Numer. Math. (1998) 81: 273–291

Numerische Mathematik

The Euler-Maclaurin expansion and finite-part integrals

G. Monegato[1,⋆], **J. N. Lyness**[2,⋆⋆]

[1] Dipartimento di Matematica, Politecnico di Torino, Cso. Duca degli Abruzzi 24, I-10129 Torino, Italy
[2] Mathematics and Computer Science Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439, USA

Received June 11, 1997 / Revised version received December 15, 1997

Summary. In this paper we compare $G(p)$, the Mellin transform (together with its analytic continuation), and $\overline{\overline{G}}(p)$, the related Hadamard finite-part integral of a function $g(x)$, which decays exponentially at infinity and has specified singular behavior at the origin. Except when p is a nonpositive integer, these coincide. When p is a nonpositive integer, $\overline{\overline{G}}(p)$ is well defined, but $G(p)$ has a pole. We show that the terms in the Laurent expansion about this pole can be simply expressed in terms of the Hadamard finite-part integral of a related function. This circumstance is exploited to provide a conceptually uniform proof of the various generalizations of the Euler-Maclaurin expansion for the quadrature error functional.

Mathematics Subject Classification (1991): 65D30

1. The one-dimensional Euler-Maclaurin expansion

The prototype problem in numerical quadrature is that of approximating an integral

$$If = \int_0^1 f(x)dx \tag{1.1}$$

⋆ This author was supported by the Ministero dell'Università e della Ricerca Scientifica e Tecnologica of Italy

⋆⋆ This author was supported in part by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Computational and Technology Research, U.S. Department of Energy, under Contract W-31-109-Eng-38. Part of this work was performed while this author was a visiting professor at the Politecnico di Torino, under the sponsorship of the Italian C.N.R.-Gruppo Nazionale per l'Informatica Matematica

Correspondence to: G. Monegato

by a sum of function values of the form

$$Qf = \sum_{i=1}^{\nu} w_i f(x_i)$$

and finding expressions for the approximation error (see Davis and Rabinowitz (1984)). An early expression of this type is the Euler-Maclaurin expansion, which appeared first in the early eighteenth century. In its modern form this is an asymptotic expansion of the discretization error associated with the μ-panel offset trapezoidal rule

$$\tilde{S}_\mu f(\beta) = \frac{1}{\mu} \sum_{k=0}^{\mu-1} f\left(\frac{\beta+k}{\mu}\right).$$

The standard form of the Euler-Maclaurin asymptotic expansion, valid when $f(x)$ is regular, is

$$\text{(1.2)} \quad \tilde{S}_\mu f(\beta) - If \simeq \sum_{n=0} \frac{f^{(n)}(0)}{n!} \frac{\zeta(-n,\beta)}{\mu^{n+1}} - \sum_{n=0} \frac{f^{(n)}(1)}{n!} \frac{\zeta(-n,\beta)}{\mu^{n+1}},$$

where $\zeta(s,\beta)$ denotes the generalized zeta function, defined in (4.4) below. (When $\beta = 1$, this reduces to the more familiar Riemann zeta function $\zeta(s)$. When s is a positive integer,

$$\text{(1.3)} \quad \zeta(-s,\beta) = -B_{1+s}(\beta)/(1+s),$$

where $B_n(x)$ is the Bernoulli polynomial of degree n.)

When $f(x)$ is $C^{(p)}[0,1]$, (1.2) may be expressed as a finite sum of p terms, and the remainder term, of order $O(\mu^{-p-1})$, has a simple integral representation.

An important extension of this expansion was discovered by Navot (1961). This applied to a situation in which $f(x)$ has an integrable algebraic singularity at an end of the integration interval. When

$$\text{(1.4)} \quad f(x) = x^\alpha g(x),$$

where $\alpha > -1$ and $g(x)$ is $C^{(p)}[0,1]$, the expansion (1.2) has to be modified by replacing the first sum by

$$\sum_{n=0} \frac{g^{(n)}(0)}{n!} \frac{\zeta(-n-\alpha,\beta)}{\mu^{n+\alpha+1}}.$$

Navot's proof is lengthy. During subsequent years, shorter proofs have appeared from time to time. Straightforward corollaries of Navot's result provide asymptotic expansions for integrand functions having algebraic-logarithmic singularities at one end and for integrand functions having this sort of singularity at both ends of the integration interval.

A second important extension was discovered by Ninham (1966). Ninham showed that Navot's expansion is valid as written for functions defined by (1.4) when α takes any value other than a negative integer. For $\alpha < -1$, the integral If must be defined as a Hadamard finite-part integral. See Lemma 2.3 below. Ninham's proof is long.

Completing this set of results is the expansion when α is a negative integer (Lyness 1994). This resembles Navot's expansion in form; however, the coefficients are different, and an additional term in $\log \mu$ has to be included.

The present paper is devoted to a general proof of the one-dimensional Euler-Maclaurin expansion. This proof, based on the Mellin transform, embraces all of the cited variants in a single proof. It is based on a recently discovered approach due to Verlinden (1993). (See also Verlinden and Haegemans 1993.) In this paper, that approach is extended to hypersingular integrals.

In Sects. 2 and 3 we collect results about Hadamard finite-part integrals and Mellin transforms, which we denote by

$$\overline{\overline{G}}(p) = \neq\!\!\!\!\!\!\int_0^\infty g(x)x^{p-1}dx \text{ and } G(p) = \int_0^\infty g(x)x^{p-1},$$

respectively. We treat functions $g(x)$ that decay at infinity faster than any power of x. Except at the poles of the Mellin transform, both $\overline{\overline{G}}(p)$ and $G(p)$ are analytic and coincide. Sect. 3 includes a treatment in the p-plane of the singularities of the Mellin transform. We show that the coefficients in the Laurent expansion of $G(p)$ about a pole may be expressed as the Hadamard finite-part integral of a related function. In Sects. 4 and 5 these results are applied in a straightforward manner to obtain various versions of the Euler-Maclaurin asymptotic expansion.

