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The practical Gauss type rules for Hadamard finite-part integrals using Puiseux expansions

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Abstract A general framework is constructed for efficiently and stably evaluating the Hadamard finite-part integrals by composite quadrature rules. Firstly, the integrands are assumed to have the Puiseux expansions at the endpoints with arbitrary algebraic and logarithmic singularities. Secondly, the Euler-Maclaurin expansion of a general composite quadrature rule is obtained directly by using the asymptotic expansions of the partial sums of the Hurwitz zeta function and the generalized Stieltjes constant, which shows that the standard numerical integration formula is not convergent for computing the Hadamard finite-part integrals. Thirdly, the standard quadrature formula is recast in two steps. In step one, the singular part of the integrand is integrated analytically and in step two, the regular integral of the remaining part is evaluated using the standard composite quadrature rule. In this stage, a threshold is introduced such that the function evaluations in the vicinity of the singularity are intentionally excluded, where the threshold is determined by analyzing the roundoff errors caused by the singular nature of the integrand. Fourthly, two practical algorithms are designed for evaluating the Hadamard finite-part integrals by

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applying the Gauss-Legendre and Gauss-Kronrod rules to the proposed framework. Practical error indicator and implementation involved in the Gauss-Legendre rule are addressed. Finally, some typical examples are provided to show that the algorithms can be used to effectively evaluate the Hadamard finite-part integrals over finite or infinite intervals.

Keywords Hadamard finite-part integral · Algebraic and logarithmic singularity · Puiseux series · Error asymptotic expansion · Roundoff error analysis · Composite Gauss-Legendre rule · Gauss-Kronrod rule

Mathematics Subject Classification (2010) MSC 65B15 · MSC 65D30

1 Introduction

Hadamard [18] introduced the concept of hypersingular integral, which was defined to be the finite part of a divergent integral by dropping some divergent terms. This form of integral is later identified as the Hadamard finite-part (HFP) integral, usually denoted by $\displaystyle{=\!\!\!\!\!\!\int}_a^b f(x)dx$ for a given integrand $f(x)$. A general HFP integral is typically expressed as

$$H[\omega, g, a, b, t, \gamma] := {=\!\!\!\!\!\!\int}_a^b \frac{\omega(x)g(x)}{|x-t|^\gamma}dx,\ a \le t \le b,\ \gamma > 1, \tag{1.1}$$

where $\omega(x)$ is a weakly singular weight function involving algebraic and logarithmic endpoint singularities and $g(x)$ is a sufficiently smooth function. A typical $\omega(x)$ reads

$$\omega(x) = (x-a)^\alpha (b-x)^\beta (\log(x-a))^\mu (\log(b-x))^\nu,\ \alpha, \beta > -1(\text{real}),\ \mu, \nu \ge 0(\text{integer}).$$

The HFP integral (1.1) can be derived by expanding $g(x)$ in a Taylor's series [12]. For instance, if $\alpha - \gamma < -1$ is not an integer and denote the integer part of $\gamma - \alpha$ by m, then

$$\begin{aligned} H[(x-a)^\alpha, g, a, b, a, \gamma] &= {=\!\!\!\!\!\!\int}_a^b (x-a)^{\alpha-\gamma} g(x)dx \\ &= \int_a^b (x-a)^{\alpha-\gamma}\left[g(x) - \sum_{k=0}^{m-1}\frac{g^{(k)}(a)}{k!}(x-a)^k\right]dx + \sum_{k=0}^{m-1}\frac{g^{(k)}(a)(b-a)^{\alpha-\gamma+k+1}}{k!(\alpha-\gamma+k+1)}. \end{aligned} \tag{1.2}$$

In addition, if $\alpha - \gamma \le -1$ is an integer and denote its absolute value by m, then

$$\begin{aligned} H[(x-a)^\alpha, g, a, b, a, \gamma] &= \int_a^b (x-a)^{\alpha-\gamma}\left[g(x) - \sum_{k=0}^{m-1}\frac{g^{(k)}(a)}{k!}(x-a)^k\right]dx \\ &+ \sum_{k=0}^{m-2}\frac{g^{(k)}(a)(b-a)^{\alpha-\gamma+k+1}}{k!(\alpha-\gamma+k+1)} + \frac{g^{(m-1)}(a)}{(m-1)!}\log(b-a). \end{aligned} \tag{1.3}$$

The HFP integrals share some of the usual properties of regular integrals. For instance, they are additive on the interval of integration, changes of variable are allowed, but they do not behave well with respect to inequalities [12]. Many applications of the HFP integrals have been found in the boundary integral equations in mechanics, electrodynamics, aerodynamics, and acoustics, which were illustrated by Monegato [35] in a concise description. Zozulya [64] also considered the regularization of some type divergent integrals in boundary integral equations and boundary element methods based on the theory of distributions.

The highly efficient and highly accurate evaluations of the HFP integrals are very important for practical applications. In the past decades, numerous work has been devoted to the study of quadrature rules for these integrals. Here we mention two main classes of the numerical methods. The first one is based on formula (1.2) or (1.3). Since the integral on the right-hand side of Eq. 1.2 or Eq. 1.3 is a regular one, we can evaluate it by the standard numerical integration methods such as the Gaussian quadratures [10, 22, 40] and the composite Newton-Cotes type rules [13, 21, 49, 50]. The second one is the interpolation formula constructed by replacing $g(x)$ in Eq. 1.1 by its (piecewise) Lagrange or Lagrange-Hermite interpolation polynomial based on a set of distinct nodes [11, 16, 20, 28, 52, 56]. Monegato [32] examined some numerical approaches for the two kinds of the methods and showed that the first one is more accurate than the second one. Linz [28] also proved that the piecewise linear interpolation formula (also called composite trapezoidal rule) has only first order accuracy for $\gamma = 2$ in Eq. 1.1. But Wu and Sun [59] found this formula has superconvergence phenomenon when the singular point coincides with some a priori known points. Since then the superconvergence of the interpolation formulas has been investigated intensively by some authors [52, 60, 63]. In addition, there are some special methods which can evaluate the hypersingular integrals, see for example, the optimal methods in the sense of accuracy [2, 3] and the numerical quadrature of undetermined coefficient in boundary element calculation [6].

The HFP integrals can be interpreted as taking the analytic continuation of weakly singular integrals. Actually, the first integral on the right-hand side of Eq. 1.2 is a weakly singular integral. Hence, we can unify the treatment of the HFP integrals and the weakly singular integrals. For the weakly singular integral involving algebraic or logarithmic singularities at one or both endpoints, for example, $H[\omega, g, a, b, t, 0]$ in Eq. 1.1, where $\omega(x) = (x-a)^\alpha$ or $\omega(x) = (x-a)^\alpha \log(x-a)$ and $\alpha > -1$ (note that here the integral is degenerated to a regular one), Navot [36, 37] gave an extension of the Euler-Maclaurin formula when the integral is computed by generalized trapezoidal rule. The results were also obtained by Lyness and Ninham [30] via the Fourier expansion and some generalized functions. Ninham [38] also showed that Navot's expansions are valid for the HFP integral $H[(x-a)^\alpha, g, a, b, t, 0]$ when α takes any value other than a negative integer. The remaining case in which α is a negative integer was completed by Lyness [31]. Monegato and Lyness [33] also discussed the various Euler-Maclaurin expansions of the HFP integrals by using the Mellin transform. Based on Navot's results, Sidi [45, 47, 48] derived some general Euler-Maclaurin expansions of offset trapezoidal rule approximations for weakly singular integrals or the HFP integrals by assuming that the integrands have asymptotic expansions at the endpoints. Sidi's assumptions about $f(x)$ can be expressed as

$$\begin{aligned} f(x) &= \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(x-a))^{\mu_{0,j}}}{x-a} + \sum_{i=1}^{u} \sum_{j=0}^{u_i} c_{i,j}^{(1)} (x-a)^{\alpha_i} (\log(x-a))^{\mu_{i,j}} + r_a(x) \\ &:= f_a(x) + r_a(x),\ x > a, \end{aligned} \tag{1.4}$$

$$\begin{aligned} f(x) &= \sum_{j=0}^{v_0} c_{0,j}^{(2)} \frac{(\log(b-x))^{\nu_{0,j}}}{b-x} + \sum_{i=1}^{v} \sum_{j=0}^{v_i} c_{i,j}^{(2)} (b-x)^{\beta_i} (\log(b-x))^{\nu_{i,j}} + r_b(x) \\ &:= f_b(x) + r_b(x),\ x < b, \end{aligned} \tag{1.5}$$

where the exponents α_i and β_i $(i = 1, 2, \ldots)$ are all real numbers except -1 satisfying $\alpha_1 < \alpha_2 < \cdots$ and $\beta_1 < \beta_2 < \cdots$. Here parts of α_i or β_i may be less than -1. It is pointed out that the $\mu_{i,j}$ and $\nu_{i,j}$ in Eqs. 1.4 and 1.5 are all nonnegative integers and the remainders $r_a(x)$ and $r_b(x)$ can be sufficiently smooth over $[a, b]$ by choosing u and v suitably large. We note that α_i and β_i are all complex numbers in Sidi's work [45, 47, 48], but here we restrict them to real numbers. If $c_{0,j}^{(1)} = c_{0,j}^{(2)} = 0$ and both $\alpha_1, \beta_1 > -1$ in Eqs. 1.4 and 1.5, then the integral of $f(x)$ over $[a, b]$ is a weakly singular integral, otherwise, it exists in the sense of HFP. Sidi considered the case in which $c_{0,j}^{(1)} = c_{0,j}^{(2)} = 0$ and α_i, β_i are different from $-1, -2, \ldots$ in [45]. He also considered the cases that the integrands possess arbitrary algebraic singularities and more general algebraic-logarithmic singularities at one or both endpoints in [47] and [48], respectively. In Sidi's work, the trapezoidal rule was considered. We further designed practical Gauss type rules for weakly singular integrals based on Eqs. 1.4 and 1.5 in [58].

Equations 1.4 and 1.5 have also been used by some authors to derive the asymptotic expansions of a class of integrals [43] and the asymptotic solution to a class of nonlinear Volterra integral equations [19]. In [43], Sellier called the function $f(x)$ possessing Eq. 1.4 or Eq. 1.5 is of the first kind on the right at $x = a$ or on the left at $x = b$. Furthermore, Sellier considered the asymptotic expansion of $f(x)$ at $x = \infty$

$$\begin{aligned} f(x) &= \sum_{j=0}^{w_0} c_{0,j}^{(3)} \frac{(\log x)^{\rho_{0,j}}}{x} + \sum_{i=1}^{w} \sum_{j=0}^{w_i} c_{i,j}^{(3)} x^{-\delta_i} (\log x)^{\rho_{i,j}} + r_\infty(x) \\ &:= f_\infty(x) + r_\infty(x),\ x \to \infty, \end{aligned} \tag{1.6}$$

where $\delta_1 < \delta_2 < \cdots < \delta_w < 1$. Based on Eq. 1.6, Sellier also defined the HFP integral over a semi-infinite interval. Monegato and Lyness [33] derived the Euler-Maclaurin expansion of the infinite range HFP integral $⨎_0^\infty x^\alpha g(x)dx$ provided that $g(x)$ decays faster than any inverse power of x at infinity. Wang, Zhang and Huybrechs [55] derived the asymptotic expansions of oscillatory Hilbert transforms in both the senses of Cauchy principal value and HFP.

Sellier [43] pointed out that Eq. 1.4 or Eq. 1.5 or Eq. 1.6 is unique. The expansions (1.4)-(1.6) are formally called the Puiseux expansions in Mathematica, Matlab and Maple and some literature [1, 42], which are obviously a generalization of

Taylor's expansions. Nowadays, the Puiseux series of a function at a point can be easily obtained by symbolic computation, for instance, by the `Series` command of Mathematica. Here we list two examples.

