J Sci Comput (2014) 60:141–159
DOI 10.1007/s10915-013-9788-7

Richardson Extrapolation on Some Recent Numerical Quadrature Formulas for Singular and Hypersingular Integrals and Its Study of Stability

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Received: 21 April 2013 / Revised: 15 September 2013 / Accepted: 1 October 2013 /
Published online: 31 October 2013

Abstract Recently, we derived some new numerical quadrature formulas of trapezoidal rule type for the integrals $I^{(1)}[g] = \int_a^b \frac{g(x)}{x-t}\, dx$ and $I^{(2)}[g] = \int_a^b \frac{g(x)}{(x-t)^2}\, dx$. These integrals are not defined in the regular sense; $I^{(1)}[g]$ is defined in the sense of Cauchy Principal Value while $I^{(2)}[g]$ is defined in the sense of Hadamard Finite Part. With $h = (b-a)/n,\ n = 1, 2, \ldots,$ and $t = a+kh$ for some $k \in \{1, \ldots, n-1\},\ t$ being fixed, the numerical quadrature formulas $Q_n^{(1)}[g]$ for $I^{(1)}[g]$ and $Q_n^{(2)}[g]$ for $I^{(2)}[g]$ are

$$Q_n^{(1)}[g] = h \sum_{j=1}^{n} f(a + jh - h/2), \quad f(x) = \frac{g(x)}{x-t},$$

and

$$Q_n^{(2)}[g] = h \sum_{j=1}^{n} f(a + jh - h/2) - \pi^2 g(t) h^{-1}, \quad f(x) = \frac{g(x)}{(x-t)^2}.$$

We provided a complete analysis of the errors in these formulas under the assumption that $g \in C^{\infty}[a,b]$. We actually show that

$$I^{(k)}[g] - Q_n^{(k)}[g] \sim \sum_{i=1}^{\infty} c_i^{(k)} h^{2i} \quad \text{as}\, n \to \infty,$$

the constants $c_i^{(k)}$ being independent of h. In this work, we apply the Richardson extrapolation to $Q_n^{(k)}[g]$ to obtain approximations of very high accuracy to $I^{(k)}[g]$. We also give a thorough analysis of convergence and numerical stability (in finite-precision arithmetic) for them. In our study of stability, we show that errors committed when computing the function $g(x)$, which form the main source of errors in the rest of the computation, propagate in a relatively

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mild fashion into the extrapolation table, and we quantify their rate of propagation. We confirm our conclusions via numerical examples.

Keywords Cauchy principal value · Hadamard finite part · Singular integral · Hypersingular integral · Numerical quadrature · Trapezoidal rule · Euler–Maclaurin expansion · Richardson extrapolation

Mathematics Subject Classification (2010) 41A55 · 41A60 · 45B05 · 45B15 · 45E05 · 45E99 · 65B05 · 65B15 · 65D30 · 65D32

1 Introduction and Background

This work concerns the use of some new numerical quadrature formulas for the finite-range integrals

$$I^{(1)}[g] = \int_a^b \frac{g(x)}{x-t}\,dx, \quad a < t < b, \quad g \in C^\infty[a,b], \tag{1.1}$$

and

$$I^{(2)}[g] = \int_a^b \frac{g(x)}{(x-t)^2}\,dx, \quad a < t < b, \quad g \in C^\infty[a,b]. \tag{1.2}$$

Clearly, neither $I^{(1)}[g]$ nor $I^{(2)}[g]$ exists in the ordinary sense; $I^{(1)}[g]$ is defined in the sense of *Cauchy Principal Value (CPV)*, while $I^{(2)}[g]$ is defined in the sense of *Hadamard Finite Part (HFP)*.[1] Both integrals arise in different problems of applied mathematics and engineering. Specifically, they appear in boundary integral equation formulations of 2D boundary value problems, for example. As such, their accurate evaluation is an important issue. Integral equations involving $I^{(1)}[g]$ are known as *singular integral equations*, while those involving $I^{(2)}[g]$ are known as *hypersingular integral equations*. In keeping with this nomenclature, we call $I^{(1)}[g]$ a *singular* integral and $I^{(2)}[g]$ a *hypersingular* integral.

For a general treatment of hypersingular integrals and their applications to hypersingular integral equations, see the books by Lifanov et al. [11] and by Ladopoulos [10]. For some recent applications arising from problems in elasticity, see Chen et al. [3] and [11], for those arising from fracture mechanics, see Chan et al. [2] and Chen [4], and for those arising from scattering from cracks, see Kress [7] and Kress and Lee [8], for example.

In this work, we shall consider two compact numerical quadrature formulas for these integrals, namely, $Q_n^{(1)}[g]$ for $I^{(1)}[g]$ and $Q_n^{(2)}[g]$ for $I^{(2)}[g]$, which are given as in

$$Q_n^{(1)}[g] = h\sum_{j=1}^{n} f(a + jh - h/2), \quad f(x) = \frac{g(x)}{x-t}, \quad h = \frac{b-a}{n}, \tag{1.3}$$

[1] The usual notation for integrals defined in the sense of CPV and HFP is $⨍_a^b f(x)\,dx$, and $⨎_a^b f(x)\,dx$, respectively. In this work, we denote both of them by $\int_a^b f(x)\,dx$, as in (1.1) and (1.2), for simplicity. For the definition and properties of CPV and HFP integrals, see Davis and Rabinowitz [5], Evans [6], or Kythe and Schäferkotter [9], for example.

and

$$Q_n^{(2)}[g] = h \sum_{j=1}^{n} f(a + jh - h/2) - \pi^2 g(t) h^{-1}, \quad f(x) = \frac{g(x)}{(x-t)^2}, \quad h = \frac{b-a}{n}. \tag{1.4}$$

Here $t = a + kh$ for some $k \in \{1, \ldots, n-1\}$. The formula $Q_n^{(1)}[g]$ was originally derived in Sidi and Israeli [18] by using the classical Euler–Maclaurin (E–M) expansion for regular integrands. The formula $Q_n^{(2)}[g]$ was derived in the recent paper Sidi [17] by making use of one of the author's generalizations of the E–M expansion for integrands with arbitrary algebraic endpoint singularities. For the classical E–M expansion, see Atkinson [1], Davis and Rabinowitz [5], and Stoer and Bulirsch [19], for example. See also Sidi [13, Appendix D]. The author's generalization of the E–M expansion alluded to here is given in Sidi [15]. For generalizations of the E–M expansion to the case of arbitrary algebraic-logarithmic endpoint singularities, see Sidi [14,16].

The results in the following theorem were proved in [17]:

Theorem 1.1 *Let $I^{(1)}[g]$ and $I^{(2)}[g]$ be as in (1.1)–(1.2), respectively, and let $Q_n^{(1)}[g]$ and $Q_n^{(2)}[g]$ be as in (1.3)–(1.4), respectively. Let also $\{\nu_k\}_{k=0}^{\infty}$ be a sequence of positive integers, $\nu_0 < \nu_1 < \nu_2 < \cdots$, and let $h_k = (b-a)/\nu_k$. Let t be such that $t \in \{a + jh_k\}_{j=1}^{\nu_k - 1}$ for every $k = 0, 1, \ldots$. (This is guaranteed if each ν_k is an integer multiple of ν_0 and $t \in \{a + jh_0\}_{j=1}^{\nu_0 - 1}$.) Let $n \in \{\nu_k\}_{k=0}^{\infty}$ and let $h = (b-a)/n$. Then $Q_n^{(1)}[g]$ and $Q_n^{(2)}[g]$ are well defined and have the asymptotic expansions*

$$Q_n^{(k)}[g] \sim I^{(k)}[g] + \sum_{i=1}^{\infty} \frac{B_{2i}}{(2i)!} (2^{1-2i} - 1) \big[f^{(2i-1)}(b) - f^{(2i-1)}(a) \big] h^{2i} \quad \text{as}\, h \to 0. \tag{1.5}$$

Here B_s are the Bernoulli numbers, $f(x)$ is as in (1.3) for $k = 1$ and as in (1.4) for $k = 2$, and $f^{(s)}$ stands for the sth derivative of f.