A refreshing feature of this theory is that it treats all cases in a fundamentally uniform way. The different expansions arise simply because the residues at poles in the complex p-plane of the Mellin transform $F(p)$ of $f(x) = x^\alpha g(x)$ are of a marginally different form when α is a negative integer than otherwise; and the $\log \mu$ term arises for negative integer α since a pole of $F(p)$ then coincides with a pole of the zeta function. The differences between these various expansions arise in this theory simply as a result of a technical difference in the formula required to calculate a set of residues.

Interesting but unrelated work on the evaluation of Hadamard finite-part integrals has recently appeared (Elliott and Venturino 1997). See also Monegato (1994) and Diligenti and Monegato (1994).

2. The Hadamard finite part integral

In this section we recall some of the standard Hadamard theory of the finite-part integral for the finite interval (Hadamard 1952) and apply it to semifinite integrals for a class of rapidly decaying functions.

We shall be interested, almost exclusively, in integrands having moderate continuity over a semi finite interval, say, $(0, \infty)$. At the lower end, the worst singularity is algebraic-logarithmic, that is, $x^\alpha \log^k x$, while at the upper limit, the integration properties are benign. (See Definition 2.4.)

For our purposes, the following definition is adequate.

Definition 2.1 Let $f(x)$ be integrable over (ϵ, b) for any ϵ satisfying $0 < \epsilon < b < \infty$. Suppose there exists a strictly monotonic increasing sequence $\alpha_0 < \alpha_1 < \alpha_2 < \ldots$ and a nonnegative integer J such that the expansion

$$\int_\epsilon^b f(x)dx = \sum_{i=0}^{\infty} \sum_{j=0}^{J} I_{i,j}(b)\epsilon^{\alpha_i} \log^j \epsilon$$

converges for all $\epsilon \in (0, h)$ for some $h > 0$. Then the corresponding Hadamard finite-part integral may be defined as follows:

$$\begin{aligned} \,\,⨍_0^b f(x)dx &:= I_{I,0}(b) \text{ when } \alpha_I = 0 \\ &:= 0 \text{ when } \alpha_i \neq 0 \text{ for all } i. \end{aligned}$$

Some of the simpler special cases of this definition are listed in Lemmas 2.2, 2.3, and 2.5. For much of the work in this paper, these lemmas together form an adequate definition.

Lemma 2.2 *For* $b > 0$,

$$⨍_0^b x^\alpha dx =: \begin{cases} \log b \textit{ when } \alpha = -1; \\ b^{\alpha+1}/(\alpha+1) \textit{ otherwise.} \end{cases}$$

This may be extended to sufficiently regular functions as follows:

Lemma 2.3 *Let* $\alpha \leq -1$ *and* $m > -\alpha - 2$ *and* $g(x) \in C^{(m+1)}[0, b)$. *Then for* $b > 0$

$$⨍_0^b g(x)x^\alpha dx =: \int_0^b x^\alpha \left[g(x) - \sum_{k=0}^{m} g^{(k)}(0)x^k/k! \right] dx$$

$$+ \sum_{k=0}^{m} \frac{g^{(k)}(0)}{k!} ⨍_0^b x^{\alpha+k} dx. \tag{2.1}$$

The first integral on the right-hand side is a standard integral. The rest of this expression involves Lemma 2.2 in order to define the finite-part integrals. Clearly, except when α is a negative integer, the function defined in (2.1) is analytic in α.

We shall be interested in a class of functions $g(x)$ whose decay rate at infinity exceeds that of any inverse power of x.

Definition 2.4 An "allowable" function $g(x)$ of class $C^{(m+1)}[0,\infty)$ is one for which

$$\left|\int_0^\infty g^{(k)}(x)x^{p-1}dx\right| < \infty, \qquad k = 0, 1, \ldots, m+1,$$

for all $p \geq 1$.

Lemma 2.5 *When g is an allowable function in $C^{(m+1)}[0,\infty)$ and $f(x) = x^\alpha g(x)$,*

$$⨎_0^\infty f(x)dx := ⨎_0^b f(x)dx + \int_b^\infty f(x)dx.$$

Notice that this definition is independent of $b > 0$. Moreover, we have

$$⨎_0^\infty x^\alpha dx = 0, \qquad \forall\alpha < -1. \tag{2.2}$$

Theorem 2.6 follows immediately from Lemmas 2.2 and 2.3.

Theorem 2.6 *When $g(x)$ is an allowable function in $C^{(m+1)}[0,\infty)$, $m \geq 0$, the function*

$$\overline{\overline{G}}(\alpha) := ⨎_0^\infty g(x)x^{\alpha-1}dx \tag{2.3}$$

is analytic in α for Re $\alpha > -m-2$, *except at nonpositive integer values of α.*

In fact, with the important exception of these integer values of α, $\overline{\overline{G}}(\alpha)$ is the analytic continuation of

$$\int_0^\infty g(x)x^{\alpha-1}dx, \qquad \text{Re}\ \alpha > 0,$$

and coincides with the Mellin transform $G(\alpha)$ defined in (3.1) below.

Our first nontrivial theorem will concern integration by parts. When $g(x)$ is $C^{(m+1)}[0,b]$ and $m > 0$, we have

$$\int_\epsilon^b \frac{g(x)}{x^{m+1}}dx = -\frac{g(b)}{mb^m} + \frac{g(\epsilon)}{m\epsilon^m} + \frac{1}{m}\int_\epsilon^b \frac{g'(x)}{x^m}dx. \tag{2.4}$$

In the limit as ϵ tends to zero, in general neither integral exists. However, we can provide an expansion of the type needed in Definition 2.1 if we note that

$$\begin{aligned} \frac{g(\epsilon)}{m\epsilon^m} = \frac{1}{m}\Bigg(& g(0)\epsilon^{-m} + g'(0)\epsilon^{-m+1} + \dots \\ & + \frac{g^{(m)}(0)}{m!} + \frac{g^{(m+1)}(0)}{(m+1)!}\epsilon + \dots \Bigg). \end{aligned} \tag{2.5}$$

We apply that definition to the integral obtained from amalgamating the two integrals in (2.4). Then, in view of the expansion (2.5), we have

$$⨍_0^b \frac{g(x)}{x^{m+1}}dx = -\frac{g(b)}{mb^m} + \frac{g^{(m)}(0)}{m.m!} + \frac{1}{m} ⨍_0^b \frac{g'(x)}{x^m}dx. \tag{2.6}$$