For the function $f_1(x) = \arcsin x/x^{10}$, the Puiseux series at $x = 0$ and $x = 1$ are given respectively by

$$f_1(x) \sim \frac{1}{x^9} + \frac{1}{6x^7} + \frac{3}{40x^5} + \frac{5}{112x^3} + \frac{35}{1152x} + \frac{63x}{2816} + \frac{231x^3}{13312} + \cdots, \quad x \to 0^+, \tag{1.7}$$

$$f_1(x) \sim \frac{\pi}{2} - \sqrt{2}\sqrt{1-x} + 5\pi(1-x) - \frac{121}{6\sqrt{2}}(1-x)^{3/2} + \frac{55}{2}\pi(1-x)^2 + \cdots, \quad x \to 1^-. \tag{1.8}$$

For the function $f_2(x) = x^{\sqrt[3]{x}-3}\log(1-x)$, the Puiseux series at $x = 0$ and $x = 1$ are given respectively by

$$\begin{aligned} f_2(x) \sim &- \frac{1}{x^2} - \frac{\log x}{x^{5/3}} - \frac{(\log x)^2}{2x^{4/3}} - \frac{3+(\log x)^3}{6x} - \frac{12\log x + (\log x)^4}{24x^{2/3}} \\ &- \frac{30(\log x)^2 + (\log x)^5}{120\sqrt[3]{x}} - \frac{1}{720}\left(240 + 60(\log x)^3 + (\log x)^6\right) \\ &- \frac{\sqrt[3]{x}\left(1680\log x + 105(\log x)^4 + (\log x)^7\right)}{5040} + \cdots, \quad x \to 0^+, \end{aligned} \tag{1.9}$$

$$f_2(x) \sim \left[1 + 2(1-x) + \frac{10}{3}(1-x)^2 + \frac{89}{18}(1-x)^3 + \cdots\right]\log(1-x), \quad x \to 1^-. \tag{1.10}$$

Obviously, $x = 0$ is a strongly singular point for both $f_1(x)$ (algebraic singularity) and $f_2(x)$ (algebraic and logarithmic singularity) and $x = 1$ is also a singular point for both $f_1(x)$ (singularity of the derivative) and $f_2(x)$ (logarithmic singularity). Here we mention that Conceicão et al [9] developed analytical algorithms to evaluate some classes of Cauchy type singular integrals on the unit circle by using the symbolic computing capability of Mathematica.

One of the best methods for non-adaptive numerical integration of arbitrary functions is the Gauss-Legendre formula [41, 53]. An attractive property of the Gauss-Legendre rule is that all the function points are inside the range of integration and do not include the endpoints, which means that the singularities at one or both endpoints are unlikely to cause the formula to fail. However, the error estimates [29, 61] showed that the convergence rate is very slow when the integrands have integrable singularities inside, or at one or both endpoints of the interval. More precisely, Verlinden [54] proved an error asymptotic expansion of the Gauss-Legendre formula for the integrand with an endpoint singularity. Sidi [46] extended the result to functions that have arbitrary algebraic-logarithmic singularities at one or both endpoints. Usually, the Gauss-Legendre rule is not progressive, so the nodes must be recomputed whenever additional degrees of accuracy are desired. An alternative is to use the Gauss-Kronrod rule [5, 27, 34]. The Gauss-Kronrod rule is a variant of Gaussian quadrature, in which the evaluation points are chosen so that an accurate approximation can be computed by reusing the information produced by the computation of a less accurate approximation. The difference between a Gaussian quadrature rule and its Kronrod extension is often used as an estimate of the approximation error.

Recently, Wang et al [57] interpreted Eq. 1.4 or Eq. 1.5 without logarithms as a general fractional Taylor's expansion by defining high-order local fractional derivatives [25, 26], from which the error asymptotic expansion of trapezoidal rule was derived to approximate the integrals with algebraic singularities at some points by using the formula of sums of non-integral powers. In our more recent paper [58], we directly derived the error asymptotic expansion of a general composite quadrature rule for weakly singular integrals based on the assumption that the integrands possess Eqs. 1.4 and 1.5 with the case that $c_{0,j}^{(1)} = c_{0,j}^{(2)} = 0$ and both $\alpha_1, \beta_1 > -1$. By applying the error asymptotic expansion to the composite Gauss type rules and by simplifying the evaluations of the derivatives of the Hurwitz zeta function, practical composite Gauss-Legendre and Gauss-Kronrod rules and their error estimates are also obtained in that paper.

Following the discretizing ideas in [58], we consider the high accuracy computation of the general HFP integrals in this paper. We aim to construct a general framework for deriving the error asymptotic expansions of a general composite quadrature rule for the HFP integrals and then design efficient and stable algorithms to evaluate these integrals. Firstly, we assume that the integrand possesses Eq. 1.4, Eq. 1.5 or Eq. 1.6 at the endpoints $x = a$, $x = b$ or $x = \infty$. Secondly, we deduce the Euler-Maclaurin expansion of a standard composite quadrature rule by using the asymptotic expansion of $\sum_{k=0}^{n-1} (k+\theta)^{\alpha} (\log(k+\theta))^m$, where α is an arbitrary real number. This Euler-Maclaurin expansion formula is very general, which reveals the essence of each composite quadrature rule. It tells us that the standard quadrature formula is not suitable for evaluating the HFP integrals since the leading error term involves a factor $h^{1+\alpha_1}$, which tends to infinity as $h \to 0$ for $\alpha_1 < -1$. Thirdly, we recast the standard quadrature formula so that it can evaluate the HFP integrals. As indicated before, the HFP integral itself is a divergent one, but endowed a finite value by discarding some divergent terms. We say a good method should reflect this feature of the integrals. We do this in two steps. In step one, we integrate the singular part analytically since the Puiseux expansion of the integrand at its singularity is known. In step two, we compute the regular integral of the remaining part using the above composite quadrature rule. In this stage, we introduce a threshold such that the function evaluations in the vicinity of the singularity are intentionally excluded and the threshold is determined by analyzing the roundoff errors caused by the singular nature of the integrand. Fourthly, the average sum of the derivatives of the Hurwitz zeta function is approximately evaluated by elementary operations with high accuracy, such that the deduced algorithms have very high efficiency. After all these steps, the general framework for accurately and stably evaluating the HFP integrals is formulated. Finally, we obtain two practical algorithms for evaluating the HFP integrals over finite or infinite intervals by applying the Gauss-Legendre and Gauss-Kronrod rules to this framework.

The remainder of the paper is organized as follows. In Section 2, a collection of the preliminaries are provided, including the definitions and properties of the Bernoulli polynomials, the Riemann zeta function, the Hurwitz zeta function, the generalized Stieltjes constants and the HFP integrals. In Section 3, we first derive the error asymptotic expansion of a general composite rule for the HFP integrals possessing algebraic or logarithmic endpoint singularities in a rather intuitive way and then design numerically stable formulas to evaluate these integrals. In Section 4, we consider two practical Gauss type formulas for evaluating the HFP integrals over finite or infinite intervals, which are the composite Gauss-Legendre and Gauss-Kronrod rules. We also provide a computable error indicator for these methods. In Section 5, some typical numerical examples are provided to show the stability and accuracy of these methods. We end with a brief conclusion in Section 6.

2 Preliminaries

In this section, we collect the preliminary knowledge about the Bernoulli polynomials, the Riemann zeta function, the Hurwitz zeta function and the Stieltjes constants. We state some fundamental lemmas about the asymptotic expansions of the Hurwitz zeta function and its higher derivatives, as well as the generalized Stieltjes constants. We also introduce the precise definition of the HFP integrals and summarize their useful properties.

Definition 1 (Bernoulli polynomials [39]) The Bernoulli polynomials $B_k(x)$ ($k = 0, 1, 2, \ldots$) are defined as the coefficients of the following series

$$\frac{z\mathrm{e}^{xz}}{\mathrm{e}^z - 1} = \sum_{k=0}^{\infty} \frac{B_k(x)}{k!} z^k, \; |z| < 2\pi.$$

Furthermore, for a positive integer k the periodic Bernoulli function with period 1 is defined by

$$\widetilde{B}_k(x) = B_k\left(x - [x]\right),$$

where $[x]$ is the greatest integer less than or equal to x.

Definition 2 (Riemann zeta function and Hurwitz zeta function [7, 23, 24]) The Riemann zeta function is defined by the setting

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s}$$

for $\mathrm{Re}(s) > 1$ and by analytic continuation to other $s \neq 1$.

The Hurwitz zeta function $\zeta(s, a)$ is a generalization of the Riemann zeta function. It is classically defined by the formula

$$\zeta(s, a) = \sum_{k=0}^{\infty} \frac{1}{(k+a)^s}$$

for $\mathrm{Re}(s) > 1$ and by analytic continuation to other $s \neq 1$, where any term with $k + a = 0$ is excluded.

Obviously, the two zeta functions have some relations, for example, $\zeta(s, a) = \zeta(s, a+1) + a^{-s}$ and $\zeta(s, 1) = \zeta(s)$. The Bernoulli polynomials and the Hurwitz zeta function have many useful properties, which are summarized in [58]. Here we state some asymptotic expansions about the Riemann and Hurwitz zeta functions.

Lemma 1 *(Some expansions of the Riemann zeta and Hurwitz zeta functions)*

(1) *$\zeta(s)$ and $\zeta(s,a)$ hold the Laurent expansions*

$$\zeta(s) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{(-1)^k}{k} \gamma_k (s-1)^k, \ \zeta(s,a) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{(-1)^k}{k} \gamma_k(a)(s-1)^k,$$

where γ_k and $\gamma_k(a)$ are the Stieltjes constants and the generalized Stieltjes constants, respectively.

(2) *For $s \neq -1$ and $0 < a \leq 1$, the asymptotic expansion*

$$\zeta(-s,a) = a^s - \frac{1}{s+1} \sum_{l=0}^{q} \binom{s+1}{l} B_l(a) + (-1)^{q-1} \binom{s}{q} \int_1^{\infty} \widetilde{B}_q(x-a) x^{s-q} dx$$

holds true on condition that $q > s+1$ [36].

In the following, we state some useful properties of the Stieltjes constants defined in the Laurent expansions of zeta functions (see Lemma 1).

Lemma 2 *(Properties of the Stieltjes constants)*

(1) *$\gamma_k = \gamma_k(1)$, $\gamma_0 = \gamma$, where γ is the Euler's constant.*
(2) *$\gamma_k(a+1) = \gamma_k(a) - (\log a)^k / a$ for $a > 0$.*
(3) *For $0 < a \leq 1$ and $m, n = 0, 1, 2, \ldots$, there holds [62]*

$$\gamma_m(a) = \sum_{k=0}^{n} \frac{(\log(k+a))^m}{k+a} - \frac{(\log(n+a))^{m+1}}{m+1} - \frac{(\log(n+a))^m}{2(n+a)} + \int_n^{\infty} \widetilde{B}_1(x) g_m'(x) dx,$$

where $g_m(x) = (\log(x+a))^m / (x+a)$.

Define $\eta_{\alpha,m}(x) = x^{\alpha} (\log x)^m$, which will be used in the remaining part of this paper. For this function, we have the following lemma.

Lemma 3 *For $\forall \alpha \in \mathbb{R}$ and $m = 0, 1, 2, \ldots$, the lth order derivative of $\eta_{\alpha,m}(x)$ reads*

$$\eta_{\alpha,m}^{(l)}(x) = x^{\alpha-l} \sum_{k=0}^{\min(l,m)} \binom{m}{k} (\log x)^{m-k} \sum_{\rho=0}^{l-k} (\rho+1)_k s(l, k+\rho) \alpha^{\rho}, \tag{2.1}$$

where $(\rho+1)_k$ is the standard Pochhammer symbol and $s(l,k)$ denote the Stirling numbers of the first kind. For $\forall \alpha$, the Pochhammer symbol is defined by $(\alpha)_0 = 1$, $(\alpha)_k = \alpha(\alpha+1)\cdots(\alpha+k-1)$. In addition, the Stirling numbers of the first kind are defined by the recurrence relation [39] $s(l,k) = s(l-1,k-1) - (l-1)s(l-1,k)$ with initial values $s(0,0) = 1$, $s(l,0) = s(0,k) = 0$ for $l, k > 0$.