It follows from this theorem that if $f(x)$, whether as in (1.3) or as in (1.4), is such that $f^{(2i-1)}(a) = f^{(2i-1)}(b)$, for $i = 1, 2, \ldots$, then the asymptotic expansion in (1.5) is empty and this implies that

$$Q_n^{(k)}[g] - I^{(k)}[g] = O(h^{\mu}) \quad \text{as}\, h \to 0, \quad \forall\, \mu > 0. \tag{1.6}$$

In words, both quadrature formulas $Q_n^{(k)}[g]$, $k = 1, 2$, have "spectral accuracy." This situation arises naturally, when $f \in C^{\infty}(\mathbb{R})$ and is T-periodic, $T = b - a$, with polar singularities at $x = t + kT$, $k = 0, \pm 1, \pm 2, \ldots$. In this case, (1.3) and (1.4) can be replaced by

$$Q_n^{(1)}[g] = h \sum_{j=1}^{n} f(t + jh - h/2), \quad f(x) = \frac{g(x)}{x-t}, \quad h = \frac{b-a}{n}, \tag{1.7}$$

and

$$Q_n^{(2)}[g] = h \sum_{j=1}^{n} f(t + jh - h/2) - \pi^2 g(t) h^{-1}, \quad f(x) = \frac{g(x)}{(x-t)^2}, \quad h = \frac{b-a}{n}, \tag{1.8}$$

and t can now assume *any* value in $[a, b]$ on account of the periodicity of $f(x)$. This case is treated in great detail in [17].

Going back to the nonperiodic case, Theorem 1.1 also suggests immediately that the *classical Richardson extrapolation process* can be applied to a sequence of the $Q_n^{(k)}[g]$, $n \in \{\nu_0, \nu_1, \ldots\}$, to accelerate its convergence to $I^{(k)}[g]$. Indeed, this has already been suggested in [17]. For a detailed treatment of the classical Richardson extrapolation, see [13, Chapters 1 and 2], for example. In this work, we give a detailed analysis of this use of the Richardson extrapolation, with special attention to the issue of numerical stability associated with it. This issue arises because of the singular nature of the problems, which causes the roundoff errors in the computation of the $Q_n^{(k)}[g]$ to tend to infinity as $h \to 0$ (equivalently, as $n \to \infty$). As will become clear, however, this issue is not very serious because close to machine accuracy in floating-point arithmetic can be achieved before these errors begin to have an impact on the accuracy given by the extrapolation procedure. This makes the quadrature formulas very effective as practical computational tools.

In Sect. 2, we review briefly the classical Richardson extrapolation process, discuss the issues of convergence and of numerical stability associated with it, and also propose a new and simple algorithm for the quantitative assessment of stability numerically. It turns out that this algorithm, after some twist, can be applied to our problems in this work quite easily. In Sect. 3, we apply the convergence theory of Sect. 2 to the Richardson extrapolation as this is being applied to the $Q_n^{(k)}[g]$. The stability issue is the subject of Sects. 4 and 5. In Sect. 4, we provide a detailed practical numerical treatment of the stability issues involved in applying the Richardson extrapolation to the $Q_n^{(k)}[g]$: (i) we develop simple but effective methods that are based on realistic assumptions having to do with computation in floating-point arithmetic and (ii) we provide recursive algorithms for these methods. In Sect. 5, we provide an analytical treatment of the stability issues; we develop the theoretical aspects of the computational methods proposed in Sect. 4 and show how initial computational errors propagate in the extrapolation process as this is being applied to the $Q_n^{(k)}[g]$. Finally, in Sect. 6, we present numerical examples that confirm the validity of the methods proposed in Sect. 4 for assessing numerical stability. The approach to numerical stability given in this work is new.

2 Convergence and Stability of the Richardson Extrapolation

2.1 Classical Richardson Extrapolation

We begin with a short description of the classical Richardson extrapolation. This will set the stage for more developments and will also fix the notation we use in the sequel. Our treatment here is based on Sidi [13, Chapter 1], but is carried out under stronger conditions suitable to the problems treated in this work.

Let $A(y)$ be a function of the continuous or discrete variable y, defined on the interval $[0, b]$ for some $b > 0$, and let $A = \lim_{y\to 0} A(y)$. Assume that $A(y)$ has an asymptotic expansion of the form

$$A(y) \sim A + \sum_{i=1}^{\infty} \alpha_i y^{\sigma_i} \quad \text{as } y \to 0, \tag{2.1}$$

where α_i are constants independent of y, and the σ_i are real and satisfy

$$0 < \sigma_1 < \sigma_2 < \cdots; \quad \lim_{i\to\infty} \sigma_i = \infty. \tag{2.2}$$

Fig. 1 Arrangement of extrapolation table

$$\begin{array}{lllll} A_0^{(0)} & & & & \\ A_0^{(1)} & A_1^{(0)} & & & \\ A_0^{(2)} & A_1^{(1)} & A_2^{(0)} & & \\ A_0^{(3)} & A_1^{(2)} & A_2^{(1)} & A_3^{(0)} & \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

$A(y)$ is assumed to be known (or computable) for $0 < y < b$, but not at $y = 0$; we want to determine (or approximate) $A(0) = \lim_{y\to 0} A(y) = A$. The σ_i are also assumed to be known. The α_i need not be known.[2]

The Richardson extrapolation process is now defined as follows:

Algorithm 1

Step 0. Input $A(y)$, $\{\sigma_n\}_{n=1}^{\infty}$, $y_0 \in (0, b)$, and $\omega \in (0, 1)$.

Step 1. Set $y_j = y_0\omega^j$, and compute $A_0^{(j)} = A(y_j)$, $j = 0, 1, \ldots$.

Step 2. For $n = 1, 2, \ldots$, and $j = 0, 1, \ldots$, compute $A_n^{(j)}$ via

$$A_n^{(j)} = \frac{A_{n-1}^{(j+1)} - c_n A_{n-1}^{(j)}}{1 - c_n}; \quad c_n = \omega^{\sigma_n}. \tag{2.3}$$

Here, the $A_n^{(j)}$ are the approximations to A, and they can be arranged in a two-dimensional array as in Fig. 1.

