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Effective Error Bounds in Euler-Maclaurin-Based Quadrature Schemes

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Abstract

We analyze the behavior of Euler-Maclaurin-based integration schemes with the intention of deriving accurate and economic estimations of the error term.

1 Introduction

The Euler-Maclaurin summation formula, while most often used for evaluating summations, is also useful for performing high-speed, high-accuracy numerical integration. In particular, quadrature schemes based on the Euler-Maclaurin formula have recently proven their utility in experimental mathematics applications, where they have permitted the preliminary analytic evaluation of integrals in terms of their high-precision numerical values. The schemes provide very high-precision results (hundreds or even thousands of digits), in reasonable run time, even in many cases where the integrand function has a blow-up singularity or infinite derivative at one or both endpoints [3, 4].

As a single example, one of the present authors (Borwein) and David Broadhurst found the following conjectured identity:

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \quad \stackrel{?}{=} \quad L_{-7}(2) \;= \tag{1}$$

$$\sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right].$$

This integral arose out of some studies in quantum field theory, in analysis of the volume of ideal tetrahedra in hyperbolic space. Note that the integrand function has a nasty

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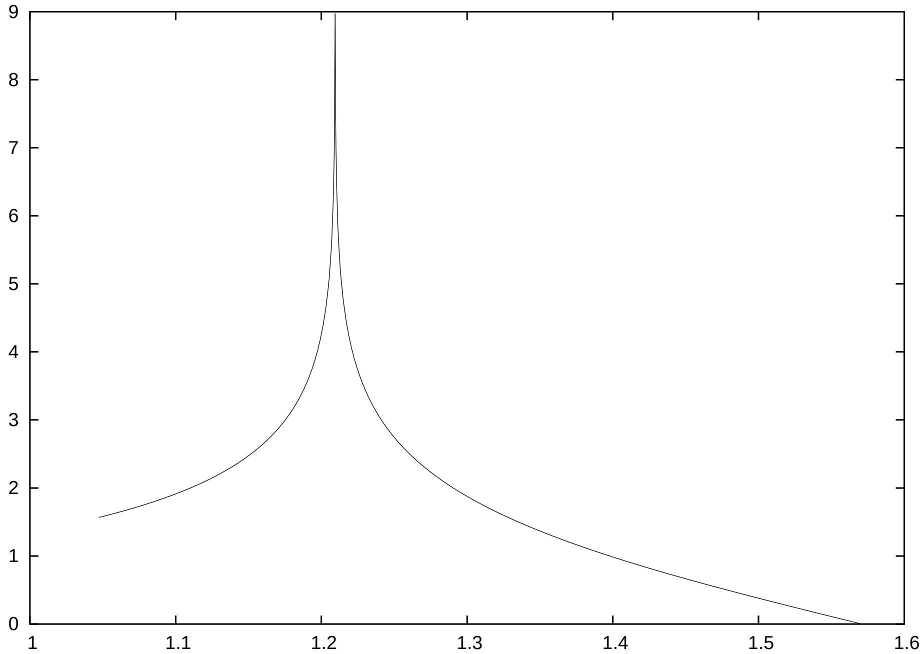

Figure 1: Integrand function with singularity

singularity at $t = \arctan(\sqrt{7})$ (see Figure 1). The question mark is used because no formal proof is yet known, but it has been verified numerically to 20,000 digit precision. We will deal with this integral further in Section 5 below.

Heretofore, researchers using these schemes have relied mostly on *ad hoc* error estimation schemes, such as to use differences between the quadrature sums of the past two halvings of the underlying interval length, h, to project the estimated error of the present iteration. In this paper, we seek to develop some more rigorous, yet highly usable schemes to estimate these errors. To do so requires that we take a close look at the error term in the Euler-Maclaurin formula.