Proof For the function x^α, we have

$$\frac{\partial^l x^\alpha}{\partial x^l} = (-1)^l(-\alpha)_l x^{\alpha-l}.$$

Then, since $\eta_{\alpha,m}(x) = \partial^m x^\alpha/\partial\alpha^m$, we obtain

$$\eta^{(l)}_{\alpha,m}(x) = \frac{\partial^l}{\partial x^l}\frac{\partial^m x^\alpha}{\partial\alpha^m} = (-1)^l \sum_{k=0}^{m} \binom{m}{k} \frac{d^k(-\alpha)_l}{d\alpha^k} x^{\alpha-l}(\log x)^{m-k}. \tag{2.2}$$

Using a formula [8, 17]

$$(\alpha)^{(k)}_l = (-1)^{l-k}\sum_{\rho=0}^{l-k}(-1)^\rho(\rho+1)_k s(l, k+\rho)\alpha^\rho, \tag{2.3}$$

and noting that $(\alpha)^{(k)}_l = 0$ for $k > l$, we know Eq. 2.1 holds. □

Lemma 4 *(The asymptotic expansion of the generalized Stieltjes constants) For* $0 < \theta \le 1$, $m = 0, 1, 2\ldots$ *and any* $q \in \mathbb{N}$, *there holds*

$$\gamma_m(\theta) = \frac{(\log\theta)^m}{\theta} - \sum_{l=1}^{q}\frac{B_l(\theta)}{l!}\eta^{(l-1)}_{-1,m}(1) + \frac{(-1)^{q-1}}{q!}\int_1^\infty \widetilde{B}_q(x-\theta)\eta^{(q)}_{-1,m}(x)dx. \tag{2.4}$$

Proof Taking $n = 0$ and replacing a by θ in the formula of Lemma 2(3) (here $g_m(x)$ is substituted by $\eta_{-1,m}(x+\theta)$) gives

$$\begin{aligned}\gamma_m(\theta) &= \frac{(\log\theta)^m}{2\theta} - \frac{(\log\theta)^{m+1}}{m+1} + \int_0^\infty \widetilde{B}_1(x)\eta'_{-1,m}(x+\theta)dx \\ &= \frac{(\log\theta)^m}{2\theta} - \frac{(\log\theta)^{m+1}}{m+1} + \int_0^{1-\theta} B_1(x)\eta'_{-1,m}(x+\theta)dx + \int_{1-\theta}^\infty \widetilde{B}_1(x)\eta'_{-1,m}(x+\theta)dx.\end{aligned} \tag{2.5}$$

Noting that $B_1(x) = x - \frac{1}{2}$, integrating by parts implies

$$\int_0^{1-\theta} B_1(x)\eta'_{-1,m}(x+\theta)dx = \frac{(\log\theta)^m}{2\theta} - B_1(\theta)\eta_{-1,m}(1) + \frac{(\log\theta)^{m+1}}{m+1}.$$

Substituting this formula into Eq. 2.5 and taking $t = x + \theta$ for the last integral in Eq. 2.5, we have

$$\gamma_m(\theta) = \frac{(\log\theta)^m}{\theta} - B_1(\theta)\eta_{-1,m}(1) + \int_1^\infty \widetilde{B}_1(t-\theta)\eta'_{-1,m}(t)dt.$$

Performing integration by parts $q - 1$ times for the integral in the above formula, noticing that $\eta^{(l)}_{-1,m}(\infty) = 0$ for $\forall l \in \mathbb{N}$ (see Eq. 2.1) and the properties of the Bernoulli polynomials ($B'_k(x) = kB_{k-1}(x)$ and $B_k(1-x) = (-1)^k B_k(x)$ for $k \ge 1$ [58]), we can obtain (2.4). The lemma is proved. □

Lemma 5 *(Euler-Maclaurin expansion for sums* [44, 48, 51]*) Let J be an integer and $\theta \in [0, 1]$. Suppose that $f(x) \in C^q[J, \infty)$, then for any integer $n > J$,*

$$\sum_{k=J}^{n-1} f(k+\theta) = \int_J^n f(x)dx + \sum_{l=1}^{q} \frac{B_l(\theta)}{l!} \left[f^{(l-1)}(n) - f^{(l-1)}(J) \right] + \overline{R}_q(n,\theta), \quad (2.6)$$

where the remainder $\overline{R}_q(n,\theta)$ reads

$$\overline{R}_q(n,\theta) = -\frac{1}{q!}\int_J^n \widetilde{B}_q(\theta - x) f^{(q)}(x)dx = \frac{(-1)^{q-1}}{q!}\int_J^n \widetilde{B}_q(x-\theta) f^{(q)}(x)dx.$$

Lemma 6 *For $\alpha \neq -1$, $0 < \theta \leq 1$, and any $n, m \in \mathbb{N}$, $q > \alpha + 1$, there holds* [58]

$$\sum_{k=0}^{n-1} (k+\theta)^{\alpha} (\log(k+\theta))^m = (-1)^m \zeta_{\alpha}^{(m)}(-\alpha,\theta) + n^{1+\alpha} \sum_{k=0}^{m} \frac{(-1)^k m!}{(m-k)!} \frac{(\log n)^{m-k}}{(1+\alpha)^{k+1}} + \sum_{l=1}^{q} \frac{B_l(\theta)}{l!} \eta_{\alpha,m}^{(l-1)}(n) + R_q(n,m,\alpha,\theta), \quad (2.7)$$

where $\zeta_{\alpha}^{(m)}(-\alpha,\theta)$ implies $\partial^m \zeta(-\alpha,\theta)/\partial(-\alpha)^m$ and the remainder $R_q(n,m,\alpha,\theta)$ reads

$$R_q(n,m,\alpha,\theta) = \frac{(-1)^q}{q!}\int_n^{\infty} \widetilde{B}_q(x-\theta)\eta_{\alpha,m}^{(q)}(x)dx. \quad (2.8)$$

Lemma 7 *For $0 < \theta \leq 1$, and any $n \in \mathbb{N}$, there holds*

$$\sum_{k=0}^{n-1} \frac{(\log(k+\theta))^m}{k+\theta} = \gamma_m(\theta) + \frac{(\log n)^{m+1}}{m+1} + \sum_{l=1}^{q} \frac{B_l(\theta)}{l!} \eta_{-1,m}^{(l-1)}(n) + \widetilde{R}_q(n,m,\theta), \quad (2.9)$$

where the remainder $\widetilde{R}_q(n,m,\theta)$ reads

$$\widetilde{R}_q(n,m,\theta) = \frac{(-1)^q}{q!}\int_n^{\infty} \widetilde{B}_q(x-\theta)\eta_{-1,m}^{(q)}(x)dx. \quad (2.10)$$

This lemma has been proved by Sidi [48]. Here we provide a modified version of the proof.

Proof Let $f(x) = \eta_{-1,m}(x)$ and $J = 1$ in Eq. 2.6, we have

$$\sum_{k=0}^{n-1} \frac{(\log(k+\theta))^m}{k+\theta} = \frac{(\log\theta)^m}{\theta} + \frac{(\log n)^{m+1}}{m+1} + \sum_{l=1}^{q} \frac{B_l(\theta)}{l!} \left[\eta_{-1,m}^{(l-1)}(n) - \eta_{-1,m}^{(l-1)}(1) \right] + \overline{R}_q(n,\theta).$$

Noticing (2.4), we can obtain Eqs. 2.9 and 2.10. The proof is complete. □

As we have indicated in Section 1, the HFP integral is a regularizing one of divergent integral by dropping some divergent terms and keeping the finite part. Here we provide a general definition for the integral.

Definition 3 (The Hadamard finite-part)[43] For $h > 0$, there exist a family of non-negative integers (M_i), (K_i), two real families (β_i), (g_{ij}) and a function G such that

$$g(\varepsilon) = \sum_{i=0}^{N} \sum_{j=K_i}^{M_i} g_{ij} \varepsilon^{\beta_i} (\log \varepsilon)^j + G(\varepsilon), \ \forall \varepsilon \in (0, h), \tag{2.11}$$

where $\beta_N < \beta_{N-1} < \cdots < \beta_1 < \beta_0 = 0$ and $g_{00} = 0$ if $\beta_0 = 0$. If $C = \lim_{\varepsilon \to 0} G(\varepsilon)$ exists, then C is called the finite part in the Hadamard sense of the quantity $g(\varepsilon)$.

Applying Definition 3 to integral, we know if

$$g(\varepsilon) = \int_{\varepsilon}^{b} f(x)dx \text{ or } g(\varepsilon) = \int_{a}^{1/\varepsilon} f(x)dx,$$

then [33]

$$\,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_0^b f(x)dx = \lim_{\varepsilon \to 0} G(\varepsilon) \text{ or } \,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_a^{\infty} f(x)dx = \lim_{\varepsilon \to 0} G(\varepsilon).$$

For some special cases, we have for $b > 0$ [12, 32, 35, 43]

$$\,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_0^b x^{\alpha} (\log x)^m dx = \begin{cases} b^{1+\alpha} \sum_{k=0}^{m} \dfrac{(-1)^k m! (\log b)^{m-k}}{(m-k)!(1+\alpha)^{k+1}}, & \alpha \neq -1, \\ \dfrac{(\log b)^{m+1}}{m+1}, & \alpha = -1, \end{cases} \tag{2.12}$$

and for $a > 0$ [43]

$$\,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_a^{\infty} x^{\alpha} (\log x)^m dx = \begin{cases} -a^{1+\alpha} \sum_{k=0}^{m} \dfrac{(-1)^k m! (\log a)^{m-k}}{(m-k)!(1+\alpha)^{k+1}}, & \alpha \neq -1, \\ -\dfrac{(\log a)^{m+1}}{m+1}, & \alpha = -1. \end{cases} \tag{2.13}$$

We note that the first equality of Eq. 2.12 is exactly the regular one for $\alpha > -1$ and the first equality of Eq. 2.13 is also the regular one for $\alpha < -1$.

Lemma 8 *(Properties of the HFP integral* [12, 32, 35, 43]*)*

(1) *The HFP integral is additive with respect to the union of integration intervals, that is*

$$\,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_a^b \frac{f(x)}{|x-t|^{\alpha}} dx = \,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_a^t \frac{f(x)}{(t-x)^{\alpha}} dx + \,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_t^b \frac{f(x)}{(x-t)^{\alpha}} dx \text{ for } t \in (a,b) \text{ and } \forall \alpha \in \mathbb{R}.$$

(2) *If $f(x) = g(x) + C_0 (\log(x-a))^m/(x-a)$, where $g(x)$ may involve the term $(x-a)^{\alpha} (\log(x-a))^m$, but $\alpha \neq -1$, then a variable transformation $x = a + (b-a)t$ yields* [43]

$$\,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_a^b f(x)dx = (b-a) \,\,\,\,\!\!\!\!\!\!\!\!=\!\!\!\!\!\!\!\!\int_0^1 f(a+(b-a)t)dt + C_0 \frac{(\log(b-a))^{m+1}}{m+1}.$$

Lemma 9 *(The infinite range HFP integral* [43]*) If $f(x)$ possesses the Puiseux expansion* (1.6) *at $x = \infty$, then*

$$\begin{aligned}\displaystyle\fint_a^\infty f(x)dx &= \fint_a^b f(x)dx - \sum_{j=0}^{w_0} c_{0,j}^{(3)} \frac{(\log b)^{1+\rho_{0,j}}}{1+\rho_{0,j}} \\ &- \sum_{i=1}^{w}\sum_{j=0}^{w_i} c_{i,j}^{(3)} b^{1-\delta_i} \sum_{k=0}^{\rho_{i,j}} \frac{(-1)^k \rho_{i,j}!(\log b)^{\rho_{i,j}-k}}{(\rho_{i,j}-k)!(1-\delta_i)^{k+1}} + \int_b^\infty r_\infty(x)dx,\end{aligned} \tag{2.14}$$

where $b \geq a$ is an arbitrary positive number such that $f(x)$ has only one singularity at $x = \infty$ over the interval $[b, \infty)$.

For $\alpha > -1$, we know $\int_0^1 \zeta(-\alpha, \theta)\, d\theta = 0$ [4]. Generally, we have the following lemma.