Note also that the c_n in (2.3) satisfy

$$1 > c_1 > c_2 > \cdots; \quad \lim_{n\to\infty} c_n = 0. \tag{2.4}$$

Define the polynomials $U_n(z)$ and their coefficients ρ_{ni} as in

$$U_n(z) = \prod_{i=1}^{n} \frac{z - c_i}{1 - c_i} = \sum_{i=0}^{n} \rho_{ni} z^i, \quad n = 0, 1, \ldots, \tag{2.5}$$

and note that, by (2.4),

$$(-1)^{n-i} \rho_{ni} > 0, \quad i = 0, 1, \ldots, n. \tag{2.6}$$

Thus,

$$U_n(1) = \sum_{i=0}^{n} \rho_{ni} = 1 \quad \text{and} \quad \big|U_n(-1)\big| = \sum_{i=0}^{n} |\rho_{ni}| = \prod_{i=1}^{n} \frac{1 + c_i}{1 - c_i}. \tag{2.7}$$

Then $A_n^{(j)}$ can also be expressed as in

$$A_n^{(j)} = \sum_{i=0}^{n} \rho_{ni} A(y_{j+i}). \tag{2.8}$$

[2] Actually, in the treatment given in [13, Chapter 1], we have considered the more general case in which (i) σ_i can be complex and satisfy $\Re\sigma_1 < \Re\sigma_2 < \cdots$; $\lim_{i\to\infty} \Re\sigma_i = \infty$, and (ii) $\lim_{y\to 0} A(y)$ may not have to exist, in which case A is said to be the *antilimit* of $A(y)$ as $y \to 0$. Divergence may take place, if $\Re\sigma_1 \leq 0$, for example.

2.2 Convergence Theory

In Table 1, the sequences $\{A_n^{(j)}\}_{j=0}^{\infty}$ with n fixed (called *column sequences*) and $\{A_n^{(j)}\}_{n=0}^{\infty}$ with j fixed (called *diagonal sequences*) are of special interest. For these, we have the following convergence theorems (see [13, Theorems 1.5.1 and 1.5.4]):

Theorem 2.1 *With $A(y)$ as in (2.1) and (2.2), and with fixed n, $A_n^{(j)}$ has the full asymptotic expansion*

$$A_n^{(j)} \sim A + \sum_{i=n+1}^{\infty} \alpha_i U_n(c_i) y_j^{\sigma_i} \quad \text{as } j \to \infty. \tag{2.9}$$

As a result,

$$A_n^{(j)} - A = O(y_j^{\sigma_{n+1}}) = O(c_{n+1}^j) \quad \text{as } j \to \infty. \tag{2.10}$$

If $\alpha_{n+\mu}$ is the first nonzero α_i with $i \geq n+1$, then we also have the asymptotic equality

$$A_n^{(j)} - A \sim \alpha_{n+\mu} U_n(c_{n+\mu}) y_j^{\sigma_{n+\mu}} \quad \text{as } j \to \infty. \tag{2.11}$$

In words, all column sequences converge linearly, *and each column converges at least as fast as the one preceding it. [Note that $U_n(c_i) \neq 0$ for $i \geq n+1$.]*

Theorem 2.2 *With $A(y)$ as in (2.1) and (2.2), and with fixed j, and assuming that the σ_i satisfy*

$$\sigma_{i+1} - \sigma_i \geq d > 0, \quad i = 1, 2, \ldots, \tag{2.12}$$

$A_n^{(j)}$ satisfies

$$A_n^{(j)} - A = O(e^{-\lambda n}) \quad \text{as } n \to \infty, \quad \forall\, \lambda > 0. \tag{2.13}$$

By imposing a mild growth condition on the α_s, the result in (3.2) can be made much stronger to read

$$A_n^{(j)} - A = O((\omega + \Delta)^{dn^2/2}) \quad \text{as } n \to \infty; \quad \Delta > 0 \text{ arbitrary}, \quad j \text{ fixed}. \tag{2.14}$$

In words, all diagonal sequences converge superlinearly, *hence faster than the column sequences.*

2.3 Assessment of Numerical Stability

The issue of numerical stability, which is relevant to floating-point computations, concerns the propagation of numerical errors in the input function values, namely, the $A(y_s)$, to the entries $A_n^{(j)}$ in Table 1. Here we tackle this issue under the assumptions made concerning $A(y)$ in the preceding subsection.

Assume that the function $A(y)$ is computed with errors, that is, assume that we are computing $\bar{A}(y_s) = A(y_s) + \Delta_s$ instead of $A(y_s)$. Then, assuming that the rest of the computation is being done in exact arithmetic, what we are computing by the Richardson extrapolation process via (2.3) are $\bar{A}_n^{(j)}$ instead of $A_n^{(j)}$. Thus, by (2.3) and (2.8), we have

$$\bar{A}_n^{(j)} = \frac{\bar{A}_{n-1}^{(j+1)} - c_n \bar{A}_{n-1}^{(j)}}{1 - c_n} = \sum_{i=0}^{n} \rho_{ni} \big[A(y_{j+i}) + \Delta_{j+i}\big] = A_n^{(j)} + \sum_{i=0}^{n} \rho_{ni} \Delta_{j+i}. \tag{2.15}$$

In view of this, the actual *absolute* error in $\bar{A}_n^{(j)}$ is

$$\bar{A}_n^{(j)} - A = \big(\bar{A}_n^{(j)} - A_n^{(j)}\big) + \big(A_n^{(j)} - A\big) = \sum_{i=0}^{n} \rho_{ni}\,\Delta_{j+i} + \big(A_n^{(j)} - A\big), \tag{2.16}$$

while the more important *relative* error is

$$\frac{\bar{A}_n^{(j)} - A}{A} = \frac{\bar{A}_n^{(j)} - A_n^{(j)}}{A} + \frac{A_n^{(j)} - A}{A} = \frac{\sum_{i=0}^{n} \rho_{ni}\,\Delta_{j+i}}{A} + \frac{A_n^{(j)} - A}{A}, \quad \text{provided} A \neq 0, \tag{2.17}$$

and numerical stability is ultimately connected with the relative error.

By Theorems 2.1 and 2.2, the term $\big(A_n^{(j)} - A\big)/A$ tends to zero as $j \to \infty$ or $n \to \infty$. This implies that, in (2.17), the term $\big(A_n^{(j)} - A\big)/A$, for all large j and n, becomes negligible compared to the term $(\bar{A}_n^{(j)} - A_n^{(j)})/A$, which is always nonzero due to errors committed in the computation of $A_n^{(j)}$. Thus, we can safely replace the equality in (2.17) by the following approximate equality:

$$\frac{\bar{A}_n^{(j)} - A}{A} \approx \frac{\bar{A}_n^{(j)} - A_n^{(j)}}{A} = \frac{\sum_{i=0}^{n} \rho_{ni}\,\Delta_{j+i}}{A}, \quad \text{for all large} j \text{ or } n, \quad \text{provided} A \neq 0. \tag{2.18}$$

Therefore, the numerical stability issue revolves around the term $\big(\sum_{i=0}^{n} \rho_{ni}\,\Delta_{j+i}\big)/A$.

In case some good upper bounds δ_s on the respective $|\Delta_s|$ are known, that is,

$$|\Delta_s| \leq \delta_s, \quad s = 0, 1, \ldots, \tag{2.19}$$

then we have

$$\left|\sum_{i=0}^{n} \rho_{ni}\,\Delta_{j+i}\right| \leq \sum_{i=0}^{n} |\rho_{ni}|\,|\Delta_{j+i}| \leq \sum_{i=0}^{n} |\rho_{ni}|\,\delta_{j+i},$$

and hence

$$\frac{\big|\bar{A}_n^{(j)} - A_n^{(j)}\big|}{|A|} \leq \frac{\sum_{i=0}^{n} |\rho_{ni}|\delta_{j+i}}{|A|} \approx \frac{\sum_{i=0}^{n} |\rho_{ni}|\delta_{j+i}}{|A_{j+n}^{(0)}|}, \quad \text{for all large } j \text{ or } n,$$

where we have also replaced the unknown limit A by $A_{j+n}^{(0)}$, the "best" approximation to A available to us from the given information, namely, from $A(y_s)$, $0 \leq s \leq j+n$. We can now use this knowledge to replace the approximate equality in (2.18) by the approximate inequality in

$$\frac{\big|\bar{A}_n^{(j)} - A\big|}{|A|} \lessapprox \frac{\widetilde{D}_n^{(j)}}{|A_{j+n}^{(0)}|}, \quad \text{for all large } j \text{ or } n; \quad \widetilde{D}_n^{(j)} = \sum_{i=0}^{n} \big|\rho_{ni}\big|\,\delta_{j+i}. \tag{2.20}$$

Since both the $A(y_s)$ and the δ_s are known, the right-hand side of (2.20) presents an effective way of assessing the relative error in $\bar{A}_n^{(j)}$ for all large j or n. That is to say, if $\widetilde{D}_n^{(j)}/|A_{j+n}^{(0)}|$ is of the order of 10^{-r} for some $r \geq 0$, then we can safely conclude that $\bar{A}_n^{(j)}$ can have up to r correct decimal digits *for sufficiently large j and/or n*.