It is interesting to note that for the marginally more complicated situation in which $\log^k x$ also occurs in the integrand, no term corresponding to $g^{(m)}(0)/m.m!$ in (2.6) occurs. Thus,

$$\begin{aligned} \int_\epsilon^b \frac{g(x)\log^k x}{x^{m+1}}dx = & -\frac{1}{m}\frac{g(x)\log^k x}{x^m}\Bigg|_\epsilon^b + \frac{1}{m}\int_\epsilon^b \frac{g'(x)\log^k x}{x^m}dx \\ & + \frac{k}{m}\int_\epsilon^b \frac{g(x)\log^{k-1} x}{x^{m+1}}dx \qquad \begin{array}{l} k > 0; \\ m > 0. \end{array} \end{aligned} \tag{2.7}$$

The cases in which $k = 0$ have been treated above. When $k > 0$ and $m = 0$, we have

$$\begin{aligned} \int_\epsilon^b \frac{g(x)\log^k x}{x}dx = & \frac{1}{k+1}g(x)\log^{k+1} x\Bigg|_\epsilon^b \\ & -\frac{1}{k+1}\int_\epsilon^b g'(x)\log^{k+1} x dx \qquad k > 0, \end{aligned} \tag{2.8}$$

and, in all cases specified in the two preceding equations, all terms in the expansion in terms of ϵ arising from the lower limit of the final term on the right contain $\log \epsilon$ as a factor.

We are interested in the case in which b becomes infinite. With this in view, we need a restriction on $g(x)$ so that the various integrals continue to exist and other terms involving b have proper limits. A simple consequence of $g(x)$ being an allowable function of class $C^{(m+1)}[0, \infty)$ is that $g'(x)$ is one of class $C^{(m)}[0, \infty)$. In view of this, we may write down our principal theorem.

Theorem 2.7 *When $g(x)$ is an allowable function of class $C^{(m+1)}[0,\infty)$, we have*

$$\begin{aligned} ⨍_0^\infty \frac{g(x)}{x^{m+1}}dx &= \frac{g^{(m)}(0)}{m.m!} + \frac{1}{m} ⨍_0^\infty \frac{g'(x)}{x^m}dx, \qquad m>0, \\ &= -\int_0^\infty g'(x)\log x dx, \qquad m=0, \end{aligned} \tag{2.9}$$

and, when $k \geq 1$,

$$\begin{aligned} ⨍_0^\infty \frac{g(x)\log^k x}{x^{m+1}}dx &= \frac{k}{m} ⨍_0^\infty \frac{g(x)\log^{k-1} x}{x^{m+1}}dx \\ &\quad + \frac{1}{m} ⨍_0^\infty \frac{g'(x)\log^k x}{x^m}dx, \qquad m>0 \\ &= -\frac{1}{k+1}\int_0^\infty g'(x)\log^{k+1} x dx, \qquad m=0. \end{aligned} \tag{2.10}$$

The importance of this theorem is twofold. First, it pinpoints an unexpected term $g^{(m)}(0)/m.m!$, which occurs in the first relation in this theorem. Second, it justifies in many cases a process of integration by parts applied directly to Hadamard finite-part integrals.

Theorem 2.8 *When $g(x)$ is an allowable function in $C^{(m+1)}[0,\infty)$, $m \geq 0$,*

$$\begin{aligned} ⨍_0^\infty \frac{g(x)}{x^{m+1}}dx &= -\frac{1}{m!}\int_0^\infty g^{(m+1)}(x)\log x dx \\ &\quad + \frac{\psi(m+1)-\psi(1)}{m!}g^{(m)}(0), \end{aligned} \tag{2.11}$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$.

Proof. This is a simple consequence of Theorem 2.7. Let us apply the first member of (2.9) iteratively m times. We find

$$\begin{aligned} ⨍_0^\infty \frac{g(x)}{x^{m+1}}dx &= \frac{g^{(m)}(0)}{m!}\left\{\frac{1}{m} + \frac{1}{m-1} + \frac{1}{m-2} + \ldots + \frac{1}{1}\right\} \\ &\quad + \frac{1}{m!} ⨍_0^1 \frac{g^{(m)}(x)}{x}dx. \end{aligned}$$

Simplifying this and applying the second member of (2.9) gives (2.11) above directly. We have used the relation

$$\frac{1}{m!}\sum_{j=1}^m \frac{1}{j} = \frac{\psi(m+1)-\psi(1)}{m!}.$$

This is a standard property of $\psi(z)$, the logarithmic derivative of the gamma function, and is given, for example, in Abramowitz and Stegun(1965) on page 258. □

3. The Mellin transform

The conventional definition is as follows.

Definition 3.1 Given a function $f(x)$, its Mellin transform $F(p)$ is defined as

$$F(p) = \int_0^\infty f(x)x^{p-1}dx \tag{3.1}$$

for all values of p for which this integral exists.

It is well known that $F(p)$ is an analytic function. Equally well known is the inversion formula

$$f(x) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} F(p)x^{-p}dp, \tag{3.2}$$

where the contour of integration may be taken to be along the line Re $p = c$, where c is any value of p for which the integral on the right in (3.1) exists.

We now treat

$$G(p) = \int_0^\infty x^{p-1}g(x)dx, \qquad p > 0, \tag{3.3}$$

the Mellin transform of an *allowable* function $g(x)$. This integral representation $G(p)$ is valid when $p > 0$ where the integral converges. When $p \leq 0$, this integral diverges and defines nothing. However, $G(p)$ is an analytic function of p and can be continued into Re $p \leq 0$. To investigate this, we proceed as follows. Setting p to some positive number, we integrate by parts to obtain

$$G(p) = \frac{x^p g(x)}{p}\bigg|_0^\infty - \int_0^\infty \frac{g'(x)x^p}{p}dx.$$

Since $p > 0$ and $x^p g(x)$ vanishes at ∞, the first term on the right disappears. Iterating this procedure n times gives

$$G(p) = \frac{(-1)^{n+1}}{p(p+1)(p+2)\dots(p+n)} \int_0^\infty g^{(n+1)}(x)x^{p+n}dx. \tag{3.4}$$