Lemma 10 *There hold*

$$\fint_0^1 \zeta_\alpha^{(m)}(-\alpha, \theta)\, d\theta = 0 \text{ for } \alpha \neq -1; \quad \fint_0^1 \gamma_m(\theta)\, d\theta = 0, \; m = 0, 1, 2, \ldots. \tag{2.15}$$

Proof Taking $n = 1$ in Eq. 2.7, noting that $\eta_{\alpha,m}^{(l-1)}(1) = 0$ for $l \leq m$, we obtain for $q > m$

$$(-1)^m \zeta_\alpha^{(m)}(-\alpha, \theta) = \theta^\alpha (\log\theta)^m - \frac{(-1)^m m!}{(1+\alpha)^{m+1}} - \sum_{l=m+1}^{q} \frac{B_l(\theta)}{l!} \eta_{\alpha,m}^{(l-1)}(1) - R_q(1, m, \alpha, \theta). \tag{2.16}$$

Noticing (2.12) ($b = 1$) and $\int_0^1 B_l(x)dx = 0$ for $l \geq 1$, we conclude that the first integral of Eq. 2.15 vanishes. Analogously, from Eq. 2.4, using the formula (2.12) ($b = 1$) for the case $\alpha = -1$, we know the second integral of Eq. 2.15 also vanishes. The lemma is proved. □

In the last of this section, we emphatically point out that the N in Eq. 2.11 can not be extended to infinity. For example, for the function $f(x) = x^{1/x}$, we have

$$f(x) = \exp\left(\frac{\log x}{x}\right) = 1 + \frac{\log x}{x} + \sum_{m=2}^{\infty} \frac{(\log x)^m}{m! x^m}, \; x > 0.$$

Then for $0 < \varepsilon < 1$

$$\begin{aligned}\int_1^{1/\varepsilon} f(x)dx &= \frac{1}{\varepsilon} + \frac{(\log\varepsilon)^2}{2} + \sum_{m=2}^{\infty} \frac{1}{(m-1)^{m+1}} - 1 + \sum_{m=2}^{\infty}\sum_{k=0}^{m} \frac{(-1)^m \varepsilon^{m-1} (\log\varepsilon)^{m-k}}{(m-k)!(1-m)^{k+1}}, \\ \int_\varepsilon^1 f(x)dx &= -\frac{(\log\varepsilon)^2}{2} - \sum_{m=2}^{\infty}\sum_{k=0}^{m} \frac{(-1)^k \varepsilon^{1-m} (\log\varepsilon)^{m-k}}{(m-k)!(1-m)^{k+1}} + 1 - \sum_{m=2}^{\infty} \frac{1}{(m-1)^{m+1}} - \varepsilon.\end{aligned} \tag{2.17}$$

Obviously, we have by Definition 3

$$\ \mathop{=\!\!\!\!\!\!\int}_{1}^{\infty} f(x)dx = \sum_{m=2}^{\infty} \frac{1}{(m-1)^{m+1}} - 1 = 0.06687278808178032\cdots . \tag{2.18}$$

Noting that $N = \infty$ in Eq. 2.17, we can not obtain

$$\mathop{=\!\!\!\!\!\!\int}_{0}^{1} f(x)dx = 1 - \sum_{m=2}^{\infty} \frac{1}{(m-1)^{m+1}}$$

since

$$\int_{0}^{1} f(x)dx = 0.35349680070488065\cdots \tag{2.19}$$

is a regular integral.

3 The general framework for evaluating the HFP integrals

Let $f(x)$ be sufficiently smooth in (a, b) with Eqs. 1.4 and 1.5 at the two endpoints $x = a, b$. In this section, we assume that $\alpha_i \neq -1$, $\beta_i \neq -1$ and $\alpha_1 < -1$ or $\beta_1 < -1$, then the integral of $f(x)$ over $[a, b]$ only exists in the sense of Hadamard finite-part. Since

$$\mathop{=\!\!\!\!\!\!\int}_{a}^{b} f(x)dx = \mathop{=\!\!\!\!\!\!\int}_{-b}^{-a} f(-t)dt, \tag{3.1}$$

the singularity $x = b$ of $f(x)$ can be treated similarly as for the singularity $x = a$. In this and next sections, we only consider the case that $f(x)$ has only one singularity $x = a$, at which the Puiseux expansion (1.4) holds. Denote by

$$I[f; a, b] = \mathop{=\!\!\!\!\!\!\int}_{a}^{b} f(x)dx = \mathop{=\!\!\!\!\!\!\int}_{a}^{b} f_a(x)dx + \int_{a}^{b} r_a(x)dx, \tag{3.2}$$

where $f_a(x), r_a(x)$ are defined by (1.4) and $\mathop{=\!\!\!\!\!\int}_{a}^{b} f_a(x)dx$ can be evaluated by Eq. 2.12.

Firstly, for a function $g(t) \in C(0, 1)$, we define a general p-point numerical quadrature formula

$$\mathop{=\!\!\!\!\!\!\int}_{0}^{1} g(t)dt \approx \sum_{\lambda=1}^{p} \sigma_\lambda g(\theta_\lambda), \tag{3.3}$$

where $\sigma_\lambda > 0$ and $\theta_\lambda \in (0, 1)$ $(\lambda = 1, 2, \ldots, p)$ are the weights and abscissas, respectively. They have different values for different formulas, see for example, [41, 53] for the Gauss-Legendre rule and [5, 27, 34] for the Gauss-Kronrod rule.

Secondly, divide $[a, b]$ into n equal subintervals with step length $h = (b-a)/n$ and the nodes are denoted by $x_i = a + ih$, where $i = 0, 1, \ldots, n$. Then by Eqs. 1.4 and 3.3, noticing Lemma 8 (2), we have

$$\begin{aligned} I[f; a, b] &= \mathop{⨍}_{x_0}^{x_1} f(x)dx + \sum_{k=1}^{n-1} \int_{x_k}^{x_{k+1}} f(x)dx \\ &= h \sum_{k=0}^{n-1} \mathop{⨍}_0^1 f\left(a + (k+t)h\right) dt + \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log h)^{\mu_{0,j}+1}}{\mu_{0,j}+1} \\ &\approx h \sum_{\lambda=1}^{p} \sigma_\lambda \sum_{k=0}^{n-1} f\left(a + (k+\theta_\lambda)h\right) + \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log h)^{\mu_{0,j}+1}}{\mu_{0,j}+1} \\ &:= Q_n[f; a, b], \end{aligned} \tag{3.4}$$

where $Q_n[f; a, b]$ can be regarded as a general composite numerical quadrature formula for the HFP integral (3.2). The remainder of the formula is denoted by

$$E_{n,Q}[f; a, b] = I[f; a, b] - Q_n[f; a, b]. \tag{3.5}$$

Next we shall derive the asymptotic expansion of $E_{n,Q}[f; a, b]$ based on Lemmas 6 and 7.

In this section, we still use the symbol $\eta_{\alpha,m}(x) = x^\alpha (\log x)^m$. For the functions $\eta_{\alpha,\mu}(x-a)$ and $\eta_{\alpha,\mu}(b-x)$, where α is an arbitrary real and $\mu \geq 0$ is an integer, we have the following theorem.

Theorem 1 *The error asymptotic expansions of the general composite numerical quadrature formulas $Q_n[\eta_{\alpha,\mu}(\cdot - a); a, b]$ and $Q_n[\eta_{\alpha,\mu}(b - \cdot); a, b]$ in* Eq. 3.4 *are expressed as follows.*

(i) *For $\alpha \neq -1$ and $q > \alpha + 1$, there holds*

$$\begin{aligned} &E_{n,Q}[\eta_{\alpha,\mu}(\cdot - a); a, b] = E_{n,Q}[\eta_{\alpha,\mu}(b - \cdot); a, b] \\ &= -h^{1+\alpha} \sum_{m=0}^{\mu} \binom{\mu}{m} (-1)^m (\log h)^{\mu-m} \sum_{\lambda=1}^{p} \sigma_\lambda \zeta_\alpha^{(m)}(-\alpha, \theta_\lambda) \\ &\quad - \sum_{l=1}^{q} \frac{h^l}{l!} \eta_{\alpha,\mu}^{(l-1)}(b-a) \sum_{\lambda=1}^{p} \sigma_\lambda B_l(\theta_\lambda) + \frac{h^q}{q!} \max_{0 \leq x \leq 1} \left| \sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x - \theta_\lambda) \right| O(1). \end{aligned} \tag{3.6}$$

(ii) *For $\alpha = -1$ and $q > 0$, there holds*

$$\begin{aligned} &E_{n,Q}[\eta_{-1,\mu}(\cdot - a); a, b] = E_{n,Q}[\eta_{-1,\mu}(b - \cdot); a, b] \\ &= -\sum_{m=0}^{\mu} \binom{\mu}{m} (\log h)^{\mu-m} \sum_{\lambda=1}^{p} \sigma_\lambda \gamma_m(\theta_\lambda) \\ &\quad - \sum_{l=1}^{q} \frac{h^l}{l!} \eta_{-1,\mu}^{(l-1)}(b-a) \sum_{\lambda=1}^{p} \sigma_\lambda B_l(\theta_\lambda) + \frac{h^q}{q!} \max_{0 \leq x \leq 1} \left| \sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x - \theta_\lambda) \right| O(1). \end{aligned} \tag{3.7}$$

Proof The case $\alpha \neq -1$ corresponding to Eq. 3.6 can be proved from Lemma 6, see for example [58], where the result was obtained for $\alpha > -1$, but the arguments also hold true for $\alpha < -1$. The case $\alpha = -1$ for offset trapezoidal rule was proved by Sidi [48]. Here we provide a concise version of the proof for this general quadrature rule.

Firstly, a straightforward computation shows $E_{n,Q}[\eta_{-1,\mu}(\cdot - a); a, b] = E_{n,Q}[\eta_{-1,\mu}(b - \cdot); a, b]$. Secondly, taking $\eta_{-1,\mu}(x-a)$ as an example, we prove (3.7). Noting that $\sum_{\lambda=1}^{p}\sigma_\lambda = 1$, we have from Eq. 2.12, Eq. 3.4 and Lemma 7

$$\begin{aligned}E_{n,Q}[\eta_{-1,\mu}(\cdot - a); a, b] &= \tfrac{(\log(b-a))^{\mu+1}}{\mu+1} - \tfrac{(\log h)^{\mu+1}}{\mu+1}\\ &- \sum_{m=0}^{\mu}\tbinom{\mu}{m}(\log h)^{\mu-m}\sum_{\lambda=1}^{p}\sigma_\lambda\sum_{k=0}^{n-1}\tfrac{(\log(k+\theta_\lambda))^m}{k+\theta_\lambda}\\ &:= T_1 + T_2 + T_3 + T_4,\end{aligned} \tag{3.8}$$

where

$$\begin{aligned}T_1 &= -\sum_{m=0}^{\mu}\binom{\mu}{m}(\log h)^{\mu-m}\sum_{\lambda=1}^{p}\sigma_\lambda\gamma_m(\theta_\lambda),\\ T_2 &= \frac{(\log(b-a))^{\mu+1}}{\mu+1} - \frac{(\log h)^{\mu+1}}{\mu+1} - \sum_{m=0}^{\mu}\binom{\mu}{m}(\log h)^{\mu-m}\frac{(\log n)^{m+1}}{m+1},\\ T_3 &= -\sum_{m=0}^{\mu}\binom{\mu}{m}(\log h)^{\mu-m}\sum_{\lambda=1}^{p}\sigma_\lambda\sum_{l=1}^{q}\frac{B_l(\theta_\lambda)}{l!}\eta_{-1,m}^{(l-1)}(n),\\ T_4 &= -\sum_{m=0}^{\mu}\binom{\mu}{m}(\log h)^{\mu-m}\sum_{\lambda=1}^{p}\sigma_\lambda\widetilde{R}_q(n,m,\theta_\lambda).\end{aligned}$$

For $\eta_{-1,m}(x) = (\log x)^m/x$, we have [48]

$$\sum_{m=0}^{\mu}\binom{\mu}{m}(\log h)^{\mu-m}\eta_{-1,m}^{(l-1)}(x) = h^l\eta_{-1,\mu}^{(l-1)}(hx). \tag{3.9}$$

For T_2, noting that $(\log n)^{m+1}/(m+1) = \int_1^n \eta_{-1,m}(x)dx$ and Eq. 3.9 ($l = 1$), we can deduce it vanishes. Analogously, we can deduce that

$$T_3 = -\sum_{l=1}^{q}\frac{h^l}{l!}\eta_{-1,\mu}^{(l-1)}(b-a)\sum_{\lambda=1}^{p}\sigma_\lambda B_l(\theta_\lambda).$$

For the remainder T_4, noting (2.10) and Eq. 3.9, we have

$$T_4 = (-1)^{q+1}\frac{h^q}{q!}\int_n^\infty\sum_{\lambda=1}^{p}\sigma_\lambda\widetilde{B}_q(x-\theta_\lambda)\eta_{-1,\mu}^{(q)}(hx)h dx.$$

Noting that $\widetilde{B}_q(x-\theta_\lambda)$ is a periodic Bernoulli polynomial with period 1, we can obtain

$$|T_4| \le \frac{h^q}{q!}\max_{0\le x\le 1}\left|\sum_{\lambda=1}^{p}\sigma_\lambda\widetilde{B}_q(x-\theta_\lambda)\right|\int_{b-a}^{\infty}\left|\eta_{-1,\mu}^{(q)}(x)\right|dx.$$

From Eq. 2.1 (with $\alpha = -1$), we know the integral on the right-hand side of the above inequality exists. Substituting the expressions of T_i ($i = 1, 2, 3, 4$) into Eq. 3.8, we know Eq. 3.7 holds. □

For the function $f(x) \in C(a,b]$ possessing the Puiseux expansion (1.4) at $x = a$, we have

$$E_{n,Q}[f;a,b] = \sum_{j=0}^{u_0} c_{0,j}^{(1)} E_{n,Q}[(\cdot - a)^{-1} (\log(\cdot - a))^{\mu_{0,j}} ; a,b]$$

$$+ \sum_{i=1}^{u} \sum_{j=0}^{u_i} c_{i,j}^{(1)} E_{n,Q}[(\cdot - a)^{\alpha_i} (\log(\cdot - a))^{\mu_{i,j}} ; a,b] + E_{n,Q}[r_a; a,b].$$

Combining with Eqs. 3.6 and 3.7, we can prove the following theorem.