We end by giving a convenient recursive algorithm for computing the $\widetilde{D}_n^{(j)}$ that is based entirely on Algorithm 1. First, by (2.6) and (2.20), we have

$$\widetilde{D}_n^{(j)} = \sum_{i=0}^{n} (-1)^{n-i} \rho_{ni} \delta_{j+i} = (-1)^{j+n} D_n^{(j)}; \quad D_n^{(j)} = \sum_{i=0}^{n} \rho_{ni} \big[(-1)^{j+i} \delta_{j+i}\big]. \quad (2.21)$$

Let us define the function $D(y)$ via

$$D(y_s) = (-1)^s \delta_s, \quad s = 0, 1, \ldots; \quad D(y) \text{ arbitrary otherwise.} \quad (2.22)$$

Then

$$D_n^{(j)} = \sum_{i=0}^{n} \rho_{ni} D(y_{j+i}), \quad j, n = 0, 1, \ldots. \quad (2.23)$$

Thus, we can apply Algorithm 1, with the $A(y_s)$ and $A_n^{(j)}$ there replaced by $D(y_s)$ and $D_n^{(j)}$, respectively.

Thus, we have the following algorithm:

Algorithm 2

Step 0. Input $\{\delta_s\}_{s=0}^{\infty}$, $\{\sigma_n\}_{n=1}^{\infty}$, $y_0 \in (0, b)$, and $\omega \in (0, 1)$.

Step 1. Compute $D_0^{(j)} = D(y_j) = (-1)^j \delta_j, \quad j = 0, 1, \ldots$.

Step 2. For $n = 1, 2, \ldots$, and $j = 0, 1, \ldots$, compute $D_n^{(j)}$ via

$$D_n^{(j)} = \frac{D_{n-1}^{(j+1)} - c_n D_{n-1}^{(j)}}{1 - c_n}; \quad c_n = \omega^{\sigma_n}. \quad (2.24)$$

Obviously, Algorithms 1 and 2 can easily be combined into one.

Invoking in (2.24) also the fact that $D_n^{(j)} = (-1)^{j+n} \widetilde{D}_n^{(j)}$, we obtain the following equivalent recursion relation for the $\widetilde{D}_n^{(j)}$:

$$\widetilde{D}_0^{(j)} = \delta_j, \quad j \geq 0; \quad \widetilde{D}_n^{(j)} = \frac{\widetilde{D}_{n-1}^{(j+1)} + c_n \widetilde{D}_{n-1}^{(j)}}{1 - c_n}, \quad j \geq 0, \ n \geq 1. \quad (2.25)$$

2.4 Examples

An immediate and commonly occurring example of this approach is that in which it is known that the $A(y_s)$ have been computed with machine accuracy, which means that

$$\bar{A}(y_s) = A(y_s)(1 + \eta_s), \quad |\eta_s| \leq \mathbf{u} \quad \forall\, s, \quad (2.26)$$

where $\mathbf{u}$ is the *unit roundoff* of the floating-point arithmetic being used. Consequently,

$$\Delta_s = \eta_s A(y_s) \quad \Rightarrow \quad |\Delta_s| \leq \mathbf{u}|A(y_s)| \quad \forall\, s. \quad (2.27)$$

We can now proceed as above by taking $\delta_s = \mathbf{u}|A(y_s)|$, $s = 0, 1, \ldots$, since these quantities are available at no additional cost.

If the $A(y_s) \approx A$ (they need not be very accurate approximations to A, it is enough if they are of the same order of magnitude), we can simplify the above approach by replacing $A(y_s)$ by A, and hence δ_s by $\mathbf{u}|A|$ in (2.27). Following this, (2.20) becomes

$$\frac{\big|\bar{A}_n^{(j)} - A\big|}{|A|} \lessapprox \mathbf{u} \sum_{i=0}^{n} |\rho_{ni}| = \mathbf{u} \sum_{i=0}^{n} (-1)^{n-i} \rho_{ni} = K_n \mathbf{u}, \quad \text{for all large } j \text{ or } n, \quad (2.28)$$

where

$$K_n = \sum_{i=0}^{n} |\rho_{ni}| = \big|U_n(-1)\big| = \prod_{i=1}^{n} \frac{1+c_i}{1-c_i}. \tag{2.29}$$

Now, being independent of j, the product $\prod_{i=1}^{n} \frac{1+c_i}{1-c_i}$ is bounded in j. In addition, by the assumption in (2.12) of Theorem 2.2, it is also bounded in n since

$$K_n = \prod_{i=1}^{n} \frac{1+c_i}{1-c_i} < \prod_{i=1}^{\infty} \frac{1+c_i}{1-c_i} = K_\infty < \infty. \tag{2.30}$$

Thus, the extrapolation process is very stable in that the relative error is bounded by $K_\infty \mathbf{u}$ for all large j and n.

3 Richardson Extrapolation Applied to $\mathbf{Q_n^{(k)}[g]}$

We now consider the application of the Richardson extrapolation to the numerical quadrature formulas $Q_n^{(1)}[g]$ and $Q_n^{(2)}[g]$, recalling that they both satisfy (1.5). Thus, (2.1) holds with

$$y = h = \frac{b-a}{n}, \quad A(y) = Q_n^{(k)}[g], \quad \text{and} \quad \sigma_i = 2i, \quad i = 1, 2, \ldots .$$

In addition, the σ_i satisfy (2.12). Clearly, both Theorems 2.1 and 2.2 apply with no changes, and we have

$$A_n^{(j)} - I^{(k)}[g] = O(\omega^{2j(n+1)}) \quad \text{as } j \to \infty; \quad n \text{ fixed}, \tag{3.1}$$

and

$$A_n^{(j)} - I^{(k)}[g] = O(e^{-\lambda n}) \quad \text{as } n \to \infty, \quad \forall\, \lambda > 0; \quad j \text{ fixed}. \tag{3.2}$$

By imposing a rather unrestrictive growth condition on the $g^{(s)}$, such as

$$\max_{a \le x \le b} \big|g^{(s)}(x)\big| = O\big(\exp(cs^\sigma)\big) \quad \text{as } s \to \infty, \quad c \ge 0, \quad \sigma < 2,$$

the result in (3.2) can be made much stronger to read

$$A_n^{(j)} - I^{(k)}[g] = O((\omega + \epsilon)^{n^2}) \quad \text{as } n \to \infty; \quad \epsilon > 0 \text{ arbitrarily small}, \quad j \text{ fixed}. \tag{3.3}$$

Here, $t = a + kh_0$, where $h_0 = (b-a)/\nu_0$ for some integer ν_0 and $k \in \{1, \ldots, \nu_0 - 1\}$. Of course, ω cannot take on arbitrary values. The fact that h can take on only the values $(b-a)/m$, $m = 1, 2, \ldots$, requires ω to take on only the values $1/s$, $s = 2, 3, \ldots$. The most common choice is $\omega = 1/2$, and this is our choice in the numerical examples in Sect. 5.