The right-hand side is an analytic function of p in all Re $p > -n-1$ except at isolated poles $p = 0, -1, \dots -n$. Since this analytic function coincides with $G(p)$ when Re $p > 0$, it represents its continuation into Re $p \in (-n-1, 0]$. It is trivial to note from (3.4) that $G(p)$ has a simple pole at $p = -n$, with residue

$$\mathrm{Res}(G(p) : p = -n) = \frac{-1}{n!} \int_0^\infty g^{(n+1)}(x)dx = \frac{g^{(n)}(0)}{n!}. \tag{3.5}$$

Theorem 3.2 *Let $g(x)$ be an allowable function in $C^{(\infty)}[0,\infty)$ and $G(p)$ be its Mellin transform. Then $G(p)$ has an analytic continuation for all p, except for simple poles at $p = 0, -1, -2, \ldots$.*

To obtain the early terms in the Laurent expansion, we seek an expansion of $G(-n+\epsilon)$ in powers of ϵ. Direct substitution of $p = -n+\epsilon$ in (3.4) gives

$$G(-n+\epsilon) = \frac{-\Gamma(1-\epsilon)}{\Gamma(n+1-\epsilon)\epsilon}\int_0^\infty g^{(n+1)}(x)x^\epsilon dx. \tag{3.6}$$

We may use

$$x^\epsilon = \mathrm{e}^{\epsilon\log x} = 1 + \epsilon\log x + \frac{(\epsilon\log x)^2}{2!} + \ldots \tag{3.7}$$

and an expansion of the form

$$\frac{\Gamma(1-\epsilon)}{\Gamma(n+1-\epsilon)} = C_0^{(n)} + C_1^{(n)}\epsilon + C_2^{(n)}\epsilon^2 + \ldots \tag{3.8}$$

to establish formulas for the individual terms of the Laurent expansion in terms of the coefficients $C_j^{(n)}$. Recurrence relations for these coefficients are given later in (3.21) and (3.22). It is trivial to verify that

$$C_0^{(0)} = 1; \qquad C_j^{(0)} = 0, \quad j \geq 1, \tag{3.9}$$

$$C_j^{(1)} = 1; \qquad C_j^{(2)} = 1 - \frac{1}{2^{j+1}}, \quad j \geq 0, \tag{3.10}$$

and

$$C_0^{(n)} = \frac{1}{n!}; \quad C_1^{(n)} = \frac{1}{n!}\{\psi(n+1) - \psi(1)\}, \qquad \forall n \geq 1. \tag{3.11}$$

Carrying out this process, we find

$$G(-n+\epsilon) = b_{-1}^{(n)}/\epsilon + b_0^{(n)} + b_1^{(n)}\epsilon + \ldots, \tag{3.12}$$

where

$$b_{-1}^{(n)} = g^{(n)}(0)/n!$$

$$b_k^{(n)} = -\sum_{i=0}^{k+1}\frac{C_{k+1-i}^{(n)}}{i!}\int_0^\infty g^{(n+1)}(x)\log^i x\,dx, \qquad k \geq 0. \tag{3.13}$$

The theory given above may be used to provide critical information about the poles and Laurent expansions of the Mellin transform $F(p)$ of the function $f(x) = x^\alpha g(x)$. Clearly, when f and g are related in this way, their Mellin transforms satisfy

$$F(p-\alpha) = G(p).$$

In view of this, we find the somewhat trite corollary.

Corollary 3.3 *Let $g(x)$ be an allowable function in $C^{(\infty)}[0,\infty)$. When $f(x) = x^\alpha g(x)$, its Mellin transform $F(p)$ has poles at $p = -\alpha - n$ $(n = 0, 1, 2, \ldots)$. The Laurent expansion $F(-\alpha - n + \epsilon)$ coincides precisely with the right-hand side of (3.12) above.*

This result is used in the later sections of this paper and extensively in forthcoming work on multidimensional quadrature.

Setting $k = 0$ in (3.13), and recalling (3.11), we find that

$$b_0^{(n)} = -\frac{1}{n!}\int_0^\infty g^{(n+1)}(x)\log x dx + \frac{\psi(n+1) - \psi(1)}{n!} g^{(n)}(0).$$

This coincides with the Hadamard finite-part integral given in (2.11). We shall now prove that all coefficients $b_j^{(n)}$ have equally simple integral representations.

Theorem 3.4 *Under the hypotheses of Theorem 3.2, the Laurent expansion coefficients $b_k^{(n)}$ of (3.12) are given by*

$$b_k^{(n)} = \frac{1}{k!} \;⨎_0^\infty \frac{g(x)\log^k x}{x^{n+1}} dx, \qquad \forall k, n \geq 0. \tag{3.14}$$

Throughout the proof, which is manipulative, we shall use the abbreviation

$$H_{j,i} := \frac{1}{i!} \;⨎_0^\infty \frac{g^{(n-j+1)}(x)\log^i x}{x^j} dx. \tag{3.15}$$

In view of expression (3.13), in order to establish (3.14), we must show

$$H_{n+1,k} = -\sum_{j=0}^{k+1} C_{k+1-j}^{(n)} H_{0,j}. \tag{3.16}$$

As a preliminary, we establish two lemmas.

Lemma 3.5 *For all $n, k \geq 1$ we have*

$$H_{n+1,k} = -\frac{H_{0,k+1}}{n!} + \sum_{i=1}^{n} \frac{(i-1)!}{n!} H_{i+1,k-1}. \tag{3.17}$$

Proof. This is based on the two members of (2.10) above. When we apply each of these relations to the function $g^{(n-m)}(x)$, m being the parameter in (2.10), we may express the result in the form

$$H_{m+1,\ell} = \frac{1}{m} H_{m+1,\ell-1} + \frac{1}{m} H_{m,\ell}, \qquad m, \ell > 0, \tag{3.18}$$

$$H_{1,\ell} = -H_{0,\ell+1}, \qquad \ell \geq 0. \tag{3.19}$$

Let us multiply each member of (3.18) by $m!/n!$ and sum the resulting equation over index $m \in [1, n]$. We find immediately

$$H_{n+1,k} + \sum_{m=1}^{n-1} \frac{H_{m+1,k}}{n(n-1)\dots(m+1)} = \sum_{m=1}^{n} \frac{H_{m+1,k-1}}{n(n-1)\dots m}$$

$$+ \frac{H_{1,k}}{n!} + \sum_{m=2}^{n} \frac{H_{m,k}}{n(n-1)\dots m}. \tag{3.20}$$

The summation on the left coincides, term by term, with the final summation on the right. Removing these terms and using (3.19) reduces (3.20) to (3.17), establishing Lemma 3.5. □

The second lemma we need is a relation between the coefficients $C_\ell^{(i)}$ defined in (3.8).