Theorem 2 *Suppose that $f(x) \in C(a,b]$ is sufficiently smooth except at $x = a$, where at this endpoint, $f(x)$ has arbitrary algebraic-logarithmic singularity and can be expanded as the Puiseux series* (1.4)*. When the HFP integral* (3.2) *is approximated by the general composite numerical quadrature formula $Q_n[f;a,b]$ defined by* Eq. 3.4*, the error asymptotic expansion reads*

$$\begin{aligned} E_{n,Q}[f;a,b] = &- \sum_{j=0}^{u_0} c_{0,j}^{(1)} \sum_{m=0}^{\mu_{0,j}} \binom{\mu_{0,j}}{m} (\log h)^{\mu_{0,j}-m} \sum_{\lambda=1}^{p} \sigma_\lambda \gamma_m(\theta_\lambda) \\ &- \sum_{i=1}^{u} \sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (-1)^m (\log h)^{\mu_{i,j}-m} \sum_{\lambda=1}^{p} \sigma_\lambda \zeta_{\alpha_i}^{(m)}(-\alpha_i, \theta_\lambda) \\ &- \sum_{l=1}^{q} \frac{h^l}{l!} f_a^{(l-1)}(b) \sum_{\lambda=1}^{p} \sigma_\lambda B_l(\theta_\lambda) + \frac{h^q}{q!} \max_{0 \le x \le 1} \left| \sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x - \theta_\lambda) \right| O(1) + E_{n,Q}[r_a; a,b]. \end{aligned} \tag{3.10}$$

Theorem 2 provides an Euler-Maclaurin type error asymptotic expansion of the general composite numerical quadrature formula for the HFP integral possessing an algebraic and logarithmic singularity at the lower endpoint. It tells us that the standard numerical integration formulas are not convergent for computing the HFP integral since $\lim_{h\to 0} h^{1+\alpha_1} = \infty$ for $\alpha_1 < -1$. Furthermore, a numerical instability problem could arise for these quadrature rules when $\theta_\lambda \to 0^+$ because $\lim_{x\to a^+} f(x) = \infty$. On the other hand, Theorem 2 also motivates us to modify the standard rules to evaluate the HFP integrals effectively. A key point is the consideration of stability. From Definition 3, we know the HFP integral is defined by discarding the divergent terms. For its numerical evaluation, we should avoid computing the integrand directly in the nearest vicinity of its each singularity.

By choosing $u^* \le u$ such that $\alpha_{u^*} < 0$ but $\alpha_{u^*+1} \ge 0$, we can split the functions $f_a(x)$ defined in (1.4) as

$$f_a(x) = f_{a,1}(x) + f_{a,2}(x),$$

where

$$\begin{aligned} f_{a,1}(x) &= \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(x-a))^{\mu_{0,j}}}{x-a} + \sum_{i=1}^{u^*} \sum_{j=0}^{u_i} c_{i,j}^{(1)} (x-a)^{\alpha_i} (\log(x-a))^{\mu_{i,j}}, \\ f_{a,2}(x) &= \sum_{i=u^*+1}^{u} \sum_{j=0}^{u_i} c_{i,j}^{(1)} (x-a)^{\alpha_i} (\log(x-a))^{\mu_{i,j}}. \end{aligned} \tag{3.11}$$

Since $\alpha_i < 0$ for $i = 1, 2, \ldots, u^*$, the function $f_{a,1}(x)$ is strongly or weakly singular at $x = a$. Meanwhile, the function $f_{a,2}(x)$ is not singular but its derivative or higher derivatives may be singular at $x = a$ due to the positive real values of α_i for $i = u^* + 1, u^* + 2 \ldots, u$.

Using Eq. 2.12, Eqs. 3.2 and 2.16, we obtain a modified version of Theorem 2.

Theorem 3 *Under the conditions of Theorem 2, the HFP integral* (3.2) *has the following asymptotic expansion*

$$\begin{aligned}
I[f;a,b] &= \ne\!\!\!\!\!\!\int_a^b f_{a,1}(x)dx + \int_a^b (f(x) - f_{a,1}(x))dx \\
&= \sum_{i=1}^{u^*}\sum_{j=0}^{u_i} c_{i,j}^{(1)} (b-a)^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log(b-a))^{\mu_{i,j}-m} \frac{(-1)^m m!}{(1+\alpha_i)^{m+1}} \\
&\quad + \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(b-a))^{\mu_{0,j}+1}}{\mu_{0,j}+1} + Q_n[f - f_{a,1}; a, b] \qquad (3.12)\\
&\quad - \sum_{i=u^*+1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j}-m} \left[\sum_{\lambda=1}^{p} \sigma_\lambda \theta_\lambda^{\alpha_i} (\log\theta_\lambda)^m - \frac{(-1)^m m!}{(1+\alpha_i)^{m+1}}\right] \\
&\quad + \sum_{i=u^*+1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j}-m} \sum_{l=m+1}^{q} \frac{1}{l!} \eta_{\alpha_i,m}^{(l-1)}(1) \sum_{\lambda=1}^{p} \sigma_\lambda B_l(\theta_\lambda) \\
&\quad + \sum_{i=u^*+1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j}-m} \frac{1}{q!} \max_{0\le x\le 1} \left|\sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x-\theta_\lambda)\right| O(1) \\
&\quad - \sum_{l=1}^{q} \frac{h^l}{l!} f_{a,2}^{(l-1)}(b) \sum_{\lambda=1}^{p} \sigma_\lambda B_l(\theta_\lambda) + \frac{h^q}{q!} \max_{0\le x\le 1} \left|\sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x-\theta_\lambda)\right| O(1) + E_{n,Q}[r_a; a, b].
\end{aligned}$$

Further by choosing $\lambda_1^* \le p$, the term

$$T_1^* := Q_n[f - f_{a,1}; a, b] - \sum_{i=u^*+1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j}-m} \sum_{\lambda=1}^{p} \sigma_\lambda \theta_\lambda^{\alpha_i} (\log\theta_\lambda)^m$$

can be approximated by

$$\begin{aligned}
T_1^* &\approx h \sum_{\lambda=1}^{p} \sigma_\lambda \sum_{k=1}^{n-1} \Bigg[f(a + (k+\theta_\lambda)h) - \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log((k+\theta_\lambda)h))^{\mu_{0,j}}}{(k+\theta_\lambda)h} \\
&\quad - \sum_{i=1}^{u^*}\sum_{j=0}^{u_i} c_{i,j}^{(1)} ((k+\theta_\lambda)h)^{\alpha_i} (\log((k+\theta_\lambda)h))^{\mu_{i,j}} \Bigg] \\
&\quad + h \sum_{\lambda=\lambda_1^*}^{p} \sigma_\lambda \left[f(a+\theta_\lambda h) - \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(\theta_\lambda h))^{\mu_{0,j}}}{\theta_\lambda h} - \sum_{i=1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} (\theta_\lambda h)^{\alpha_i} (\log(\theta_\lambda h))^{\mu_{i,j}} \right]
\end{aligned} \qquad (3.13)$$

We note that λ_1^* *is the minimal number of* λ *such that*

$$\varepsilon_{\text{round}}(\theta_\lambda) \le \varepsilon_{\text{rem}}(\theta_\lambda), \tag{3.14}$$

where

$$\begin{aligned} \varepsilon_{\text{round}}(\theta_\lambda) &= \varepsilon_{\text{mac}}(\theta_\lambda h)^{\alpha_1 - 1} \left| \sum_{j=0}^{u_1} c_{1,j}^{(1)} \left[\alpha_1 + \mu_{1,j} \left(\log(\theta_\lambda h)\right)^{-1}\right] \left(\log(\theta_\lambda h)\right)^{\mu_{1,j}} \right|, \\ \varepsilon_{\text{rem}}(\theta_\lambda) &= (\theta_\lambda h)^{\alpha_u} \left| \sum_{j=0}^{u_u} c_{u,j}^{(1)} \left(\log(\theta_\lambda h)\right)^{\mu_{u,j}} \right|, \end{aligned} \tag{3.15}$$

and $\varepsilon_{\text{mac}} = 2.22045 \times 10^{-16}$ *is the machine precision number.*

Proof (3.12) is a straightforward corollary of Eq. 3.10 combining with Eq. 2.12, Eqs. 2.16 and 3.11. As for Eq. 3.13, noting that

$$h^{\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j} - m} \sum_{\lambda=1}^{p} \sigma_\lambda \theta_\lambda^{\alpha_i} (\log \theta_\lambda)^m = \sum_{\lambda=1}^{p} \sigma_\lambda (\theta_\lambda h)^{\alpha_i} \left(\log(\theta_\lambda h)\right)^{\mu_{i,j}} .$$

we have by Eq. 3.4

$$\begin{aligned} T_1^* &= h \sum_{\lambda=1}^{p} \sigma_\lambda \sum_{k=1}^{n-1} \left[f\left(a + (k+\theta_\lambda)h\right) - f_{a,1}\left(a + (k+\theta_\lambda)h\right)\right] \\ &\quad + h \sum_{\lambda=1}^{p} \sigma_\lambda \left[f\left(a + \theta_\lambda h\right) - f_{a,1}\left(a + \theta_\lambda h\right) - f_{a,2}\left(a + \theta_\lambda h\right)\right]. \end{aligned} \tag{3.16}$$

For the evaluation of the second term on the right-hand side of Eq. 3.16, we should consider two problems, one is the severe cancellation when calculating the difference between $f\left(a + \theta_\lambda h\right)$ and $f_{a,1}\left(a + \theta_\lambda h\right) + f_{a,2}\left(a + \theta_\lambda h\right)$ for small θ_λ and the other is the roundoff errors when calculating $(\theta_\lambda h)^{\alpha_i}$ for negative α_i and small θ_λ. For the first problem, we can discard very small values by computing $\varepsilon_{\text{rem}}(\theta_\lambda)$ defined by Eq. 3.15. For the second problem, we need to evaluate the roundoff error for $\eta_{\alpha_i,\mu}(x) = x^{\alpha_i} (\log x)^\mu$. Given a perturbation ε for x, we have

$$\begin{aligned} &\eta_{\alpha_i,\mu}(x+\varepsilon) - \eta_{\alpha_i,\mu}(x) \\ &= \left(x^{\alpha_i} + \alpha_i \varepsilon x^{\alpha_i - 1} + \cdots\right) \left((\log x)^\mu + \frac{\mu\varepsilon}{x} (\log x)^{\mu-1} + \cdots\right) - x^{\alpha_i} (\log x)^\mu \\ &= \varepsilon x^{\alpha_i - 1} \left(\alpha_i + \frac{\mu}{\log x}\right) (\log x)^\mu + O(\varepsilon^2). \end{aligned}$$

Hence, for the function $(x-a)^{\alpha_1} \sum_{j=0}^{u_1} c_{1,j}^{(1)} \left(\log(x-a)\right)^{\mu_{1,j}}$, we can obtain its roundoff error $\varepsilon_{\text{round}}(\theta_\lambda)$ defined by Eq. 3.15 assuming that $x - a = \theta_\lambda h$ has a perturbation ε_{mac}. Since α_1 is the smallest value of all α_i, we can say $\varepsilon_{\text{round}}(\theta_\lambda)$ is the leading roundoff error for the function $f_{a,1}(x)$. From Eq. 3.15, we know $\varepsilon_{\text{round}}(\theta_\lambda)$ varies from large to small as θ_λ increases for $\alpha_1 < 0$, but $\varepsilon_{\text{rem}}(\theta_\lambda)$ varies from small to large as θ_λ increases for $\alpha_u > 0$, see the logarithmic plots of them in Fig. 1 for the function $f(x) = \arcsin x/x^{10}$. Hence, the best choice of λ_1^* is such that $\varepsilon_{\text{round}}(\theta_\lambda) \approx \varepsilon_{\text{rem}}(\theta_\lambda)$, or Eq. 3.14 holds for practical purpose. The proof is complete. □