2 Quadrature and the Euler-Maclaurin Formula

Atkinson's version of the Euler-Maclaurin formula is as follows [2, pg 285]: Let $m > 0$ be an integer, and, for notational convenience throughout this paper assume that h evenly divides a and b (in general it is only necessary that h divide $b - a$). Further assume that the function $f(x)$ is at least $(2m+2)$-times continuously differentiable on $[a, b]$. Then

$$\begin{aligned}\int_a^b f(x)\,dx &= h \sum_{j=a/h}^{b/h} f(jh) - \frac{h}{2}[f(a) + f(b)] \\ &\quad - \sum_{i=1}^{m} \frac{h^{2i} B_{2i}}{(2i)!} \left[D^{2i-1} f(b) - D^{2i-1} f(a)\right] + E(h, m), \qquad (2)\end{aligned}$$

where B_j denotes the j-th Bernoulli number, D denotes the differentiation operator, and the *error* is given by

$$E(h,m) \quad := \quad \frac{h^{2m+2}}{(2m+2)!} \int_a^b \bar{A}_{2m+2}[(t-a)/h] D^{2m+2} f(t)\, dt, \tag{3}$$

where $\bar{A}_k$ denotes Atkinson's variant of the k-th order Bernoulli polynomials, extended periodically beyond $[0,1]$.

Atkinson's variant of the Bernoulli polynomials, $A_j(x)$, is defined implicitly by the exponential generating function

$$\frac{t(e^{tx}-1)}{e^t-1} \quad = \quad \sum_{j=1}^{\infty} \frac{A_j(x)\, t^j}{j!}.$$

The standard Bernoulli polynomials, $B_j(x)$, are defined implicitly by [1, pg 804]

$$\frac{te^{tx}}{e^t-1} \quad = \quad \sum_{j=1}^{\infty} \frac{B_j(x)\, t^j}{j!}.$$

Since the Bernoulli numbers, $B_j = B_j(0)$, satisfy

$$\frac{t}{e^t-1} \quad = \quad \sum_{j=1}^{\infty} \frac{B_j\, t^j}{j!},$$

it follows that Atkinson's polynomials and the standard Bernoulli polynomials are related by $A_j(x) = B_j(x) - B_j$, so that Atkinson's variants have a zero constant term.

A second form of the error term, which can be easily derived from the above, is [2, pg 288]:

$$E(h,m) \quad = \quad \frac{(a-b)\, B_{2m+2}\, D^{2m+2} f(\xi)}{(2m+2)!}\, h^{2m+2} \tag{4}$$

for some $\xi \in (a,b)$.

A third form of the error term in the Euler-Maclaurin formula is the following [6]:

$$E(h,m) \quad = \quad \frac{h^{2m}}{(2m)!} \int_a^b \bar{B}_{2m}[(t-a)/h]\, D^{2m} f(t)\, dt, \tag{5}$$

where $\bar{B}_{2m}(x)$ denotes the periodic extension of the Bernoulli polynomial $B_{2m}(x)$ beyond $[0,1]$.

In the circumstance where the function $f(t)$ and all of its derivatives are zero at the endpoints a and b (as with a smooth, bell-shaped function), note that the second and third terms of the Euler-Maclaurin formula are zero. Thus, for such functions, the error of a simple step-function approximation to the integral, with interval h, is simply $E(h,m)$. But since, for any m, $E(h,m)$ is less than a constant (independent of h) times h^{2m+2}, as we see by applying the second form of the error term, namely (4), we conclude that the error goes to zero more rapidly than any fixed power of h.