Lemma 3.6 *The identity*

$$\sum_{i=1}^{n} (i-1)! C_\ell^{(i)} = n! C_{\ell+1}^{(n)} \tag{3.21}$$

holds for all $n \geq 1$ *and* $\ell \geq 0$.

Proof. We first establish a recursion relation (3.22). This may be used to calculate numerical values of $C_j^{(n)}$ recursively starting with the values of $C_j^{(1)}$ and $C_0^{(n)}$ given in (3.10) and (3.11). Using the identity $\Gamma(m+1-\epsilon) = (m-\epsilon)\Gamma(m-\epsilon)$, we find immediately that

$$\frac{m\Gamma(1-\epsilon)}{\Gamma(m+1-\epsilon)} = \frac{\epsilon\Gamma(1-\epsilon)}{\Gamma(m+1-\epsilon)} + \frac{\Gamma(1-\epsilon)}{\Gamma(m-\epsilon)}.$$

Applying expansion (3.8) to each quotient of gamma functions, we find

$$m \sum_{j=0}^{\infty} C_j^{(m)} \epsilon^j = \epsilon \sum_{j=1}^{\infty} C_{j-1}^{(m)} \epsilon^{j-1} + \sum_{j=0}^{\infty} C_j^{(m-1)} \epsilon^j.$$

Examination of the coefficient of ϵ^j in this relation gives

$$m C_j^{(m)} = C_{j-1}^{(m)} + C_j^{(m-1)}, \qquad j \geq 1. \tag{3.22}$$

To establish the lemma, we multiply each element in (3.22) by $(m-1)!$ and sum over index $m \in [1, n]$. Then

$$\sum_{m=1}^{n} m! C_j^{(m)} = \sum_{m=1}^{n} (m-1)! C_{j-1}^{(m)} + \sum_{m=0}^{n-1} m! C_j^{(m)}.$$

The first $n-1$ terms in the first summation coincide with the final $n-1$ terms in the third summation. Removing the common terms leaves (3.21) as written. □

We now proceed to the proof of Theorem 3.4, which is by induction.

Proof of Theorem 3.4. The case $k = 0$ has been already proved, while the case $n = 0$ follows immediately from (3.13) and (3.9).

When $k, n \geq 1$, we proceed as follows. First we wish to establish that

$$H_{i,\kappa} = -\sum_{j=0}^{\kappa+1} C_{\kappa-j+1}^{(i-1)} H_{0,j} \qquad i = 0, 1, \ldots, \tag{3.23}$$

with $\kappa = k$. In Theorem 2.8, we established this for all $i \geq 0$ with $\kappa = 0$. Thus, we may use that as a basis for induction on κ, assume that (3.23) is valid for $\kappa \in [0, k-1]$ and derive the same result for $\kappa = k$. To this end, we invoke Lemma 3.5 and substitute for $H_{i,k-1}$ using (3.23). We find

$$\begin{aligned} H_{n+1,k} + \frac{H_{0,k+1}}{n!} &= \sum_{i=1}^{n} \frac{(i-1)!}{n!} H_{i+1,k-1} \\ &= -\sum_{i=1}^{n} \sum_{j=0}^{k} \frac{(i-1)!}{n!} C_{k-j}^{(i)} H_{0,j} \\ &= -\sum_{j=0}^{k} C_{k-j+1}^{(n)} H_{0,j}. \end{aligned}$$

This final equality results from Lemma 3.6 with $\ell = k - j$. Since $C_0^{(n)} = 1/n!$, the second term on the left may be treated as the $(k+1)$th element of the sum on the right. This establishes (3.16), which is an abbreviated statement of Theorem 3.4. □

Remark 3.7 There are two significant results in the last two sections. The first, Theorem 2.7, introduces an anomalous term which has to be included in some (specified) cases in the standard formula for integration by parts, when the integrals involved diverge and are replaced by Hadamard finite part integrals. One of the consequences of this is the second significant result (Theorem 3.4). This deals with the Laurent expansion coefficients at a pole of (the analytic continuation of) the Mellin transform. This expansion has the form

$$G(p+\epsilon) = \frac{A_{-1}}{\epsilon} + A_0 + A_1\epsilon + A_2\epsilon^2 + \ldots$$

and, for all $p \leq 0$, A_0 is the Hadamard finite part integral. That is:

$$A_0 = \,=\!\!\!\!\!\!\int_0^\infty g(x) x^{p-1} dx$$

whether or not $A_{-1} = 0$ or, when p is a negative integer, $A_{-1} \neq 0$. Thus the Mellin transform, through its analytic continuation, provides an alternative definition of Hadamard finite part integral, one which unifies the noninteger and the integer cases.

4. Quadrature error expansions for the semifinite interval $[0, \infty)$

Our ultimate purpose is to obtain expansions such as (1.2) for the discretization error of an offset trapezoidal rule over a finite interval [0,1]. The major part of the derivation appears in this section, where corresponding expansions for the semifinite interval are established. A straightforward subtraction procedure to obtain expansions for the finite interval is given in the next section. Following Verlinden (1993), we denote an offset trapezoidal rule operator for the semifinite interval by

$$S_\mu f(\beta) = \frac{1}{\mu}\sum_{k=0}^{\infty} f\left(\frac{\beta+k}{\mu}\right). \tag{4.1}$$

It follows immediately from the Mellin inversion formula (3.2) that

$$f\left(\frac{x+k}{\mu}\right) = \frac{1}{2\pi \mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} F(p)\left(\frac{x+k}{\mu}\right)^{-p} dp. \tag{4.2}$$

Substituting this into (4.1) and inverting the order of summation and integration, we find

$$S_\mu f(\beta) = \frac{1}{2\pi \mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} F(p)\zeta(p,\beta)\mu^{p-1} dp. \tag{4.3}$$

Here we have used a standard definition of the Riemann zeta function, namely

$$\zeta(p,x) = \sum_{k=0}^{\infty}(x+k)^{-p}, \qquad x \in (0,1]. \tag{4.4}$$

Since $F(p)$ is the Mellin transform (3.1) of $f(x)$, it follows that c in (4.2) may take any value of p for which the integral on the right of (3.1) exists. We shall be applying this result only in cases where $f(x)$ is an allowable function, or closely related to one, and no problem in finding a suitable value of c is encountered.