Theorem 3 is somewhat lengthy, but its idea is rather simple. Firstly, the HFP integral can be decomposed as $I[f; a, b] = I[f_{a,1}; a, b] + I[f_{a,2}; a, b] + I[r_a; a, b]$. Since $r_a(x)$ is not small when x is far away from the lower endpoint a, the remaining integral $I[r_a; a, b]$ can not be neglected. Hence, we split the integral as $I[f; a, b] = I[f_{a,1}; a, b] + I[f - f_{a,1}; a, b]$. Secondly, the HFP integral $I[f_{a,1}; a, b]$ is evaluated analytically, see the first and second terms on the right-hand side of Eq. 3.12. Thirdly, the regular integral $I[f - f_{a,1}; a, b]$ is approximated by quadrature formula $Q_n[f - f_{a,1}; a, b]$ with error terms involving the evaluations of $\zeta_{\alpha_i}^{(m)}(-\alpha_i, \theta_\lambda)$, which is heavy in computation. Hence, $\zeta_{\alpha_i}^{(m)}(-\alpha_i, \theta_\lambda)$ is substituted by Eq. 3.16, which yields the fourth to sixth terms on the right-hand side of Eq. 3.12. Finally, since $\lim_{x\to a^+} f(x) = \infty$, as well as $\lim_{x\to a^+} f_{a,1}(x) = \infty$, the direct evaluation of $f(x) - f_{a,1}(x)$ will cause large roundoff error when x tends to a. The best treatment for this difficulty is avoiding such function evaluations. Observing Eq. 3.12 carefully, we find that the term T_1^* defined by Eq. 3.16 is the only one needing to treat specially. By computing $\varepsilon_{\text{round}}(\theta_\lambda)$ (perturbation error of $\eta_{\alpha,\mu}(x)$) and $\varepsilon_{\text{rem}}(\theta_\lambda)$ (the last term of $f_{a,2}(x)$) defined by Eq. 3.15, we can solve this problem perfectly.

Since the function evaluations at the points near the singularity are intentionally excluded in Eq. 3.13 and the choice of λ_1^* is nearly optimal, the algorithm based on Eq. 3.12 is numerically stable and highly efficient.

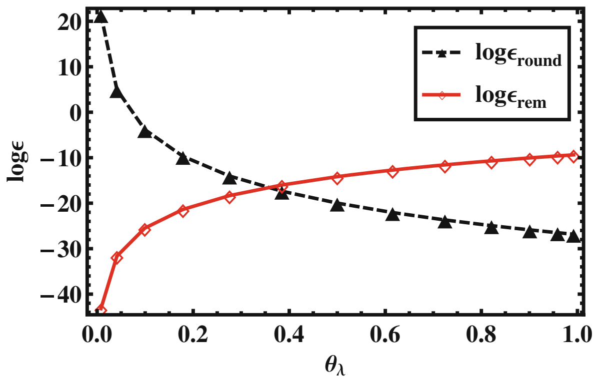

Fig. 1 The logarithmic graphs of $\varepsilon_{\text{round}}(\theta_\lambda)$ and $\varepsilon_{\text{rem}}(\theta_\lambda)$

The Puiseux expansion of a function at its singularity is needed in Eq. 3.12. This is not hard since it can be easily proceeded by symbolic computation. Hence, we can use Eq. 3.12 combining with Eq. 3.13 to evaluate the HFP integrals. Noting that the last five terms on the right-hand side of Eq. 3.12 are not easy to evaluate, the quadrature formulas with high degree of accuracy are preferable. In next section, we present two practical composite Gaussian type rules to effectively compute the HFP integrals.

4 Practical composite Gaussian type rules

In this section, we shall design practical Gauss-Legendre and Gauss-Kronrod quadrature rules based on Theorem 3 to efficiently evaluate the HFP integrals.

4.1 Composite Gauss-Legendre algorithm

The p-point Gauss-Legendre quadrature rule has degree of accuracy as high as $2p-1$. Hence, for the Bernoulli polynomial $B_l(x)$, we have [58]

$$\sum_{\lambda=1}^{p} \sigma_\lambda B_l(\theta_\lambda) = \begin{cases} 0, & l = 1, 2, \ldots, 2p-1, \\ -\dfrac{(p!)^4}{(2p+1)[(2p)!]^2}, & l = 2p, \\ 0, & l > 2p \text{ is odd}, \\ -\dfrac{(p!)^4 l!}{(2p+1)[(2p)!]^3 (l-2p)!} B_{l-2p}(\xi), & 0 < \xi < 1,\ l > 2p \text{ is even}, \end{cases} \tag{4.1}$$

where θ_λ, σ_λ are the abscissas and weights of p-point Gauss-Legendre quadrature formula over [0, 1], respectively. For $\widetilde{B}_q(x-\theta)$, it can be easily proved that [58]

$$\max_{0\le x\le 1} \left| \sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x-\theta_\lambda) \right| = \frac{(2p+2)(p!)^4}{12[(2p)!]^2} \text{ for } q = 2p+2. \tag{4.2}$$

From (1.4), we can choose u such that $\alpha_u < 2p$ and $r_a(x) \in C^{2p}[a,b]$. Hence, the error of the composite p-point Gauss-Legendre rule for $r_a(x)$, denoted by $E_{n,GL}[r_a; a, b]$, reads [58]

$$E_{n,GL}[r_a; a, b] = \tfrac{h^{2p}(p!)^4(b-a)}{(2p+1)[(2p)!]^3} r_a^{(2p)}(\xi_a),\ a < \xi_a < b. \tag{4.3}$$

Taking $q = 2p+2$ in Eq. 3.12 and noticing (3.13), then by substituting (4.1)-(4.2) into Eq. 3.12, we can prove the following theorem.

Theorem 4 *Suppose that $f(x) \in C(a,b]$ has an algebraic-logarithmic singularity at $x = a$ with the Puiseux expansion (1.4), then the HFP integral (3.2) can be* *evaluated by a modified version of p-point composite Gauss-Legendre quadrature rule. The formula and the error read, respectively*

$$
\begin{aligned}
MGL_n[f;a,b] &:= \sum_{i=1}^{u^*}\sum_{j=0}^{u_i} c_{i,j}^{(1)} (b-a)^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log(b-a))^{\mu_{i,j}-m} \frac{(-1)^m m!}{(1+\alpha_i)^{m+1}} \\
&+ \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(b-a))^{\mu_{0,j}+1}}{\mu_{0,j}+1} + h\sum_{\lambda=1}^{p}\sigma_\lambda \sum_{k=1}^{n-1}\Bigg[f\,(a+(k+\theta_\lambda)h) \qquad (4.4)\\
&- \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log((k+\theta_\lambda)h))^{\mu_{0,j}}}{(k+\theta_\lambda)h} - \sum_{i=1}^{u^*}\sum_{j=0}^{u_i} c_{i,j}^{(1)} ((k+\theta_\lambda)h)^{\alpha_i} (\log((k+\theta_\lambda)h))^{\mu_{i,j}} \Bigg] \\
&+h\sum_{\lambda=\lambda_1^*}^{p}\sigma_\lambda \left[f\,(a+\theta_\lambda h) - \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(\theta_\lambda h))^{\mu_{0,j}}}{\theta_\lambda h} - \sum_{i=1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} (\theta_\lambda h)^{\alpha_i} (\log(\theta_\lambda h))^{\mu_{i,j}} \right] \\
&+ \sum_{i=u^*+1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j}-m} \frac{(-1)^m m!}{(1+\alpha_i)^{m+1}},
\end{aligned}
$$

$$
\begin{aligned}
&EGL_n[f;a,b] := \\
&h\sum_{\lambda=1}^{\lambda_1^*-1}\sigma_\lambda \left[f\,(a+\theta_\lambda h) - \sum_{j=0}^{u_0} c_{0,j}^{(1)} \frac{(\log(\theta_\lambda h))^{\mu_{0,j}}}{\theta_\lambda h} - \sum_{i=1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} (\theta_\lambda h)^{\alpha_i} (\log(\theta_\lambda h))^{\mu_{i,j}} \right] \\
&- \frac{(p!)^4}{(2p+1)[(2p)!]^3} \sum_{i=u^*+1}^{u}\sum_{j=0}^{u_i} c_{i,j}^{(1)} h^{1+\alpha_i} \sum_{m=0}^{\mu_{i,j}} \binom{\mu_{i,j}}{m} (\log h)^{\mu_{i,j}-m} \left[\eta_{\alpha_i,m}^{(2p-1)}(1) + O\,(1)\right] \quad (4.5)\\
&+ \frac{h^{2p}(p!)^4}{(2p+1)[(2p)!]^3} \left[f_{a,2}^{(2p-1)}(b) + O(h^2)\right] + \frac{h^{2p+2}(p!)^4}{12(2p+1)[(2p)!]^3} O\,(1) \\
&+ \frac{h^{2p}(p!)^4(b-a)}{(2p+1)[(2p)!]^3} r_a^{(2p)}(\xi_a),
\end{aligned}
$$

where u^* is defined such that $\alpha_{u^*} < 0$, but $\alpha_{u^*+1} \geq 0$ and λ_1^* is defined by Eq. 3.14-3.15.

Theorem 4 shows that the Gauss-Legendre rule can be used to accurately and stably evaluate the HFP integrals. In practical computation, some issues need to be addressed.

Firstly, we should know in prior the power exponents α_i, $\mu_{i,j}$ and the corresponding coefficients $c_{i,j}^{(1)}$ in the Puiseux expansion (1.4), which can be easily obtained by symbolic computation. For instance, by using the `Series` command of Mathematica, we have the Puiseux series

```
s=Normal[Series[f[x], {x, a, 8}, Assumptions → a < x < b]]
s=s/.{x − a → t, x → t + a}
```

From the series expansion `s` we can obtain the power exponents and their coefficients. For the HFP integral, the power exponents α_i may be any real numbers or even complex ones.

Secondly, the first error term in Eq. 4.5 can be approximated by

$$\begin{aligned} e_a^{(0)} &:= h\sum_{\lambda=1}^{\lambda_1^*-1}\sigma_\lambda\sum_{j=0}^{u_u}c_{u,j}^{(1)}(\theta_\lambda h)^{\alpha_u}(\log(\theta_\lambda h))^{\mu_{u,j}} \\ &\approx h\sum_{\lambda=1}^{\lambda_1^*-1}\sigma_\lambda\left[f(a+\theta_\lambda h)-\sum_{j=0}^{u_0}c_{0,j}^{(1)}\frac{(\log(\theta_\lambda h))^{\mu_{0,j}}}{\theta_\lambda h}-\sum_{i=1}^{u}\sum_{j=0}^{u_i}c_{i,j}^{(1)}(\theta_\lambda h)^{\alpha_i}(\log(\theta_\lambda h))^{\mu_{i,j}}\right]. \end{aligned} \tag{4.6}$$

For the second error term in Eq. 4.5, we should choose p moderately large such that this term has precision 10^{-16} in most cases. For example, for the term

$$\varepsilon_p=\frac{(p!)^4}{(2p+1)[(2p)!]^3}\eta_{\alpha,m}^{(2p-1)}(1)=\frac{(p!)^4}{(2p+1)[(2p)!]^3}\sum_{\rho=0}^{2p-m-1}(\rho+1)_m s(2p-1,m+\rho)\alpha^\rho,$$

when $p=13$, we list some absolute values of ε_p for typical values of α and m in Table 1 (note: 4.31E−20 = 4.31×10^{-20}).

Table 1 shows that $|\varepsilon_p|$ decays as α increases, but $|\varepsilon_p|$ increases as m increases. It also tells us that $p\geq 13$ can guarantee the approximation of the second error term in Eq. 4.5 does not affect the total accuracy if we set double precision as our computational goal. In most cases, we can set $p=13$. If m is large, for example, $m\geq 10$, we can also set $p=15$. As for the last three terms in Eq. 4.5, because all of them involve a factor h^{2p} ($h<1$), they are much smaller than the second error term.