4 Numerical Assessment of Stability for Richardson Extrapolation on $\mathbf{Q_n^{(k)}[g]}$

To assess the numerical stability of the Richardson extrapolation process while computing the $A_n^{(j)}$ obtained as in the preceding section, we start by searching for good and *computable* upper bounds on $|\bar{Q}_n^{(k)}[g] - Q_n^{(k)}[g]|$, where $\bar{Q}_n^{(k)}[g]$ is the *computed* $Q_n^{(k)}[g]$. We aim at obtaining these bounds in terms of the quantities we use to compute $Q_n^{(k)}[g]$, no additional information being needed, and hence at *no* extra cost.

Clearly, the computational errors in $g(x)$ are the main source of error in $\bar{Q}_n^{(k)}[g]$. We now make the reasonable assumption that $g(x)$ is being computed with machine accuracy, which means that what is being computed instead of $g(x)$ is $\bar{g}(x)$, and that

$$\bar{g}(x) = g(x)[1+\eta(x)], \quad |\eta(x)| \leq \mathbf{u}, \quad \forall\, x \in [a,b]. \tag{4.1}$$

In the sequel, we also use the short-hand notation

$$x_j = a + jh - h/2, \quad j = 1,\ldots,n. \tag{4.2}$$

4.1 Preliminary Treatment of $Q_n^{(1)}[g]$

By (1.3) and (4.1),

$$\bar{Q}_n^{(1)}[g] = Q_n^{(1)}[\bar{g}] = h\sum_{i=1}^{n}\frac{\bar{g}(x_j)}{x_j - t} = Q_n^{(1)}[g] + h\sum_{i=1}^{n}\frac{g(x_j)\eta(x_j)}{x_j - t}. \tag{4.3}$$

Thus,

$$\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g] = h\sum_{i=1}^{n}\frac{g(x_j)\eta(x_j)}{x_j - t}, \tag{4.4}$$

which, upon taking absolute values on both sides, and invoking the fact that $|\eta(x)| \leq \mathbf{u}$ for all $x \in [a,b]$, gives

$$\left|\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g]\right| \leq \mathbf{u}\left[h\sum_{j=1}^{n}|f(x_j)|\right] \equiv \epsilon_n^{(1)}; \quad f(x) = \frac{g(x)}{x-t}. \tag{4.5}$$

Obviously, $\epsilon_n^{(1)}$ provides an upper bound for $|\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g]|$ that can be computed simultaneously with $Q_n^{(1)}[g]$ with no extra effort.

4.2 Preliminary Treatment of $Q_n^{(2)}[g]$

By (1.4) and (4.1),

$$\begin{aligned}\bar{Q}_n^{(2)}[g] = Q_n^{(2)}[\bar{g}] &= h\sum_{i=1}^{n}\frac{\bar{g}(x_j)}{(x_j - t)^2} - \pi^2\bar{g}(t)h^{-1}\\ &= Q_n^{(2)}[g] + h\sum_{i=1}^{n}\frac{g(x_j)\eta(x_j)}{(x_j - t)^2} - \pi^2 g(t)\eta(t)h^{-1}.\end{aligned} \tag{4.6}$$

Thus,

$$\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g] = h\sum_{i=1}^{n}\frac{g(x_j)\eta(x_j)}{(x_j - t)^2} - \pi^2 g(t)\eta(t)h^{-1}, \tag{4.7}$$

which, upon taking absolute values on both sides, and invoking the fact that $|\eta(x)| \leq \mathbf{u}$ for all $x \in [a,b]$, gives

$$\left|\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g]\right| \leq \mathbf{u}\left[h\sum_{j=1}^{n}|f(x_j)| + \pi^2|g(t)|h^{-1}\right] \equiv \epsilon_n^{(2)}; \quad f(x) = \frac{g(x)}{(x-t)^2}. \tag{4.8}$$

Of course, $\epsilon_n^{(2)}$ provides an upper bound for $|\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g]|$ that can be computed simultaneously with $Q_n^{(2)}[g]$ with no extra effort.

4.3 Completion of Numerical Assessment of Stability

With $\epsilon_n^{(1)}$ and $\epsilon_n^{(2)}$ available as above, we can now complete the *numerical* assessment of the stability of the extrapolation process on $Q_n^{(1)}[g]$ and $Q_n^{(2)}[g]$.

Let us recall the details of the computational process: In accordance with what is proposed in Theorem 1.1, we choose some positive integer ν_0, fix $t = a+kh_0$ with $h_0 = (b-a)/\nu_0$ and $k \in \{1, \dots, \nu_0 - 1\}$, and choose the integers $\nu_1, \nu_2, \dots$, according to $\nu_s = \nu_0/\omega^s$. Of course, $\omega = 1/m$ for some integer $m \geq 2$, as mentioned earlier. Thus, in applying the Richardson extrapolation process, we have

$$y_s = h_s = h_0\omega^s, \quad A_0^{(s)} = Q_{\nu_s}^{(k)}[g], \quad \widetilde{D}_0^{(s)} = \epsilon_{\nu_s}^{(k)}, \quad s = 0, 1, \dots.$$

Then, we also have

$$A_n^{(j)} = \sum_{i=0}^{n} \rho_{ni} A_0^{(j+i)} \quad \text{and} \quad \widetilde{D}_n^{(j)} = \sum_{i=0}^{n} |\rho_{ni}| \widetilde{D}_0^{(j+i)},$$

where the ρ_{ni} are defined via

$$U_n(z) = \prod_{i=1}^{n} \frac{z - c_i}{1 - c_i} = \sum_{i=0}^{n} \rho_{ni} z^i; \quad c_i = \omega^{2i}, \quad i = 1, 2, \dots,$$

and that the $A_n^{(j)}$ and $\widetilde{D}_n^{(j)}$ can be computed via the recursion relations

$$A_n^{(j)} = \frac{A_{n-1}^{(j+1)} - c_n A_{n-1}^{(j)}}{1 - c_n} \quad \text{and} \quad \widetilde{D}_n^{(j)} = \frac{\widetilde{D}_{n-1}^{(j+1)} + c_n \widetilde{D}_{n-1}^{(j)}}{1 - c_n}, \quad j \geq 0, \ n \geq 1.$$

We also recall that, since $\lim_{n\to\infty} Q_n^{(k)}[g] = I^{(k)}[g]$, we finally have

$$\frac{|\bar{A}_n^{(j)} - A|}{|A|} \lessapprox \frac{\widetilde{D}_n^{(j)}}{|A_{j+n}^{(0)}|}, \quad \text{for all large } j \text{ or } n.$$

5 Theoretical Assessment of Stability for Richardson Extrapolation on $\mathbf{Q_n^{(k)}[g]}$

In this section, we analyze the *theoretical* (as opposed to *numerical*) behavior of the $\widetilde{D}_n^{(j)}$ of (2.20) as n increases, because diagonal sequences $\{A_n^{(j)}\}_{n=0}^{\infty}$, with fixed j, have the best convergence properties. We do this by developing tight upper bounds denoted $\widetilde{E}_n^{(j)}$ on the $\widetilde{D}_n^{(j)}$ that are simple to express and easy to handle theoretically. The end result is

$$\frac{|\bar{A}_n^{(j)} - A|}{|A|} \lessapprox \frac{\widetilde{D}_n^{(j)}}{|A_{j+n}^{(0)}|} \leq \frac{\widetilde{E}_n^{(j)}}{|A_{j+n}^{(0)}|}, \quad \text{for all large } j \text{ or } n. \tag{5.1}$$

As we will see from the examples of Sect. 6, the three quantities in (5.1) are practically of the same order of magnitude. (i) This confirms our claim that $\widetilde{D}_n^{(j)}/|A_{j+n}^{(0)}|$ is an excellent *numerical on-the-fly* estimator of the relative error in $\bar{A}_n^{(j)}$. (ii) It also shows that the *theoretical* quantity $\widetilde{E}_n^{(j)}/|A_{j+n}^{(0)}|$ describes the rate at which errors propagate throughout the extrapolation table in an exact manner.

