b u(x)\,dx + R_p(h) + K(C-\log h) + \sum_{\substack{s=0\\ \gamma_s\notin\{2,4,6,\dots\}}}^{\infty} c_s\,\zeta(-\gamma_s)\,h^{\gamma_s+1}$$
$$+ L(C-\log h) + \sum_{\substack{s=0\\ \delta_s\notin\{2,4,6,\dots\}}}^{\infty} d_s\,\zeta(-\delta_s)\,h^{\delta_s+1}, \tag{A.8}$$

where $R_p(h) = O(h^p)$ as $h \to 0$ and $C = 0.577\cdots$ is Euler's constant.[9]

Remark 1. Note that if $K = L = 0$ and $\mathrm{Re}\,\gamma_0 > -1$ and $\mathrm{Re}\,\delta_0 > -1$, then $\int_a^b u(x)\,dx$ exists as a regular integral. Otherwise, it does not, but its HFP $\oint_a^b u(x)\,dx$ exists.

2. When $u(x)$ is infinitely differentiable at $x = a$ and $x = b$, its Taylor series at $x = a$ and at $x = b$, whether convergent or divergent, are also (i) its asymptotic expansions as $x \to a+$ and as $x \to b-$, respectively, and (ii) they can be differentiated term by term any number of times. Thus, Theorem A.2 applies without further assumptions on $u(x)$ in this case.
3. When $u \in C^\infty(a, b)$, we have that $p = \infty$; therefore, $R_p(h)$ is absent from (A.8) since its contribution is smaller than each of the terms in the infinite sums there. That is, when $u \in C^\infty(a, b)$, the generalization of the E–M expansion is completely determined by the asymptotic expansions of $u(x)$ as $x \to a+$ and as $x \to b-$, nothing else being needed. What happens in (a, b) is immaterial. Precisely this result was obtained in Sidi [26, Theorem 2.3] and we shall make use of it when proving Theorem A.2. Thus, Theorem A.2 is a nontrivial extension of Theorem 2.3 in [26].
4. It is clear from (A.8) that the positive even powers of $(x - a)$ and $(b - x)$, if present in the asymptotic expansions of $u(x)$ as $x \to a+$ and $x \to b-$, do not contribute to the asymptotic expansion of $h\sum_{j=1}^{n-1} u(a + jh)$ as $h \to 0$, the reason being that $\zeta(-2k) = 0$ for $k = 1, 2, \dots$. We have included the "limitations" $\gamma_s \notin \{2, 4, 6, \dots\}$ and $\delta_s \notin \{2, 4, 6, \dots\}$ in the sums on the right-hand side of (A.8) only as "reminders."
5. Theorem 2.3 in [26] is only a special case of a more general theorem there involving the so-called *offset trapezoidal sum* $h\sum_{i=0}^{n-1} u(a + jh + \theta h)$, with $\theta \in (0, 1]$ fixed,[10] that contains as special cases all previously known generalizations of the E–M expansions for integrals with *algebraic* endpoint singularities. For a further generalization pertaining to arbitrary *algebraic-logarithmic* endpoint singularities, see Sidi [27].

Proof To prove (A.8), we begin by constructing two so-called *neutralizers* $R_\pm(x) \in C^\infty[a, b]$, such that $R_+(x) + R_-(x) = 1$ for all x, as follows: Choosing a', b' such

9 Note that the constants K and/or L in (A.6) hence in (A.8) can be zero.

10 When $u \in C[a, b]$ and $I[u] = \int_a^b u(x)\,dx$ exists as a regular integral, $Q_n[u] = h\sum_{i=0}^{n-1} u(a+jh+\theta h)$, is the *offset trapezoidal rule* for $I[u]$ and $\lim_{n\to\infty} Q_n[u;\theta] = I[f]$. Note that, with $\theta = 1/2$, the offset trapezoidal rule becomes the classical mid-point rule.
In case $\int_a^b u(x)\,dx$ does not exist as a regular integral, referring to $h\sum_{i=0}^{n-1} u(a+jh+\theta h)$ as an integration *rule* is meaningless. This is why we are referring to it as a *sum* and not as a *rule*.