Thirdly, the assumption $\alpha_u\approx 2p$ in the derivation of Eqs. 4.4 and 4.5 are needed. But in practical computation, we usually set $\alpha_u\approx 8$. This results in another error term in Eq. 4.4. For example, the leading error term in Eq. 4.4 reads

$$\begin{aligned} e_a^{(1)} &= -h\sum_{\lambda=\lambda_1^*}^{p}\sigma_\lambda\sum_{j=0}^{u_u}c_{u,j}^{(1)}(\theta_\lambda h)^{\alpha_u}(\log(\theta_\lambda h))^{\mu_{u,j}} \\ &\quad+\sum_{j=0}^{u_u}c_{u,j}^{(1)}h^{1+\alpha_u}\sum_{m=0}^{\mu_{u,j}}\binom{\mu_{u,j}}{m}(\log h)^{\mu_{u,j}-m}\frac{(-1)^m m!}{(1+\alpha_u)^{m+1}} \\ &= e_a^{(0)}-\sum_{j=0}^{u_u}c_{u,j}^{(1)}h^{1+\alpha_u}\sum_{m=0}^{\mu_{u,j}}\binom{\mu_{u,j}}{m}(\log h)^{\mu_{u,j}-m}\left[\sum_{\lambda=1}^{p}\sigma_\lambda\theta_\lambda^{\alpha_u}(\log\theta_\lambda)^m-\frac{(-1)^m m!}{(1+\alpha_u)^{m+1}}\right]. \end{aligned} \tag{4.7}$$

Table 1 Gauss-Legendre rule($p=13$): values of $|\varepsilon_p|$ for some values of α and m

$m\backslash\alpha$	$\frac{1}{7}$	$\frac{4}{5}$	$\frac{3}{2}$	$\frac{7}{3}$	$\frac{13}{4}$	$\frac{13}{3}$	$\frac{13}{2}$
0	4.31E−20	7.20E−21	1.93E−21	2.59E−22	3.76E−23	8.37E−24	7.58E−25
1	1.28E−19	5.18E−20	4.68E−21	6.18E−23	5.30E−23	3.24E−24	7.15E−25
5	1.77E−16	1.54E−17	8.72E−19	9.33E−20	2.56E−20	3.98E−21	2.45E−22
10	1.56E−14	4.57E−15	9.83E−16	8.42E−17	6.45E−18	6.08E−20	4.60E−20
15	8.90E−14	4.47E−14	2.00E−14	6.74E−15	1.60E−15	1.39E−16	1.74E−18

Verlinden [54] proved for the p-point Gauss-Legendre quadrature rule

$$\sum_{\lambda=1}^{p} \sigma_\lambda \theta_\lambda^s - \frac{1}{1+s} = \sum_{k=1}^{\infty} c_k(s) \left(p + \frac{1}{2}\right)^{-2(s+k)}, \quad s > -1, \tag{4.8}$$

where the coefficients $c_k(s)$ are very difficult to evaluate. By differentiating (4.8) m times with respect to s and denoting by $\omega = (p + 1/2)^{-2}$, Sidi [46] further obtained

$$\sum_{\lambda=1}^{p} \sigma_\lambda \theta_\lambda^s (\log \theta_\lambda)^m - \frac{(-1)^m m!}{(1+s)^{m+1}} = \sum_{k=1}^{\infty} \omega^{s+k} \sum_{j=0}^{m} \binom{m}{j} c_k^{(m-j)}(s) (\log \omega)^j . \tag{4.9}$$

Hence, we have

$$e_a^{(1)} \approx e_a^{(0)} + O\left(h^{1+\alpha_u} (\log h)^{\mu_{u,uu}} \omega^{1+\alpha_u} (\log \omega)^{\mu_{u,uu}}\right). \tag{4.10}$$

Since the error term $e_a^{(0)}$ is a part of $e_a^{(1)}$, we output $e_a^{(1)}$ as the leading error term, from which we can adjust the input parameters to get satisfactory result.

Remark 1 For the case that $f(x) \in C(a, b)$ possesses a singularity at $x = b$ with the Puiseux expansion (1.5), the transform (3.1) is enough to get the error asymptotic expansion for the HFP integral (3.2). If $f(x)$ has two endpoint singularities, we can also evaluate the integral by splitting $I[f; a, b] = I[f; a, (a+b)/2] + I[f; (a+b)/2, b]$. For interior singularity $c \in (a, b)$, we further split the integral as $I[f; a, b] = I[f; a, c] + I[f; c, b]$. Hence, the algorithm in this section is valid for all the algebraic and logarithmic singularities inside or at the endpoints of the interval.

4.2 Composite Gauss-Kronrod algorithm

Gauss-Kronrod formulas are extensions of the Gauss quadrature rules generated by adding $r + 1$ points to a r-point rule in such a way that the resulting rule is of order $3r + 1$ at least (actually, the order is $3r + 2$ for odd r). These extra points are the zeros of the Stieltjes polynomials. This allows for computing higher order estimates while reusing the function values of a lower order estimate. In Eq. 3.3, $p = 2r + 1$ is set and θ_λ, σ_λ are the nodes and weights of the p-point Gauss-Kronrod rule over [0, 1], respectively, which can be computed by the algorithms in [5, 27]. Ehrich [14, 15] obtained the precise order of the remainder of the Gauss-Kronrod quadrature formula, which satisfies

$$|R_p(g)| = \left| \int_0^1 g(t)dt - \sum_{\lambda=1}^{p} \sigma_\lambda g(\theta_\lambda) \right| \leq c_{3r+2+\kappa} \left\| g^{(3r+2+\kappa)}(t) \right\|_\infty , \tag{4.11}$$

where

$$\kappa = \left[\frac{r+1}{2}\right] - \left[\frac{r}{2}\right] \text{ and } c_{3r+2+\kappa} \sim \frac{2^{-6r-3-\kappa} r^{-5/2}}{(3r+2+\kappa)!}. \tag{4.12}$$

Setting $q = 3r + 4 + \kappa$, we have

$$\max_{0 \le x \le 1} \left| \sum_{\lambda=1}^{p} \sigma_\lambda \widetilde{B}_q(x - \theta_\lambda) \right| \sim \frac{(3r+3+\kappa)(3r+4+\kappa)}{12} 2^{-6r-3-\kappa} r^{-5/2}. \quad (4.13)$$

The composite Gauss-Kronrod quadrature formula for the HFP integral can be easily derived by simply replacing the abscissas and weights in Eq. 4.4 with the ones of the p-point Gauss-Kronrod rule. But the remainder (4.5) should be modified by using the formulas (4.11)-(4.13). On the other hand, the practical error indicator (4.7) is still valid for the Gauss-Kronrod rule. We note that $p \ge 15$ (corresponding to $r = 7$) should be chosen to guarantee the integral having double precision evaluations.

4.3 Extension to infinite range finite-part integrals

In this subsection, we show the modified composite Gauss-Legendre and Gauss-Kronrod rules are capable of computing infinite range finite-part integrals.

Assume that $f(x)$ is defined on the interval (a, ∞), which can yield the Puiseux expansion (1.6) at the singularity $x = \infty$. Hence, there holds Eq. 2.14 for the HFP integral $⨍_a^\infty f(x)dx$, where in Eq. 2.14, we have indicated that b is a positive number such that $f(x)$ has only one singularity $x = \infty$ over the interval $[b, \infty)$. Here, we only need to show that the infinite range integral on the right-hand side of Eq. 2.14 can be effectively evaluated by the composite Gauss-Legendre and Gauss-Kronrod rules. Actually, for the integrand $r_\infty(x)$ defined over $[b, \infty)$, the simple variable transformation $x = 1/t$ yields

$$\int_b^\infty r_\infty(x)dx = \int_0^{1/b} r_\infty\left(\frac{1}{t}\right)\frac{1}{t^2}dt := \int_0^{1/b} g_0(t)dt. \quad (4.14)$$

We note that Eq. 4.14 may be a weakly singular integral with singularity $x = \infty$ or $t = 0$ and the Puiseux expansion of $r_\infty(1/t)$ at $t = 0$ is exactly the same one of $f(x)$ at $x = \infty$ except the strongly singular terms. Hence, we can perform the Puiseux expansion (1.6) only once by setting $\delta_w \approx 8$. Then the formula (4.4) with a minor modification can be used to evaluate this integral efficiently. For example, for the function $f(x) = x^{5/2}e^{1/x}\log x$, its Puiseux expansion at $x = \infty$ reads

$$f(x) = f_{\infty,1}(x) + f_{\infty,2}(x) + \widetilde{r}_\infty(x), \quad (4.15)$$

where

$$\begin{aligned} f_{\infty,1}(x) &= \left(x^{5/2} + x^{3/2} + \tfrac{\sqrt{x}}{2} + \tfrac{x^{-1/2}}{6}\right)\log x, \\ f_{\infty,2}(x) &= \left(\tfrac{x^{-3/2}}{24} + \tfrac{x^{-5/2}}{120} + \tfrac{x^{-7/2}}{720} + \cdots + \tfrac{x^{-15/2}}{3628800}\right)\log x, \end{aligned} \quad (4.16)$$

and $\widetilde{r}_\infty(x)$ is the remainder. From (4.15), we know

$$⨍_1^\infty f(x)dx = ⨍_1^\infty f_{\infty,1}(x)dx + \int_1^\infty \left(f(x) - f_{\infty,1}(x)\right)dx,$$

where the strongly singular part $⨎_1^{\infty} f_{\infty,1}(x)dx$ is evaluated analytically and $f_{\infty,2}(x)$ is used to effectively evaluate the remaining regular integral, see Eq. 3.12 or Eq. 4.4 for detail.

Analogously, if the integrand $f(x)$ is defined on $(-\infty, a)$, then the variable transformation $x = -y$ yields [12]

$$⨎_{-\infty}^{a} f(x)dx = ⨎_{-a}^{\infty} f(-y)dy,$$

from which we know the above method is also valid for this integral.

At the end of this section, we conclude that there are three ways to get highly accurate evaluations for the HFP integrals, which are decreasing the step length of the composite formula, increasing the order of the Puiseux expansion and increasing the nodal points of the Gauss-Legendre or Gauss-Kronrod rule. In the following, we summarize the selection of these parameters. Firstly, we note that the computational goal is getting double precision evaluations. Secondly, since the second error term in Eq. 4.5 does not count into the output error, we should select p suitably large such that this term is small enough. From Table 1, we know the number of the nodal points in the Gauss quadrature rules can reasonably set $p = 13$ for the Gauss-Legendre rule and $p = 15$ for the Gauss-Kronrod rule. Thirdly, from Eq. 3.16, we need to evaluate $f(a + \theta_\lambda h) - f_{a,1}(a + \theta_\lambda h) - f_{a,2}(a + \theta_\lambda h)$ in the computation. Obviously, large α_u in the Puiseux expansion (1.4) will result in more computational burdens. On the other hand, since $f(x)$ is singular at $x = a$, we know $\lim_{x\to a^+} f(x) = \infty$ and also $\lim_{x\to a^+} f_{a,1}(x) = \infty$, which will result in the lost of numerical accuracy in function evaluations. The selection of α_u should avoid these computations when $\theta_\lambda h$ is very small, that is, we should guarantee $\varepsilon_{\text{rem}}(\theta_\lambda)$ in Eq. 4.15 is less than 10^{-16} for some λ. Empirically, the setting $\alpha_u \approx 8$ satisfies these demands. Analogously, we set $\beta_v, \delta_w \approx 8$ in Eqs. 1.5 and 1.6, respectively. Finally, we point out that the step length h should not be too small, otherwise, the roundoff error will enlarge. In our computation in next section, $h = 0.5$ is chosen.

5 Numerical examples

In this section, some typical examples are provided to illustrate the high efficiency of the modified composite Gauss-Legendre and Gauss-Kronrod rules for evaluating the HFP integrals. Since Mathematica can easily formulate the Puiseux expansions of a function at some special points and can achieve arbitrary precision in numerical computation, we write two Mathematica functions to implement the algorithms, which are `Hfpcgl[f,a,b,xfd]` and `Hfpcgk[f,a,b,xfd]`, corresponding to the modified composite Gauss-Legendre rule and Gauss-Kronrod rule, respectively. In the above Mathematica functions, `b` may be an infinity and `xfd` is a one-dimensional array indicating all the algebraic and logarithmic (weakly or strongly) singular points inside or at the endpoints of the interval, which should be known in advance. If `xfd` is an empty set, written as `xfd`= {} in Mathematica, then the algorithms automatically implement the standard composite Gauss-Legendre or Gauss-Kronrod quadrature rule, which means that the integral is regular.