Everything here is as in the preceding section with the same notation. In addition, we use the notation

$$\|g\| = \max_{a\leq x\leq b} |g(x)|. \tag{5.2}$$

5.1 Treatment of $Q_n^{(1)}[g]$

Recalling that $t = a + kh$ for some $k \in \{1, \ldots, n-1\}$, (4.5) gives

$$\left|\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g]\right| \leq \mathbf{u}\left[h\sum_{j=1}^{n}\frac{|g(x_j)|}{|x_j - t|}\right] \leq \mathbf{u}\|g\|\sum_{j=1}^{n}\frac{1}{|j - 1/2 - k|}.$$

Now,

$$\sum_{j=1}^{n}\frac{1}{|j-1/2-k|} = \sum_{i=0}^{k-1}\frac{1}{i+1/2} + \sum_{i=0}^{n-k-1}\frac{1}{i+1/2}.$$

It is clear that this summation is $O(\log n)$ as $n \to \infty$ for every k and hence for every t. In addition, the sum $\sum_{i=1}^{m}\frac{1}{i+1/2}$ is the midpoint rule approximation for the integral $\int_1^m \frac{dx}{x}$ with $h = 1$, and since the second derivative of $1/x$ is positive for $x > 0$, we have (see [1], for example)

$$\sum_{i=1}^{m-1}\frac{1}{i+1/2} < \int_1^m \frac{dx}{x} = \log m, \tag{5.3}$$

and, therefore, we have the inequality

$$\sum_{j=1}^{n}\frac{1}{|j-1/2-k|} < 4 + \log[k(n-k)],$$

whose right-hand side achieves its maximum for $k = n/2$, and we have

$$\sum_{j=1}^{n}\frac{1}{|j-1/2-k|} < 4 + 2\log(n/2).$$

As a result, for all $t = a + kh,\ k \in \{1, \ldots, n-1\}$,

$$\left|\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g]\right| \leq \mathbf{u}\|g\|\left[4 + 2\log(n/2)\right]. \tag{5.4}$$

We now turn to the application of the Richardson extrapolation. As we have already seen, we need to study the behavior of $\widetilde{D}_n^{(j)}$ for large n. First, by (2.20), with $\delta_s = \mathbf{u}\|g\|[4 + 2\log(\nu_s/2)]$, which follows from (5.4), we have

$$\widetilde{D}_n^{(j)} \leq \sum_{i=0}^{n}|\rho_{ni}|\delta_{j+i} = \mathbf{u}\|g\|\sum_{i=0}^{n}|\rho_{ni}|\left[4 + 2\log(\nu_{j+i}/2)\right]. \tag{5.5}$$

By the fact that $\nu_{j+i} = \nu_j \omega^{-i}$, we also have

$$\widetilde{D}_n^{(j)} \le \mathbf{u}\|g\| \sum_{i=0}^{n} |\rho_{ni}| \big[4 + 2\log(\nu_j/2) + 2i \log \omega^{-1}\big]. \tag{5.6}$$

Therefore,

$$\widetilde{D}_n^{(j)} \le \mathbf{u}\|g\| \left\{ \big[4 + 2\log(\nu_j/2)\big] \sum_{i=0}^{n} |\rho_{ni}| + 2\log \omega^{-1} \sum_{i=0}^{n} i\, |\rho_{ni}| \right\}. \tag{5.7}$$

Now, by (2.29), $\sum_{i=0}^{n} |\rho_{ni}| = K_n$, whose properties are known by (2.30). We thus turn to the analysis of $\sum_{i=0}^{n} i\, |\rho_{ni}|$. First, we observe that

$$U_n'(z) = \sum_{i=0}^{n} i \rho_{ni} z^{i-1}, \tag{5.8}$$

and hence that

$$\sum_{i=0}^{n} i |\rho_{ni}| = (-1)^{n-1} \sum_{i=0}^{n} i\, \rho_{ni} (-1)^{i-1} = |U_n'(-1)|. \tag{5.9}$$

By the fact that $U_n(z)$ has $c_1 > c_2 > \cdots > c_n$ as its zeros, it follows by Rolle's theorem that $U_n'(z)$ has $n-1$ real and distinct zeros, which we denote by $c_1' > c_2' > \cdots > c_{n-1}'$. Clearly,

$$1 > c_1 > c_1' > c_2 > c_2' > \cdots > c_{n-1} > c_{n-1}' > c_n > 0. \tag{5.10}$$

As a result,

$$U_n'(z) = n\rho_{nn} \prod_{i=1}^{n-1} (z - c_i') \quad \Rightarrow \quad \sum_{i=0}^{n} i\, |\rho_{ni}| = n\rho_{nn} \prod_{i=1}^{n-1} (1 + c_i'); \quad \rho_{nn} = \prod_{i=1}^{n} \frac{1}{1 - c_i}. \tag{5.11}$$

Noting the fact that

$$\prod_{i=2}^{n} (1 + c_i) < \prod_{i=1}^{n-1} (1 + c_i') < \prod_{i=1}^{n-1} (1 + c_i),$$

which follows from (5.10), and multiplying through by $n\rho_{nn}$, we obtain

$$\frac{K_n n}{1 + c_1} < \sum_{i=0}^{n} i |\rho_{ni}| < \frac{K_n n}{1 + c_n} < K_n n. \tag{5.12}$$

Since K_n are bounded in n, this inequality implies that $\sum_{i=0}^{n} i\, |\rho_{ni}|$ grows *strictly* like n as n increases. Substituting this in (5.7), we obtain

$$\begin{aligned} \widetilde{D}_n^{(j)} &\le \mathbf{u}\|g\| \big\{ \big[4 + 2\log(\nu_j/2)\big] K_n + 2\log \omega^{-1} K_n n \big\} \\ &= \mathbf{u}\|g\| K_n \big[4 + 2\log(\nu_{j+n}/2)\big] \equiv \widetilde{E}_n^{(j)}. \end{aligned} \tag{5.13}$$

Thus, we see that the computational errors in $g(x)$ propagate in the diagonal sequence $\{A_n^{(j)}\}_{n=0}^{\infty}$ very slowly, *exactly* like n or, equivalently, like $\log h_{j+n}^{-1}$.