For a function defined on $(-\infty, \infty)$, the Euler-Maclaurin summation formula still applies to the resulting doubly-infinite sum approximation, provided much as before that the function and all of its derivatives decay to zero rapidly for large positive and negative arguments. This principle is utilized in some state-of-the-art numerical integration schemes schemes, which proceed by transforming the integral of $F(x)$ on the interval $[-1, 1]$ to an integral of $f(t) = F(g(t))g'(t)$ on $(-\infty, \infty)$, by using the change of variable $x = g(t)$. Here $g(x)$ is any monotonic, infinitely-differentiable function with the property that $g(x) \to \pm 1$ as $x \to \pm\infty$, respectively, that also has the property that $g'(x)$ and all higher derivatives rapidly approach zero for large positive and negative arguments. In this case we can write, for $h > 0$,

$$\int_{-1}^{1} F(x)\,dx \;=\; \int_{-\infty}^{\infty} F(g(t))g'(t)\,dt \;=\; h \sum_{j=-\infty}^{\infty} w_j F(x_j) + E(h) \tag{6}$$

where $x_j = g(hj)$ and $w_j = g'(hj)$. If $g'(t)$ and its derivatives tend to zero sufficiently rapidly for large t, positive and negative, then—even in cases where $F(x)$ has an infinite derivative or an integrable singularity at one or both endpoints—the resulting integrand $f(t) = F(g(t))g'(t)$ will be a smooth bell-shaped function for which the prior Euler-Maclaurin argument applies. Thus, in such cases, the error $E(h)$ in our approximation decreases faster than any power of h.

There are various such functions g that work well in practice. Using $g(t) := \tanh t$ gives rise to *tanh quadrature*. Using $g(t) := \mathrm{erf}(t)$ gives rise to "error function" or *erf quadrature*. Using $g(t) := \tanh(\pi/2 \cdot \sinh t)$ or $g(t) := \tanh(\sinh t)$ gives rise to *tanh-sinh quadrature*. For integrand functions to be integrated on $(-\infty, \infty)$, so that a transformation from a finite interval to the entire real line is unnecessary, one can use $g(t) := \sinh t$, $g(t) := \sinh(\pi/2 \cdot \sinh t)$ or $g(t) := \sinh(\sinh t)$. Tanh-sinh quadrature was first introduced by Takahasi and Mori [8].

When one studies the results of implementing and testing these schemes on various integrand functions, using high-precision arithmetic, one phenomenon that readily becomes apparent is "quadratic convergence," that is, the tendency for the actual error, as a function of the interval h, to be squared when h is halved. In other words, for many problems of interest, the number of correct digits in the result is approximately doubled when h is halved, making it possible to efficiently evaluate these integrals to very high precision. Table 1 shows this phenomenon for a subset of the test problems used in a previous study [3], with results listed to the nearest order of magnitude. These results were computed with erf quadrature, that is, using the transformation $g(t) = \mathrm{erf}(t)$.

The test integrals are:

$$\mathbf{e2} \;:\; \int_0^1 t^2 \arctan t\,dt \;=\; (\pi - 2 + 2\log 2)/12$$

$$\mathbf{e4} \;:\; \int_0^1 \frac{\arctan(\sqrt{2+t^2})}{(1+t^2)\sqrt{2+t^2}}\,dt \;=\; 5\pi^2/96$$

$$\mathbf{e6} \;:\; \int_0^1 \sqrt{1-t^2}\,dt \;=\; \pi/4$$

h	**e2**	**e4**	**e6**	**e8**	**e10**	**e12**	**e14**
1	10^{-2}	10^{-5}	10^{-3}	10^{-3}	10^{-3}	10^{-1}	10^{-1}
1/2	10^{-6}	10^{-6}	10^{-8}	10^{-10}	10^{-8}	10^{-3}	10^{-2}
1/4	10^{-13}	10^{-12}	10^{-17}	10^{-21}	10^{-16}	10^{-6}	10^{-3}
1/8	10^{-26}	10^{-25}	10^{-34}	10^{-43}	10^{-33}	10^{-11}	10^{-5}
1/16	10^{-52}	10^{-51}	10^{-68}	10^{-87}	10^{-66}	10^{-20}	10^{-10}
1/32	10^{-104}	10^{-102}	10^{-134}	10^{-173}	10^{-132}	10^{-37}	10^{-19}
1/64	10^{-206}	10^{-204}	10^{-266}	10^{-348}	10^{-264}	10^{-70}	10^{-37}
1/128	10^{-411}	10^{-409}	10^{-529}	10^{-696}	10^{-527}	10^{-132}	10^{-68}
1/256	10^{-821}	10^{-819}	10^{-1056}	10^{-1392}	10^{-1053}	10^{-249}	10^{-128}