Formula (4.3) is of wide validity, being meaningful whenever $f(x)$ is such that its Mellin transform (3.1) exists for any value of p. We now specialize to functions $f(x)$ of the form

$$f(x) = x^\alpha g(x), \tag{4.5}$$

where $g(x)$ is an allowable function. Note that we need not at the moment restrict α in any way. Recalling that $F(p) = G(\alpha+p)$, one may readily show that the expression on the right in (4.3) is $O(\mu^{c-1})$ as $\mu \to \infty$. Consequently, we may displace the contour in (4.3) to the left from Re $p = c$ to Re $p = c'$ so long as we include the sum of residues of the integrand at poles in the strip Re $p \in [c'_1, c_1)$. This process introduces a finite set of residue terms, but replacing c by c' in the integral reduces its order from $O(\mu^{c-1})$ to $O(\mu^{c'-1})$.

These poles occur at $p = 1$, where the zeta function has a simple pole and at $p = -\alpha - n$ $n = 0, 1, 2, \ldots$; at each of these points $F(p)$ has a simple pole. When α is not a negative integer, all these poles are distinct. When α is a negative integer, the pole of $F(p)$ with $n = -1 - \alpha$ coincides with the pole of the zeta function resulting in a pole of order 2 of the integrand function at this point.

We deal first with the case in which the poles are distinct. It is well known that

$$\text{Res}(\zeta(p, x) : p = 1) = 1, \tag{4.6}$$

and in view of (3.12) we have

$$\text{Res}(F(p) : p = -n - \alpha) = g^{(n)}(0)/n!. \tag{4.7}$$

This gives the following theorem.

Theorem 4.1 *Let $f(x) = x^\alpha g(x)$; let $g(x)$ be allowable in $C^{(N+1)}[0, \infty)$, and let α not be a negative integer. Then,*

$$\begin{aligned} S_\mu f(\beta) &= \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} F(p)\zeta(p, \beta)\mu^{p-1} dp \\ &= F(1) + \sum_{n=0}^{N} \frac{g^{(n)}(0)}{n!} \frac{\zeta(-n-\alpha, \beta)}{\mu^{n+\alpha+1}} \\ &\quad + \frac{1}{2\pi \mathrm{i}} \int_{c'-\mathrm{i}\infty}^{c'+\mathrm{i}\infty} F(p)\zeta(p, \beta)\mu^{p-1} dp, \end{aligned} \tag{4.8}$$

where N is a nonnegative integer, $c > \alpha - 1$, $c' \in (-N-\alpha-2, -N-\alpha-1)$, and $F(p)$ is the (analytic continuation of the) Mellin transform of $f(x)$ (in the p-plane).

Our immediate task is to identify $F(1)$. When $\alpha > -1$, the integral representation in Definition 3.1 exists, giving

$$F(1) = \int_0^\infty f(x) dx.$$

When $\alpha < -1$, $F(1)$ is the analytic continuation of $F(p)$, which exists for higher values of p. Since α is not a negative integer, we may invoke Theorem 2.6 to give

$$F(1) = \;⨍_0^\infty f(x) dx. \tag{4.9}$$

There remains the case in which α is a negative integer. The expansion (4.8) is based on the assumption that all the poles of the integrand function in (4.3) are distinct and simple and their residues given by (4.6) and (4.7). When α is a negative integer, the poles for $n \neq -1-\alpha$ are unchanged in character. However, there is a pole of order 2 at $p = 1$. We need to make a technical adjustment to (4.8) replacing $F(1)$ and the term in the sum with $n = -1-\alpha$ by the residue of $F(p)\zeta(p,x)\mu^{p-1}$ at $p = 1$. The calculation of this residue is straightforward but tedious. Briefly, we require the coefficient of ϵ^{-1} in the expansion of $F(1+\epsilon)\zeta(1+\epsilon,x)\mu^{\epsilon}$. Using the result of Corollary 3.3 with $n = 1$ and setting $m = -1-\alpha$, a nonnegative integer, we find

$$F(1+\epsilon) = \frac{1}{\epsilon}\frac{g^{(m)}(0)}{m!} + \,\,\,\,\,\,\,\,\neq\!\!\!\!\!\!\int_0^{\infty} f(x)dx + O(\epsilon).$$

In view of the standard expansions

$$\zeta(1+\epsilon,x) = \frac{1}{\epsilon} - \psi(x) + O(\epsilon),$$

$$\mu^{\epsilon} = \mathrm{e}^{\epsilon\log\mu} = 1 + \epsilon\log\mu + O(\epsilon^2),$$

we find immediately that the required coefficient is

$$\neq\!\!\!\!\!\!\int_0^{\infty} f(x)dx - \frac{g^{(m)}(0)}{m!}\psi(\beta) + \frac{g^{(m)}(0)}{m!}\log\mu.$$

Replacing the two terms mentioned above leads to a variant theorem.

Theorem 4.2 *When α is a negative integer, Theorem 4.1 is valid as written except that, in the expansion (4.8) the term with $n = m = -\alpha-1$ is omitted from the sum and replaced by*

$$-\frac{g^{(m)}(0)}{m!}\psi(\beta) + \frac{g^{(m)}(0)}{m!}\log\mu;$$

as before, $F(1)$ remains the finite-part integral (4.9).