5.2 Treatment of $Q_n^{(2)}[g]$

Recalling that $t = a + kh$ for some $k \in \{1, \ldots, n-1\}$, (4.8) gives

$$\left|\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g]\right| \leq \mathbf{u}\left[h\sum_{j=1}^{n}\frac{|g(x_j)|}{(x_j-t)^2} + \pi^2|g(t)|h^{-1}\right]$$
$$\leq \mathbf{u}\|g\|h^{-1}\left[\pi^2 + \sum_{j=1}^{n}\frac{1}{(j-1/2-k)^2}\right].$$

Now,

$$\sum_{j=1}^{n}\frac{1}{(j-1/2-k)^2} = \sum_{i=0}^{k-1}\frac{1}{(i+1/2)^2} + \sum_{i=0}^{n-k-1}\frac{1}{(i+1/2)^2}.$$

It is clear that this summation is $O(1)$ as $n \to \infty$ for every k and hence for every t. Using the fact that the Hurwitz Zeta function (see Olver et al. [12], for example) that is defined via

$$\zeta(z,\theta) = \sum_{i=0}^{\infty}\frac{1}{(i+\theta)^z}, \quad \Re z > 1,$$

also satisfies

$$\zeta(z, 1/2) = (2^z - 1)\zeta(z),$$

where $\zeta(z) = \zeta(z, 1)$ is the Riemann Zeta function, we have the inequality

$$\sum_{j=1}^{n}\frac{1}{(j-1/2-k)^2} < 2\zeta(2, 1/2) = 6\zeta(2) = \pi^2.$$

As a result, for all $t = a + kh,\ k \in \{1, \ldots, n-1\}$,

$$\left|\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g]\right| \leq 2\pi^2\mathbf{u}\|g\|h^{-1}. \tag{5.14}$$

We now turn to the application of the Richardson extrapolation. As we have already seen, we need to study the behavior of $\widetilde{D}_n^{(j)}$ for large n. First, by (2.20), with $\delta_s = 2\mathbf{u}\|g\|\pi^2 h_s^{-1}$, which follows from (5.14), and by the fact that $h_{j+i} = h_j\omega^i$,

$$\widetilde{D}_n^{(j)} \leq 2\mathbf{u}\|g\|\pi^2\sum_{i=0}^{n}|\rho_{ni}|h_{j+i}^{-1} = 2\mathbf{u}\|g\|\pi^2 h_j^{-1}\sum_{i=0}^{n}|\rho_{ni}|\omega^{-i}. \tag{5.15}$$

By (2.4)–(2.6),

$$\sum_{i=0}^{n}|\rho_{ni}|\omega^{-i} = (-1)^n\sum_{i=0}^{n}\rho_{ni}(-\omega^{-1})^i = \left|U_n(-\omega^{-1})\right| = L_n\omega^{-n}; \quad L_n = \prod_{i=1}^{n}\frac{1+\omega c_i}{1-c_i}.$$

Therefore,

$$\widetilde{D}_n^{(j)} \leq 2\pi^2\mathbf{u}\|g\|L_n h_{j+n}^{-1} \equiv \widetilde{E}_n^{(j)}. \tag{5.16}$$

Now, by the fact that $\omega c_i < c_i$ for all i,

$$L_n = \prod_{i=1}^{n}\frac{1+\omega c_i}{1-c_i} < \prod_{i=1}^{\infty}\frac{1+\omega c_i}{1-c_i} = L_\infty < \infty.$$

This implies that the computational errors in $g(x)$ propagate in the diagonal sequence $\{A_n^{(j)}\}_{n=0}^{\infty}$ like h_{j+n}^{-1}, hence like ω^{-n}. Since convergence is very quick as n increases, this propagation is not severe. For example, if we take $\omega = 1/2$ in the extrapolation procedure, which is what we would normally do, for $n = 10$, we will have $\omega^{-n} = 1024 \approx 10^3$.

6 Numerical Examples

In this section, we illustrate the conclusions of the preceding section with two numerical examples. In these examples, $I^{(1)}[g]$ and $I^{(2)}[g]$ are as defined in (1.1) and (1.2), respectively, and

$$g(x) = \frac{x}{x^2+1} \quad \text{and} \quad [a,b] = [-R, R].$$

Consequently,

$$I^{(1)}[g] = \frac{1}{t^2+1}\left(t \log \frac{R-t}{R+t} + 2 \arctan R\right)$$

and

$$I^{(2)}[g] = \frac{d}{dt} I^{(1)}[g] = -\frac{2t}{(t^2+1)^2}\left(t \log \frac{R-t}{R+t} + 2 \arctan R\right) + \frac{1}{t^2+1}\left(\log \frac{R-t}{R+t} - \frac{2Rt}{R^2-t^2}\right).$$

Here we have made use of the fact that

$$\int_a^b \frac{g(x)}{(x-t)^2}\,dx = \frac{d}{dt}\int_a^b \frac{g(x)}{x-t}\,dx, \quad a < t < b.$$

It is easy to verify that

$$\|g\| = \begin{cases} R/(R^2+1) & \text{if } R \le 1, \\ 1/2 & \text{if } R > 1. \end{cases}$$

In the computations reported here, we took $R = 2$ and $t = 1$. We also took $\nu_0 = 4$ and $\nu_s = \nu_0 2^s$, $s = 1, 2, \ldots$. These computations were done in both double-precision and quadruple-precision arithmetic in FORTRAN 77, for which, we have

$$\mathbf{u} = 2.22 \times 10^{-16} \text{ for double-precision,}$$
$$\mathbf{u} = 1.93 \times 10^{-34} \text{ for quadruple-precision,}$$

rounded to three significant decimal digits.

The results for $I^{(1)}[g]$ are given in Tables 1 and 2, while those for $I^{(2)}[g]$ are given in Tables 3 and 4, and they all pertain to the approximations $A_n^{(0)}$, $n = 0, 1, \ldots$. In both examples and both arithmetics, we see that the quantities $\widetilde{D}_n^{(j)}/|A_n^{(0)}|$ and $\widetilde{E}_n^{(j)}/|A_n^{(0)}|$ in (5.1), which estimate $\big|\bar{A}_n^{(j)} - A_n^{(j)}\big|/|A|$ for large n, and the actual relative error $\big|\bar{A}_n^{(j)} - A\big|/|A|$ as well, are of the same order of magnitude at the bottoms of the respective tables.

Table 1 Double-precision numerical results for the integral $I^{(1)}[g]$ in Sect. 6, with $t = 1$ throughout

n	$\mathcal{E}_n$	$\widetilde{D}_n^{(0)}/\lvert A_n^{(0)}\rvert$	$\widetilde{E}_n^{(0)}/\lvert A_n^{(0)}\rvert$
0	2.96D − 02	8.40D − 16	1.04D − 15
1	4.63D − 03	1.76D − 15	2.24D − 15
2	2.00D − 04	2.48D − 15	3.07D − 15
3	3.38D − 06	3.08D − 15	3.70D − 15
4	4.08D − 09	3.64D − 15	4.27D − 15
5	1.99D − 11	4.19D − 15	4.82D − 15
6	3.26D − 14	4.74D − 15	5.37D − 15
7	1.19D − 15	5.28D − 15	5.91D − 15
8	1.79D − 15	5.83D − 15	6.46D − 15
9	7.96D − 16	6.37D − 15	7.00D − 15
10	2.99D − 15	6.91D − 15	7.54D − 15

Here $\mathcal{E}_n = |\bar{A}_n^{(0)} - I^{(1)}[g]|/|I^{(1)}[g]|$, $\widetilde{D}_n^{(j)}$ as in Sect. 4.3, and $\widetilde{E}_n^{(j)}$ as in (5.13)