Table 1: 'QUADERF' errors at successive values of h

$$
\begin{aligned}
\mathbf{e8} &: \int_0^1 \log^2 t\, dt = 2 \\
\mathbf{e10} &: \int_0^{\pi/2} \sqrt{\tan t}\, dt = \pi\sqrt{2}/2 \\
\mathbf{e12} &: \int_0^\infty \frac{e^{-t}}{\sqrt{t}}\, dt = \int_0^1 \frac{e^{1-1/s}\, ds}{\sqrt{s^3 - s^4}} = \sqrt{\pi} \\
\mathbf{e14} &: \int_0^\infty e^{-t}\cos t\, dt = \int_0^1 \frac{e^{1-1/s}\cos(1/s-1)\, ds}{s^2} = 1/2.
\end{aligned}
$$

3 Estimates of the Error Term

In an attempt to understand why and when this very favorable phenomenon occurs, we need to better understand the error term in Euler-Maclaurin. Indeed, it is clearly very advantageous, for both theoretical understanding and practical reasons, to find a formulation (even an approximate formulation) of the error term that is amenable to simple calculation and estimation. To that end, we state and prove two alternate forms of the error term.

Theorem 1 *The error term of the Euler-Maclaurin formula is given by:*

$$E(h, m) = 2(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m}\sum_{k=1}^{\infty}\frac{1}{k^{2m}}\int_a^b \cos[2k\pi(t-a)/h]\, D^{2m} f(t)\, dt. \qquad (7)$$

Proof: This follows by noting that the even-indexed Bernoulli polynomials have a rather compact and fairly rapidly convergent Fourier series representation [1, pg 805]:

$$B_{2m}(x) = \frac{2(-1)^{m-1}(2m)!}{(2\pi)^{2m}}\sum_{j=1}^{\infty}\frac{\cos(2j\pi x)}{j^{2m}} = B_{2m}\sum_{j=1}^{\infty}\frac{\cos(2j\pi x)}{j^{2m}}. \qquad (8)$$

Substituting this expression into the third form of the error term (5), and applying the Dominated convergence theorem, we obtain the result. □

Theorem 2 *Suppose that $f(t)$ is defined on $[a, b]$, and has the property that $f(a) = f(b) = 0$. Suppose further that the f is at least $2m$-times continuously differentiable on $[a, b]$, with $D^k f(a) = D^k f(b) = 0$ for $1 \le k \le 2m$. Also, as before assume that h divides a and b. Then $E(h, 1) = E(h, k)$ for $1 \le k \le m$.*

Proof: This follows immediately from the Euler-Maclaurin formula (2), since the second and third terms are zero, leaving only the first summation (which is independent of m) and the error term. □

It is important to note that for many integrand functions of interest, even the first term of the infinite summation in (7) is an excellent approximation to the error. In other words, we can consider the approximation

$$E_1(h, m) \quad := \quad 2\,(-1)^{m-1} \left(\frac{h}{2\pi}\right)^{2m} \int_a^b \cos[2\pi(t-a)/h] D^{2m} f(t)\, dt. \tag{9}$$

We shall also introduce a second approximation, which we first noticed because of a 'bug' in our computer program. In implementing formula (9), we employed a numerical summation as the approximation to the integral involved in the formula, using for the integration interval the value of h (one should use a much smaller interval, such as $h/8$ or $h/16$, to accurately resolve the oscillations in the integrand). In so doing, all the cosine evaluations were at multiples of 2π, giving the result of '1.0'. As a result of this "petri dish" error, our numerical evaluations of the formula gave results almost precisely twice the actual error. This observation led to the interesting result below:

Theorem 3 *Assume the same hypotheses as in Theorem 2, and further let $n \ge 1$ be any integer such that these conditions are also met with $m + n$ replacing m. Then*

$$\begin{aligned} E(h, m) \quad &= \quad h(-1)^{m-1} \left(\frac{h}{2\pi}\right)^{2m} \sum_{j=a/h}^{b/h} D^{2m} f(jh) \qquad (10) \\ &+ 2\,(-1)^{n-1} \left(\frac{h}{2\pi}\right)^{2m+2n} \sum_{k=1}^{\infty} \left(\frac{1}{k^{2n}} + \frac{(-1)^m}{k^{2m+2n}}\right) \int_a^b \cos[2k\pi(t-a)/h] D^{2m+2n} f(t)\, dt. \end{aligned}$$

Proof. To derive this result, note first that

$$\int_a^b D^{2m} f(t)\, dt \quad = \quad D^{2m-1} f(t)|_a^b \; = 0,$$

since we assume here that $f(t)$ and $m + n$ derivatives are zero at the endpoints a and b. Thus we can now write, by applying the Euler-Maclaurin formula of degree n (with the error term as given in Theorem 1) to the function $D^{2m} f(t)$:

$$0 \quad = \quad \left(\frac{h}{2\pi}\right)^{2m} \int_a^b D^{2m} f(t)\, dt$$

$$
\begin{aligned}
= \;& h\left(\frac{h}{2\pi}\right)^{2m}\sum_{j=a/h}^{b/h} D^{2m}f(jh) - \frac{h}{2}\left(\frac{h}{2\pi}\right)^{2m}\left[D^{2m}f(b) - D^{2m}f(a)\right] \\
& - \left(\frac{h}{2\pi}\right)^{2m}\sum_{k=1}^{n}\frac{h^k B_{2k}}{(2k)!}\left[D^{2m+2k-1}f(b) - D^{2m+2k-1}f(a)\right] \\
& + 2(-1)^{n-1}\left(\frac{h}{2\pi}\right)^{2m+2n}\sum_{k=1}^{\infty}\frac{1}{k^{2n}}\int_a^b \cos[2k\pi(t-a)/h]D^{2m+2n}f(t)\,dt.
\end{aligned}
$$

As before, the second and third terms on the right-hand side are zero, since we assume that $f(t)$ and $m+n$ derivatives are zero at a and b. Thus we are left with the equivalence

$$
\begin{aligned}
h\left(\frac{h}{2\pi}\right)^{2m}\sum_{j=a/h}^{b/h} D^{2m}f(jh) \;=\; & \\
& -2\,(-1)^{n-1}\left(\frac{h}{2\pi}\right)^{2m+2n}\sum_{k=1}^{\infty}\frac{1}{k^{2n}}\int_a^b \cos[2k\pi(t-a)/h]D^{2m+2n}f(t)\,dt.
\end{aligned}
$$

and the result follows from Theorems 1 and 2 (with m replaced by $m+n$). □

Theorem 3 immediately suggests the simple approximation

$$
E_2(h,m) \;:=\; h(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m}\sum_{j=a/h}^{b/h} D^{2m}f(jh). \tag{11}
$$

We will make use E_2 in the computer implementations described in the next section.

One other estimate is worth mentioning. Note that the Fourier expansion (8) leads immediately to the the bound

$$
|B_{2k}(x)/B_{2k} - \cos(2\pi x)| \;\le\; \zeta(2k) - 1
$$

where $\zeta(\cdot)$ denotes the Riemann zeta function. This permits us to derive:

Corollary 1 *Under the hypotheses of Theorem 1 one has*

$$
|E(h,m) - E_1(h,m)| \;\le\; 2\,(\zeta(2m)-1)\left(\frac{h}{2\pi}\right)^{2m}\int_a^b \left|D^{2m}f(t)\right|\,dt.
$$

This bound can be used, for instance, to establish a rigorous "certificate" of the estimate $E_1(h,m)$, and thus (after computation of $E_1(h,m)$) of the quadrature result itself. Other useful bounds can also be derived. For example, integrating repeatedly by parts yields:

Corollary 2 *Under the hypotheses of Theorem 3, one has*

$$
\int_a^b \cos[2k\pi(t-a)/h]\,D^{2m}f(t)\,dt \;=\; \left(\frac{i\,h}{2k\pi}\right)^{2n}\int_a^b \cos[2k\pi(t-a)/h]\,D^{2m+2n}\,f(t)\,dt.
$$

Moreover, by the Riemann-Lebesgue lemma,

$$\int_a^b \cos[2k\pi(t-a)/h] D^{2m} f(t)\, dt \to 0$$

as $k \to \infty$.

In particular, we can mirror Corollary 1:

Corollary 3 *Under the hypotheses of Theorem 3 with n=1, one obtains*

$$|E(h,m) - E_2(h,m)| \leq 2\left[\zeta(2m) + (-1)^m \zeta(2m+2)\right] \left(\frac{h}{2\pi}\right)^{2m} \int_a^b \left|D^{2m} f(t)\right| dt. \tag{12}$$

This highlights what is gained by using $E_2(h,m)$ rather than $E_1(h,m)$ (note that (12) is particularly advantageous when m is odd). In each of Corollary 1 and Corollary 3, by using the Cauchy-Schwarz inequality to obtain the bound

$$\int_a^b \cos[2k\pi(t-a)/h]\, D^{2m} f(t)\, dt \leq h\sqrt{\int_a^b |D^{2m} f(t)|^2\, dt},$$

we may replace

$$\int_a^b \left|D^{2m} f(t)\right| dt$$

by

$$h\sqrt{\int_a^b |D^{2m} f(t)|^2\, dt}, \tag{13}$$

which is often significantly smaller.

4 Implementations and Tests

We have implemented the error estimation formula (9) for $E_1(h,m)$, which requires integrations with the cosine terms, using *Mathematica*. We have also tried numerical integrations, using the computer programs described in [3], where it is important to use a much smaller integration interval than the h that appears in the formula (we typically use $h/8$ or $h/16$).

Implementing the formula (11) for $E_2(h,m)$ is even easier, and requires no symbolic manipulation except for finding the derivatives of the input function $F(t)$. Evaluation of $E_2(h,1)$, for instance, can be done as follows: Let $g(t)$ be the function defining the quadrature scheme to be used. Then we can write

$$\begin{aligned} D^2 f(t) &= D^2[F(g(t))g'(t)]] \\ &= F(g(t))g'''(t) + F'(g(t))[3g'(t)g''(t)] + F''(g(t))[g'(t)]^3 \end{aligned} \tag{14}$$

So for instance when $g(t) = \tanh(\sinh t)$,

$$
\begin{aligned}
D^2 f(t) = \; & F(\tanh(\sinh t)) \Big[\mathrm{sech}^2(\sinh t)\cosh t - 2\,\mathrm{sech}^4(\sinh t)\cosh^3 t \\
& \quad - 6\,\mathrm{sech}^2(\sinh t)\tanh(\sinh t)\cosh t \sinh t \\
& \quad + 4\,\mathrm{sech}^2(\sinh t)\tanh^2(\sinh t)\cosh^3 t\Big] \\
& + F'(\tanh(\sinh t)) \Big[3\,\mathrm{sech}^4(\sinh t)\cosh t \sinh t \\
& \quad - 6\,\mathrm{sech}^4(\sinh t)\tanh(\sinh t)\cosh^3 t\Big] \\
& + F''(\tanh(\sinh t))[\mathrm{sech}^6(\sinh t)\cosh^3 t]
\end{aligned}
$$