that

$$a < a' < a'' < b'' < b' < b,$$

we let

$$\begin{aligned} R_+(x) &= 1 \quad \text{for } x \in [a, a'] \cup [b', b]; \qquad & R_+(x) &= 0 \quad \text{for } x \in [a'', b''], \\ R_-(x) &= 0 \quad \text{for } x \in [a, a'] \cup [b', b]; \qquad & R_-(x) &= 1 \quad \text{for } x \in [a'', b''], \end{aligned}$$

such that $R_+(x)$ decreases on (a', a'') and increases on (b'', b'), while $R_-(x)$ increases on (a', a'') and decreases on (b'', b'), and

$$R_\pm^{(i)}(a') = R_\pm^{(i)}(a'') = R_\pm^{(i)}(b'') = R_\pm^{(i)}(b') = 0, \quad i = 1, 2, \ldots. \tag{A.9}$$

With the functions $R_\pm(x)$ available, we now split $u(x)$ as in

$$u(x) = u_+(x) + u_-(x); \quad u_+(x) = R_+(x)u(x), \quad u_-(x) = R_-(x)u(x). \tag{A.10}$$

First, $u_+(x) \equiv u(x)$ for $x \in [a, a'] \cup [b', b]$ and $u_+(x) \equiv 0$ for $x \in [a'', b'']$; therefore, $u_+ \in C^\infty(a, b)$ and has the asymptotic expansions given in (A.6). Consequently, Theorem 2.3 in [26] applies (recall Remark 3 following the statement of Theorem A.2), and we have, as $h \to 0$,

$$\begin{aligned} h \sum_{j=1}^{n-1} u_+(a + jh) \sim \,&⨍_a^b u(x)\,dx + K(C - \log h) + \sum_{\substack{s=0 \\ \gamma_s \notin \{2,4,6,\ldots\}}}^{\infty} c_s\,\zeta(-\gamma_s)\,h^{\gamma_s+1} \\ &+ L(C - \log h) + \sum_{\substack{s=0 \\ \delta_s \notin \{2,4,6,\ldots\}}}^{\infty} d_s\,\zeta(-\delta_s)\,h^{\delta_s+1}. \end{aligned} \tag{A.11}$$

Next, $u_-(x) \equiv u(x)$ for $x \in [a'', b'']$ and $u_-(x) \equiv 0$ for $x \in [a, a'] \cup [b', b]$; therefore, $u_- \in C^{p-1}[a, b]$ and $u_-^{(i)}(a) = u_-^{(i)}(b) = 0$, $i = 0, 1, \ldots, p-1$, and $u_-^{(p)}(x)$ is absolutely integrable in $[a, b]$. Consequently, Lemma A.1 applies to $⨍_a^b u_-(x)\,dx$, which is now the regular integral $\int_a^b u_-(x)\,dx$, and we have

$$h \sum_{j=1}^{n-1} u_-(a + jh) = \int_a^b u_-(x)\,dx + R_p(h), \quad R_p(h) = O(h^p) \quad \text{as } h \to 0. \tag{A.12}$$

Finally, adding (A.12) to (A.11), noting that

$$h\sum_{j=1}^{n-1}u_+(a+jh)+h\sum_{j=1}^{n-1}u_-(a+jh)=h\sum_{j=1}^{n-1}u(a+jh),$$

and recalling also that

$$\neq\!\!\!\!\!\!\int_a^b u_+(x)\,dx+\neq\!\!\!\!\!\!\int_a^b u_-(x)\,dx=\neq\!\!\!\!\!\!\int_a^b u(x)\,dx,$$

we obtain (A.8). This completes the proof. □

Remark In [17], Navot extended the classical E–M expansion to integrands $f(x)$ with an algebraic end-point singularity of the form $f(x)=(x-a)^{\alpha}g(x)$ with $\alpha>-1$, $g\in C^{\infty}[a,b]$. Using a different approach, Lyness and Ninham [14], extended the E–M expansion further to singular integrands of the form $f(x)=(x-a)^{\alpha}g_a(x)=(b-x)^{\beta}g_b(x)$ with $\alpha,\beta>-1$, $g_a\in C^{\infty}[a,b)$, $g_b\in C^{\infty}(a,b]$. Theorem 2.3 in Sidi [26], generalizes all the above in that (i) it applies to finite-range integrals of integrands that have *arbitrary* algebraic endpoint singularities and (ii) these integrals can be defined in the regular sense or in the sense of HFP. Thus, it contains as special cases, but is not contained in, the classical E–M expansion and its extensions given in [14,17]. Being an extension of Theorem 2.3 in [26], Theorem A.2 is thus a further extension of the classical E–M expansion.

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