Table 2 Quadruple-precision numerical results for the integral $I^{(1)}[g]$ in Sect. 6, with $t = 1$ throughout

n	$\mathcal{E}_n$	$\widetilde{D}_n^{(0)}/\lvert A_n^{(0)}\rvert$	$\widetilde{E}_n^{(0)}/\lvert A_n^{(0)}\rvert$
0	2.96D − 02	7.31D − 34	9.05D − 34
1	4.63D − 03	1.53D − 33	1.94D − 33
2	2.00D − 04	2.16D − 33	2.67D − 33
3	3.38D − 06	2.68D − 33	3.22D − 33
4	4.08D − 09	3.17D − 33	3.71D − 33
5	1.99D − 11	3.65D − 33	4.19D − 33
6	3.31D − 14	4.12D − 33	4.67D − 33
7	8.03D − 18	4.59D − 33	5.14D − 33
8	5.11D − 22	5.06D − 33	5.61D − 33
9	5.68D − 27	5.54D − 33	6.09D − 33
10	5.35D − 33	6.01D − 33	6.56D − 33
11	1.04D − 33	6.48D − 33	7.03D − 33
12	6.90D − 34	6.95D − 33	7.50D − 33
13	8.29D − 33	7.43D − 33	7.97D − 33
14	1.04D − 32	7.90D − 33	8.45D − 33
15	2.04D − 32	8.37D − 33	8.92D − 33

Here $\mathcal{E}_n = |\bar{A}_n^{(0)} - I^{(1)}[g]|/|I^{(1)}[g]|$, $\widetilde{D}_n^{(j)}$ as in Sect. 4.3, and $\widetilde{E}_n^{(j)}$ as in (5.13)

7 The Periodic Case Revisited

As we mentioned in the paragraph following the statement of Theorem 1.1 in Sect. 1, if $f \in C^\infty(\mathbb{R})$ and is T-periodic, $T = b - a$, with polar singularities at $x = t + kT$, $k = 0, \pm 1, \pm 2, \ldots$, then $Q_n^{(k)}[g]$, $k = 1, 2$, have spectral accuracy, since their associated E–M expansions are empty; see (1.6). This means that *no* extrapolation is needed to improve their accuracies, which are already excellent. Here we would like to analyze the numerical stability properties of $Q_n^{(k)}[g]$, $k = 1, 2$, as they are (i.e., without extrapolation).

Note that these quadrature formulas can be used, as they are, in the numerical solution of singular and hypersingular integralequations

Table 3 Double-precision numerical results for the integral $I^{(2)}[g]$ in Sect. 6, with $t = 1$ throughout

n	$\mathcal{E}_n$	$\widetilde{D}_n^{(0)}/\lvert A_n^{(0)}\rvert$	$\widetilde{E}_n^{(0)}/\lvert A_n^{(0)}\rvert$
0	1.89D − 02	1.10D − 15	1.26D − 15
1	1.57D − 07	3.44D − 15	3.71D − 15
2	1.07D − 04	7.84D − 15	8.15D − 15
3	4.47D − 07	1.64D − 14	1.67D − 14
4	4.71D − 09	3.33D − 14	3.36D − 14
5	1.32D − 11	6.69D − 14	6.73D − 14
6	1.11D − 14	1.34D − 13	1.35D − 13
7	2.54D − 14	2.69D − 13	2.69D − 13
8	2.44D − 13	5.38D − 13	5.38D − 13
9	1.54D − 12	1.08D − 12	1.08D − 12
10	9.37D − 12	2.15D − 12	2.15D − 12

Here $\mathcal{E}_n = |\bar{A}_n^{(0)} - I^{(2)}[g]|/|I^{(2)}[g]|$, $\widetilde{D}_n^{(j)}$ as in Sect. 4.3, and $\widetilde{E}_n^{(j)}$ as in (5.16)

Table 4 Quadruple-precision numerical results for the integral $I^{(2)}[g]$ in Sect. 6, with $t = 1$ throughout

n	$\mathcal{E}_n$	$\widetilde{D}_n^{(0)}/\lvert A_n^{(0)}\rvert$	$\widetilde{E}_n^{(0)}/\lvert A_n^{(0)}\rvert$
0	1.89D − 02	9.57D − 34	1.09D − 33
1	1.57D − 07	2.99D − 33	3.22D − 33
2	1.07D − 04	6.82D − 33	7.09D − 33
3	4.47D − 07	1.42D − 32	1.45D − 32
4	4.71D − 09	2.89D − 32	2.92D − 32
5	1.33D − 11	5.82D − 32	5.85D − 32
6	5.44D − 15	1.17D − 31	1.17D − 31
7	3.70D − 18	2.34D − 31	2.34D − 31
8	7.11D − 23	4.68D − 31	4.68D − 31
9	3.93D − 27	9.36D − 31	9.36D − 31
10	2.65D − 30	1.87D − 30	1.87D − 30
11	2.17D − 29	3.74D − 30	3.74D − 30
12	3.33D − 29	7.49D − 30	7.49D − 30
13	5.88D − 29	1.50D − 29	1.50D − 29
14	8.20D − 29	3.00D − 29	3.00D − 29
15	3.65D − 28	5.99D − 29	5.99D − 29

Here $\mathcal{E}_n = |\bar{A}_n^{(0)} - I^{(2)}[g]|/|I^{(2)}[g]|$, $\widetilde{D}_n^{(j)}$ as in Sect. 4.3, and $\widetilde{E}_n^{(j)}$ as in (5.16)

$$u(t) + \lambda \int_a^b K(t,x)u(x)\,dx = w(t), \quad a \le t \le b,$$

where $K(t,x)$ is T-periodic in t and x and infinitely differentiable for all real t and x except for $t = x$ and $w(x)$ is T-periodic in x and infinitely differentiable for all real x. This guarantees that the solution $u(x)$ is also T-periodic in x and infinitely differentiable throughout the real line. For this use of the quadrature formulas, see the discussions in [18] and [17, Section 7].

Using the techniques of Sect. 5.1, we first have,

$$\left|\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g]\right| \le \mathbf{u}\left[h \sum_{j=1}^{n} \frac{|g(t + jh - h/2)|}{jh - h/2}\right] \le \mathbf{u}\|g\| \sum_{j=0}^{n-1} \frac{1}{j + 1/2},$$

which, by (5.3), gives

$$\left|\bar{Q}_n^{(1)}[g] - Q_n^{(1)}[g]\right| \leq \mathbf{u}\|g\|\,(2 + \log n). \tag{7.1}$$

Next, using the technique of Sect. 5.2, we have

$$\begin{aligned}\left|\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g]\right| &\leq \mathbf{u}\left[h\sum_{j=1}^{n}\frac{|g(t+jh-h/2)|}{(jh-h/2)^2} + \pi^2|g(t)|h^{-1}\right]\\ &\leq \mathbf{u}\|g\|h^{-1}\left[\pi^2 + \sum_{j=0}^{n}\frac{1}{(j+1/2)^2}\right]\\ &\leq \mathbf{u}\|g\|h^{-1}\left[\pi^2 + \zeta(2,1/2)\right],\end{aligned}$$

which finally gives

$$\left|\bar{Q}_n^{(2)}[g] - Q_n^{(2)}[g]\right| \leq \tfrac{3}{2}\pi^2\mathbf{u}\|g\|h^{-1}. \tag{7.2}$$

From (7.1) and (7.2), it is clear that the relative errors in the quadrature formulas $Q_n^{(1)}[g]$ and $Q_n^{(2)}[g]$ increase very mildly with increasing n.

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