The three hyperbolic function expressions, as well as the abscissas $\tanh(\sinh t)$, can be pre-calculated for a range of arguments—note that in formula (11) for $E_2(h, m)$, the function $D^{2m} f(t)$ is evaluated at the same equi-spaced arguments that are used in the quadrature calculation itself, namely $\{jh,\ a/h \le j \le b/h\}$. Further, we have found that by avoiding unnecessary duplication when evaluating the function and its two derivatives, it is often possible to compute $E_2(h, 1)$, in particular, with only a modest increase in the quadrature run time. This increase ranges from only about 10% for integrands involving transcendental functions to at most 200%, as in the case of simple algebraic integrands where there is little or no potential for avoiding duplication. It may also be possible to do these calculations using somewhat less than the full precision used for quadrature, although in this paper we use full precision. In any event, these estimates can be computed quite rapidly.

Tables 2 through 5 include some computational analysis of $E_2(h, m)$, based on the test functions

f1 : $F_1(t) = 1/(1 + t^2 + t^4 + t^6)$
f2 : $F_2(t) = (1 - t^4)^{1/2}$
f3 : $F_3(t) = (1 - t^2)^{-1/2}$
f4 : $F_4(t) = (1 + t)^2 \sin(2\pi/(1 + t))$.

In each case the interval of integration is $[-1, 1]$, and the tanh-sinh rule was used for quadrature. In problems f1, f2 and f4, 400-digit arithmetic was employed. In problem f3, 1100-digit arithmetic was used, although 550-digit arithmetic suffices here if one employs a "secondary epsilon" technique described in [3].

Note that $F_2(t)$ has an infinite derivative at the endpoints, and $F_3(t)$ has a blow-up singularity at the endpoints, while $F_4(t)$ represents a worst case for these methods, since it is highly oscillatory near -1. In particular, while the first two derivatives of the transformed function $f_4(t)$ tend to zero with large positive and negative arguments, the third and higher derivatives do not. Plots of these four test functions are shown in Figures 2 and 3.

Recall that for the tanh-sinh scheme, a function $F(t)$ to be integrated on $[-1, 1]$ is transformed to the function $f(t) = F(\tanh(\sinh t))\,\mathrm{sech}^2(\sinh t)\cosh t$, integrated over $(-\infty, \infty)$. For the problems f1, f2 and f4, the "infinite" integration interval $[a, b]$ is taken