We point out that all the experiments are performed on the desktop computer with Intel Core i5 CPU (2.80GHZ) and 4GB RAM by using Mathematica 8.0. The abscissas and weights of the quadrature rule are obtained by the command `NIntegrate`GaussBerntsenEspelidRuleData` (the Gauss-Legendre rule) or `NIntegrate`GaussKronrodRuleData` (the Gauss-Kronrod rule).

Example 1 Compute the following HFP integrals over finite intervals using the modified composite Gauss-Legendre (MGL) and Gauss-Kronrod (MGK) rules.

$$
\begin{aligned}
&(1) \; ⨎_0^1 f_1(x)dx = \frac{35\log 2}{1152} - \frac{1319}{82944} - \frac{\pi}{18}, \;\; f_1(x) = \frac{\arcsin x}{x^{10}};\\
&(2) \; ⨎_{-1}^1 f_2(x)dx = 0, \;\; f_2(x) = \frac{1}{\sqrt{(1-x^2)^3}\left(x-\frac{1}{2}\right)^3};\\
&(3) \; ⨎_{-\pi/2}^{\pi/2} f_3(x)dx = \frac{3240\log 2 - 3409}{180\sqrt{2}}, \;\; f_3(x) = \frac{1}{(1-\sin x)^{3/2}(1-\cos x)^{5/2}};\\
&(4) \; ⨎_0^1 f_4(x)dx = \frac{1}{50}\left(-63 + 5\sqrt{3}\pi + 45\log 3\right), \;\; f_4(x) = \frac{1}{x^{8/3}}\log\left(\frac{x}{1-x}\right);\\
&(5) \; ⨎_0^1 f_5(x)dx, \;\; f_5(x) = x^{\sqrt[3]{x}-3}\log(1-x).
\end{aligned}
$$

In this example, all the parameters are taken as the ones stated in the last of Section 4. The computational results are shown in Table 2, where C-value, O-error, T-error and Time(s) represent the computational value, the absolute output error computed by Eq. 4.7, the true error and the CPU time in second, respectively.

Table 2 The computational results in Example 1

	C-value	O-error	T-error	Time(s)
(1)(MGL)	−0.16937606162779417	5.92272E−10	3.52654E−11	0.015
(1)(MGK)	−0.16937606163507724	9.40976E−10	4.25485E−11	0.015
(2)(MGL)	−7.60281E−13	2.04759E−11	7.60281E−13	0.031
(2)(MGK)	2.60059E−12	2.76051E−11	−2.60059E−12	0.047
(3)(MGL)	−4.56949347023129	3.68268E−11	−2.36762E−11	0.047
(3)(MGK)	−4.56949347021662	8.67494E−11	−3.83462E−11	0.047
(4)(MGL)	0.27289086907151305	9.43868E−13	5.09592E−14	0.031
(4)(MGK)	0.27289086907157634	4.25524E−14	−1.23235E−14	0.032
(5)(MGL)	−199.59943991061854	3.01292E−16	—	0.063
(5)(MGK)	−199.59943991061854	1.52752E−14	—	0.063

For the results in Table 2, we give the following expositions.

(**i**) The exact values of the HFP integrals are obtained by analytic method, which is illustrated by $f_1(x)$. Let $I(\varepsilon) = \int_{\varepsilon}^{1} f_1(x)dx$, then by Mathematica

$$I(\varepsilon) = \frac{\arcsin\varepsilon}{9\varepsilon^9} + \frac{\sqrt{1-\varepsilon^2}}{3456\varepsilon^8}\left(105\varepsilon^6 + 70\varepsilon^4 + 56\varepsilon^2 + 48\right) - \frac{35}{1152}\log\varepsilon + \frac{35}{1152}\log\left(\sqrt{1-\varepsilon^2}+1\right) - \frac{\pi}{18}.$$

Expanding $I(\varepsilon)$ at $\varepsilon = 0$ yields

$$I(\varepsilon) = \frac{1}{8\varepsilon^8} + \frac{1}{36\varepsilon^6} + \frac{3}{160\varepsilon^4} + \frac{5}{224\varepsilon^2} - \frac{35\log\varepsilon}{1152} + \left(\frac{35\log 2}{1152} - \frac{1319}{82944} - \frac{\pi}{18}\right) - \frac{63\varepsilon^2}{5632} + O\left(\varepsilon^4\right),$$

from which we can obtain by Definition 3

$$⨎_0^1 f_1(x)dx = \frac{35\log 2}{1152} - \frac{1319}{82944} - \frac{\pi}{18}.$$

We can also evaluate the integrals in this example using the method for calculating the integral $⨎_1^{\infty} x^{1/x}dx$ in Section 2. But there are some integrals that can not be evaluated by analytic methods. In such cases, the exact value is not provided and the T-error in Table 2 shows "—", see for example, the integral (5) in this example.

(**ii**) Table 2 shows all the evaluations are highly accurate and very fast, as well as numerically stable. It also verifies that the error indicator (O-error) is a good one in practical computation since the O-error is well matched with the T-error (true error).

(**iii**) A prerequisite to proceed the algorithms efficiently is to know all the algebraic and logarithmic singular points over the interval, indicated by a one-dimensional array `xfd`. Generally speaking, `xfd` is easy to be determined by observing and analyzing the integrand. For instance, for the function $f_1(x)$, $x = 0$ is obviously a strong algebraic singularity. We also know $\arcsin x$ is insufficiently smooth at $x = 1$. Hence, `xfd`=$\{0, 1\}$ for this function, see Eqs. 1.7 and 1.8, the Puiseux expansions of $f_1(x)$ at $x = 0$ and $x = 1$, respectively. Analogously, it can be seen that `xfd`=$\{-1, 1/2, 1\}$ for $f_2(x)$, `xfd`=$\{0, \pi/2\}$ for $f_3(x)$ and `xfd`=$\{0, 1\}$ for both $f_4(x)$ and $f_5(x)$. We note that both $f_2(x)$ and $f_3(x)$ possess an interior strong singularity. For such cases, the algorithms automatically decompose the interval into some subintervals that have singularities at the endpoints. We also point out that $f_5(x)$ has Eqs. 1.9 and 1.10 at $x = 0$ and $x = 1$, respectively.

(**iv**) In our algorithms, the parameters p (number of the nodal points), h (step length) and α_u, β_v (orders of the Puiseux expansions) can be adjusted to increase the accuracy. In Tables 3-5, we list the true errors for different parameters when applying

Table 3 The true errors of Example 1 (1) for different h

h	0.1	1/6	0.25	0.5
T-error	−9.79532E−10	5.63579E−12	2.92513E−13	3.52654E−11

Table 4 The true errors of Example 1 (1) for different p

p	11	13	15	17
T-error	1.43648E−9	3.52654E−11	8.08717E−12	5.85854E−11

the Gauss-Legendre rule to Example 1 (1), where the primary parameters are set $p = 13$, $h = 0.5$ and $\alpha_u, \beta_v \approx 8$. As is well known, the roundoff errors in the computation of the standard quadrature formulas may tend to infinity as $h \to 0$ or $p \to \infty$ for strongly singular integrals. The results in Tables 3-5 verify that the technique to control the roundoff error (see Eqs. 3.13–3.15) is successful. These results show that moderately small h and large p, as well as moderately large α_u, β_v are preferred for the practical computation of the HFP integrals.

(**v**) It can be seen from Table 2 that the Gauss-Legendre (MGL) and the Gauss-Kronrod (MGK) rules have almost the same accuracy. Noting that $p = 13$ for the MGL and $p = 15$ for the MGK, we can conclude that the Gauss-Legendre rule is more powerful than the Gauss-Kronrod rule.

Example 2 Compute the following HFP integrals over infinite intervals using the modified composite Gauss-Legendre and Gauss-Kronrod rules.

$$(6)\ \neq\!\!\!\!\int_0^\infty f_6(x)dx = -0.52941084553842824707\cdots,\quad f_6(x) = \frac{e^{-x}(\log x)^3}{x^{3/2}};$$

$$(7)\ \neq\!\!\!\!\int_1^\infty f_7(x)dx = 1.30113165436459561 57\cdots,\quad f_7(x) = x^{5/2}e^{1/x}\log x;$$

$$(8)\ \neq\!\!\!\!\int_5^\infty f_8(x)dx = -144.66944956258316844\cdots,\quad f_8(x) = x^{7/2}(\log x)^2\sin\left(\frac{1}{x}\right);$$

$$(9)\ \neq\!\!\!\!\int_0^\infty f_9(x)dx = 0.42036958878320229719\cdots,\quad f_9(x) = x^{1/x};$$

$$(10)\ \neq\!\!\!\!\int_0^\infty f_{10}(x)dx,\quad f_{10}(x) = \frac{K_0(x)}{x^{7/2}I_0(x)},$$

where in (9), the exact value can be obtained by Eqs. 2.18 and 2.19 and in (10), $I_0(x)$ and $K_0(x)$ are the modified Bessel functions of the first kind and second kind of order zero, respectively.

In this example, all the integrals are computed via Eq. 1.4 or Eq. 1.6, Eqs. 2.14 and 4.14 and the results are shown in Table 6. We point out that $x = 0$ is the only algebraic and logarithmic singularity for both $f_6(x)$ and $f_{10}(x)$ since

Table 5 The true errors of Example 1 (1) for different α_u, β_v

α_u, β_v	6	7	8	9
T-error	6.26913E−10	3.52441E−11	3.52654E−11	1.19667E−11

Table 6 The computational results in Example 2

	C-value	O-error	T-error	Time(s)
(6)(MGL)	−0.5294108455384139	2.40293E−14	−1.39888E−14	0.015
(6)(MGK)	−0.5294108455384243	5.79474E−14	−3.55271E−15	0.016
(7)(MGL)	1.3011316543645832	5.77417E−13	1.24345E−14	0.016
(7)(MGK)	1.3011316543645914	8.05516E−13	4.21885E−15	0.016
(8)(MGL)	−144.66944956258305	5.84902E−13	−1.13687E−13	0.016
(8)(MGK)	−144.66944956258305	6.28433E−13	−1.13687E−13	0.016
(9)(MGL)	0.42036958878319247	3.95039E−16	9.82547E−15	0.015
(9)(MGK)	0.42036958878320335	2.18518E−13	−1.05471E−15	0.016
(10)(MGL)	−0.34165816425517354	1.37281E−12	—	0.359
(10)(MGK)	−0.34165816425518225	1.30499E−13	—	0.39

$f_{10}(x) = (-\log x - \gamma + \log 2)/x^{7/2} + \cdots$ and e^{-x}, $K_0(x)/I_0(x) \sim e^{-2x}/\pi$ are rapidly decaying functions when $x \to \infty$. We further point out that $x = \infty$ is the only algebraic and logarithmic singularity for all the functions $f_7(x)$ (see Eqs. 4.15 and 4.16 for its Puiseux expansion), $f_8(x)$ and $f_9(x)$. It can be seen from Table 6 that all the five integrals get accurate numerical values with less CPU time.

From Examples 1-2, we conclude that the modified Gauss-Legendre and Gauss-Kronrod rules in this paper can be used to effectively and stably evaluate the HFP integrals over finite and infinite intervals.

6 Conclusions

In this paper, we construct a general framework to derive the error asymptotic expansion of a general composite quadrature formula for approximating the HFP integrals, where the integrands are assumed to have the Puiseux expansions at the endpoints with arbitrary algebraic and logarithmic singularities. By applying the framework to the Gauss-Legendre and Gauss-Kronrod rules, two practical composite Gauss type rules and their error indicators are obtained. The proposed methods have the following features.

(1) The algorithms need the Puiseux expansions of the integrand at its singularities, which can be easily obtained by symbolic computation.
(2) The algorithms are numerically stable since the roundoff errors caused by the singular nature of the integrand are considered.
(3) The algorithms are not only suitable for evaluating the HFP integrals over finite intervals, but also valid for infinite range integrals with singularity at infinity.
(4) Since the canonical algorithms are the standard Gauss-Legendre and Gauss-Kronrod rules, the abscissas and weights are easily obtained from numerical books or algorithm libraries.

(5) The algorithms treat some kinds of singularities (weak or strong, algebraic or logarithmic) in a uniform way by defining a one-dimensional array.
(6) The algorithms can be used to numerically solve hypersingular integral equations by combining with collocation method, which will be studied in the near future.

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