5. Quadrature error expansions for the finite interval $[0, 1]$

The results of the preceding section are expansions for the infinite sum

$$S_{\mu}f(\beta) = \frac{1}{\mu}\sum_{j=0}^{\infty} f\left(\frac{j+\beta}{\mu}\right),$$

where $f(x) = x^{\alpha}g(x)$ and $g(x)$ is an allowable function. In this section we exploit those expansions to obtain corresponding results pertaining to a finite interval [0,1] and a quadrature rule

$$\tilde{S}_{\mu}f(\beta) = \frac{1}{\mu}\sum_{j=0}^{\mu-1} f\left(\frac{j+\beta}{\mu}\right).$$

This is a discretization of the finite integral $\int_0^1 f(x)dx$. We shall treat three cases: $f(x)$ has no singularities, has a singularity at one end of the interval, and has singularities at both ends.

Definition 5.1 A *neutralizer* function $\nu(x;\kappa_1;\kappa_2)$ with $\kappa_2 > \kappa_1$ is a function satisfying

$$\begin{aligned} \nu(x) &= 1 \qquad x \leq \kappa_1, \\ \nu(x) &= 0 \qquad x \geq \kappa_2, \\ \nu(x) &\in C^{\infty}(-\infty,\infty). \end{aligned}$$

Example:

$$\nu(x) = \frac{1}{2}\left\{1 + \tanh\left(\frac{1}{\kappa_2 - t} - \frac{1}{t-\kappa_1}\right)\right\}, \qquad t \in (\kappa_1, \kappa_2).$$

A familiar result is the following lemma.

Lemma 5.2 *Let* $f(x) \in C^{(p)}[0,1]$. *There exists a* $C^{(p)}[0,\infty)$ *continuation of* $f(x)$ *that is allowable. This is*

$$f(x) = \begin{cases} f(x), & 0 \leq x \leq 1, \\ \left(\sum_{j=0}^{p} \frac{f^{(j)}(1)}{j!}(x-1)^j\right)\nu(x;\kappa_1;\kappa_2), & 1 < x, \end{cases}$$

where $\nu(x)$ *is any neutralizer function with* $1 \leq \kappa_1 < \kappa_2 < \infty$.

In the sequel, in situations in which $f(x)$ is defined only in [0,1], we shall assume a continuation of the above form without any further comment.

To obtain the classical Euler-Maclaurin expansion for [0,1] for $f(x) \in C^{(p)}[0,1]$, we define its continuation as just described with $\kappa_1 \geq 1$. Then we may set

$$\tilde{f}(x) = f(x+1),$$

and clearly

$$\tilde{S}_\mu f(\beta) = S_\mu f(\beta) - S_\mu \tilde{f}(\beta).$$

We apply the result of Theorem 4.1 to both terms. Since $\alpha = 0$, we readily find

$$\begin{aligned} \tilde{S}_\mu f(\beta) = F(1) - \tilde{F}(1) \\ + \sum_{n=0}^{N} \frac{\zeta(-n,\beta)}{n!\mu^{n+1}}(f^{(n)}(0) - f^{(n)}(1)) \\ + \frac{1}{2\pi \mathrm{i}}\int_{c'-\mathrm{i}\infty}^{c'+\mathrm{i}\infty}(F(p) - \tilde{F}(p))\zeta(p,\beta)\mu^{p-1}dp. \end{aligned} \tag{5.1}$$

Here we have denoted the Mellin transform of $\tilde{f}(x)$ by $\tilde{F}(p)$. Since $f(x)$ is regular and allowable, it follows that

$$F(1) - \tilde{F}(1) = \int_0^\infty (f(x) - f(x+1))dx = \int_0^1 f(x)dx$$

and the zeta function in the summation may be re-expressed in terms of Bernoulli polynomials, using (1.3) above.

An expansion for the error functional when there is an integrand singularity at one end of the interval is obtained by using the same procedure. Let $f(x) = x^\alpha g(x)$, where $g(x) \in C^{(p)}[0,1]$.

Let $\alpha \neq$ negative integer and $\beta > 0$. Then, applying Theorem 4.1, we find

$$\begin{aligned}(5.2)\quad \tilde{S}_\mu f(\beta) &= S_\mu f(\beta) - S_\mu \tilde{f}(\beta)\\ &= F(1) - \tilde{F}(1)\\ &\quad + \sum_{n=0}^{N} \frac{\zeta(-n-\alpha,\beta)}{\mu^{n+\alpha+1}} \frac{g^{(n)}(0)}{n!} + \sum_{n=0}^{N} \frac{\zeta(-n,\beta)}{\mu^{n+1}} \frac{f^{(n)}(1)}{n!}\\ (5.3)\quad &\quad + \frac{1}{2\pi \mathrm{i}} \int_{c'-\mathrm{i}\infty}^{c'+\mathrm{i}\infty} (F(p) - \tilde{F}(p))\zeta(p,\beta)\mu^{p-1}dp.\end{aligned}$$

Since $\alpha \neq$ negative integer, the first term here is

$$\begin{aligned}F(1) - \tilde{F}(1) &= \neq\!\!\!\!\!\!\int_0^\infty f(x)dx - \int_1^\infty f(x)dx\\ &= \neq\!\!\!\!\!\!\int_0^1 f(x)dx.\end{aligned}$$

When $\alpha > -1$, this is Navot's result. When $\alpha < -1$ and is not an integer, this is Ninham's result. This derivation is the same for these two cases.

When α is a negative integer, say, $-m-1$, where m is a nonnegative integer, the expansion given above has to be adjusted in accordance with Theorem 4.2. Doing this leads to the following replacement for (5.2). Here, $f(x) = x^\alpha g(x) = g(x)/x^{m+1}$.

$$\begin{aligned}\tilde{S}_\mu f(\beta) &= \neq\!\!\!\!\!\!\int_0^1 f(x)dx - \frac{g^{(m)}(0)}{m!}\psi(\beta) + \frac{g^{(m)}(0)}{m!}\log\mu\\ &\quad + \sum_{\substack{n=0\\ n\neq m}}^{N} \frac{\zeta(-n+m+1,\beta)}{\mu^{n-m}} \frac{g^{(n)}(0)}{n!} + \sum_{n=0}^{N} \frac{\zeta(-n,\beta)}{\mu^{n+1}} \frac{f^{(n)}(1)}{n!}\\ (5.4)\quad &\quad + \frac{1}{2\pi \mathrm{i}} \int_{c'-\mathrm{i}\infty}^{c'+\mathrm{i}\infty} (F(p) - \tilde{F}(p))\zeta(p,\beta)\mu^{p-1}dp.\end{aligned}$$

We have now treated all values of α. When α is a negative integer, expansion (5.4) (with the $\log\mu$ term) is valid. Otherwise, the expansion (5.2) is valid. The regular expansion (5.1) coincides with (5.2) when α is set to zero.

One may obtain variants of these results relating to an integrand function that has a singularity at both ends of the finite interval. Let

$$f(x) = x^{\alpha}(1-x)^{\gamma}g(x),$$

where $g(x) \in C^{(p)}[0,1]$. To handle this, we re-express $f(x)$ as follows:

$$\begin{aligned} f(x) &= f(x)\nu(x;\frac{1}{3},\frac{2}{3}) + f(x)(1-\nu(x;\frac{1}{3},\frac{2}{3})) \\ &= f_0(x) + f_1(x) = f_0(x) + f_2(1-x). \end{aligned}$$

Then,

$$\tilde{S}_{\mu}f(\beta) = \tilde{S}_{\mu}f_0(\beta) + \tilde{S}_{\mu}f_1(\beta) = \tilde{S}_{\mu}f_0(\beta) + \tilde{S}_{\mu}f_2(1-\beta).$$

Geometrically, we have replaced the original $f(x)$ by two functions whose support is localized to $[0,\kappa_2]$ and to $[\kappa_1,1]$, respectively ($\kappa_i = i/3$). The second of these has been reflected about $x = \frac{1}{2}$. This has left the two functions $f_0(x)$ and $f_2(x)$, both of which have a singularity at $x=0$ but are allowable in $C[0,\infty)$. It remains only to apply Theorem 4.1 to $f_0(x)$ and $f_2(x)$ separately. Setting

$$g_0(x) = (1-x)^{\gamma}g(x), \qquad g_1(x) = x^{\alpha}g(x),$$

we obtain

$$\begin{aligned} \tilde{S}_{\mu}f(\beta) &= \tilde{S}_{\mu}f_0(\beta) + \tilde{S}_{\mu}f_2(1-\beta) \\ &= F_0(1) + F_2(1) + \sum_{n=0}^{N} \frac{\zeta(-n-\alpha,\beta)}{\mu^{n+\alpha+1}}\frac{g_0^{(n)}(0)}{n!} \\ &\quad + \sum_{n=0}^{N} \frac{\zeta(-n-\gamma,1-\beta)}{\mu^{n+\gamma+1}}\frac{g_1^{(n)}(1)(-1)^n}{n!} \\ &\quad + \frac{1}{2\pi\mathrm{i}}\int_{c'-\mathrm{i}\infty}^{c'+\mathrm{i}\infty} (F_0(p)+F_2(p))\zeta(p,\beta)\mu^{p-1}dp. \qquad (5.5) \end{aligned}$$

Here,

$$F_0(1) + F_2(1) = \nsubseteq\!\!\!\!\int_0^1 f(x)dx.$$

In the case that one or both of α or γ are negative integers, say $-m-1$ or $-\bar{m}-1$, respectively, there is an adjustment of the same type as was made to obtain (5.4) from (5.2). In the extreme case that both are negative integers, the sums over n are adjusted by omitting the terms for which $n=m$ and $n=\bar{m}$, respectively, and by including two sets of extra terms each set being of the type specified in Theorem 4.2.

6. Concluding remarks

In this paper we have presented a unified approach for deriving the one-dimensional Euler-Maclaurin expansions for quadrature error functionals defined on a finite interval when the integrand function has an algebraic singularity, of any order, at one or both endpoints. We have been able to include, in a general framework, the case of nonintegrable singularities, that is, integrals defined as Hadamard finite-parts.

Our approach is based on properties of the Mellin transform; in particular, using integration by parts, we have continued an investigation initiated by Verlinden into the sequence of poles in the negative real axis. Critical to our theory is the nature of the Laurent expansion at each pole. We have shown that each individual term in this expansion has a simple integral representation in terms of a Hadamard finite-part integral. This is an extension of the theory recently developed by Verlinden to higher-order terms and nonintegrable singularities.

As mentioned in the introduction, a refreshing feature of this theory is that it treats all possible cases of singularities in a fundamentally uniform way. The different expansions arise simply as a result of a technical difference in the formula required to calculate the residues at the poles of the Mellin transform.

References

1. Abramowitz M., Stegun, I.A. (1965): Handbook of Mathematical Functions. Dover, New York
2. Davis, P.J., Rabinowitz, P.(1984): Methods of Numerical Integration. 2nd edition, Academic Press, London
3. Diligenti, M., Monegato, G. (1994): Finite-Part Integrals: Their Occurrence and Computation. Rend. Circolo Mat. di Palermo. **33** 39–61
4. Elliott, D., Venturino, E. (1997): Sigmoidal transformations and the Euler-Maclaurin expansion for evaluating certain Hadamard finite-part integrals, Numer. Math. **77**, 453–465
5. Hadamard, J. (1952): Lectures on Cauchy's Problem in Linear Partial Differential Equations. Yale Univ. Press, New Haven, 1923 / Dover, New York, 1952
6. Lyness, J.N. (1994): Finite-Part Integrals and the Euler-Maclaurin Expansion. In Approximation and Computation, Zahar, R.V.M. ed. Birkhäuser Verlag, pp. 397–407
7. Monegato, G. (1994): Numerical Evaluation of Hypersingular Integrals. JCAM **50**, 9–31
8. Navot, I. (1961): An Extension of the Euler-Maclaurin Summation Formula to Functions with a Branch Singularity. J. Math. and Phys. **40**, 271–276
9. Ninham, B.W. (1966): Generalised Functions and Divergent Integrals. Num. Math. **8**, 444–457
10. Verlinden, P. (1993): Cubature Formulas and Asymptotic Expansions. thesis, Katholieke Universiteit Leuven
11. Verlinden, P., Haegemans, A. (1993): An Error Expansion for Cubature with an Integrand with Homogeneous Boundary Singularities. Numer. Math. **65**, 383–406