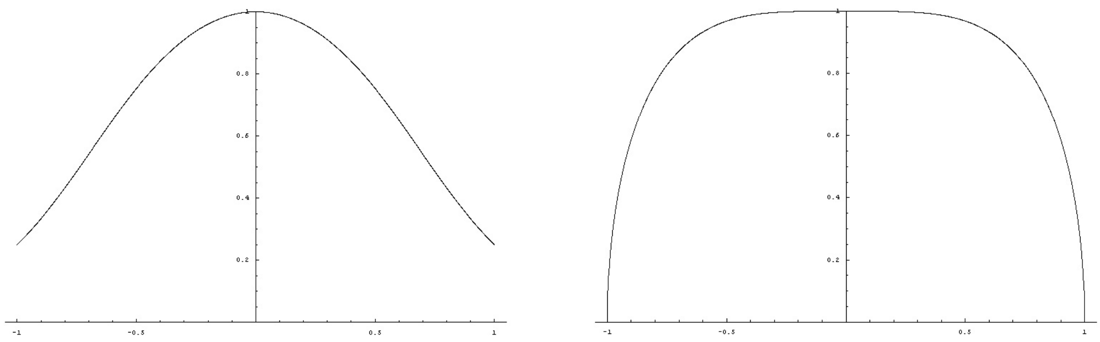

Figure 2: $F_1(t) = 1/(1 + t^2 + t^4 + t^6)$ and $F_2(t) = (1 - t^4)^{1/2}$

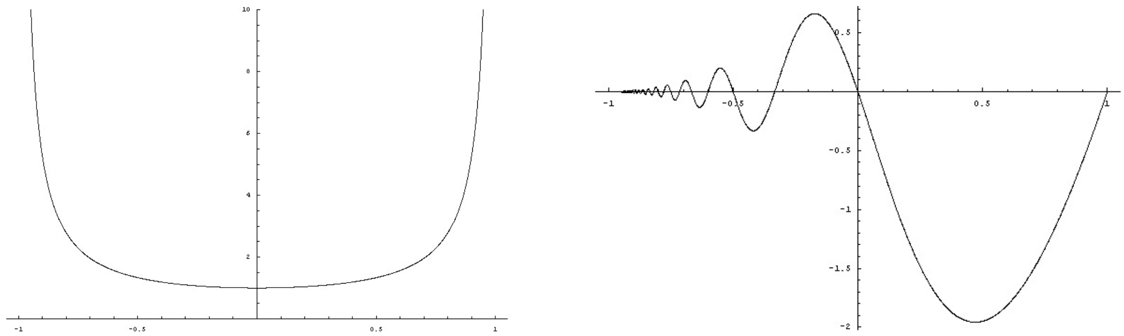

Figure 3: $F_3(t) = (1 - t^2)^{-1/2}$ and $F_4(t) = (1 + t)^2 \sin(2\pi/(1 + t))$

to be $[-7, 7]$, which is (provably) sufficient to insure that all of these computations agree with values on $(-\infty, \infty)$ to within 10^{-400} in each case. For the problem f3, the interval is $[-8, 8]$, which is sufficient to insure accuracy to within 10^{-600}.

The values $E(h)$ shown in the first column of the four tables are the actual errors of the quadrature results, namely

$$E(h) \;=\; \int_{-1}^{1} F(t)dt - Q(h),$$

where $Q(h)$ is the numerical approximation to the integral using the tanh-sinh rule:

$$Q(h) \;=\; h \sum_{j=a/h}^{b/h} f(jh) \;=\; h \sum_{j=a/h}^{b/h} F(\tanh(\sinh(jh)))\,\mathrm{sech}^2(\sinh(jh))\cosh(jh).$$

The correct quadrature results for the first three problems are $\pi/4 + \log(1+\sqrt{2})/\sqrt{2}$, $\sqrt{\pi}\,\Gamma(5/4)/\Gamma(7/4)$ and π, respectively. We know of no classical closed-form evaluation for problem f4, but in terms of the *cosine integral* the result equals

$$-\frac{4}{15}\pi^5\,\mathrm{Ci}\,(\pi) + \frac{4}{15}\,\pi^3 - \frac{8}{5}\,\pi,$$

whose numerical value is $-2.76989612386024129018\ldots$. Here

$$\mathrm{Ci}(x) \quad := \quad \gamma + \ln(x) + \int_0^x \frac{\cos(t)-1}{t}\,dt,$$

and γ is Euler's constant.

Except for the problem f4, we include results for $E_2(h,m)$ with $m = 1,2,3,4$, or, in other words, estimates based on the second, fourth, sixth and eighth derivatives of $f(t)$, respectively. In the case of the problem f4, computing $E_2(h,m)$ for $m > 1$ does not make mathematical sense, since the conditions of Theorem 3 are not met for the transformed function $f_4(t)$: while the second derivative of $f_4(t)$ tends to zero rapidly for large positive and large negative arguments, higher derivatives do not—the third derivative, for instance, oscillates between roughly -4000 and 4000 for negative t, and the fourth derivative oscillates with sharply increasing amplitude for negative t.

It is clear from these results that the estimates $E_2(h,m)$ are extremely accurate in the first three test problems. In each of these problems, $E_2(h,1)$ through $E_2(h,4)$ all agree with the actual errors to at least eight significant digits when $h = 1/4$, and to more than 120 significant digits when $h = 1/64$ (in the problem f3, the four estimates are correct to 270 significant digits when $h = 1/64$). Indeed, as h is reduced the estimates actually increase in *relative* precision as well as in absolute precision, approximately *doubling* in relative precision (in digits) with each halving of the interval h (in other words, exhibiting quadratic convergence). The estimate $E_2(h,1)$ is always the most accurate, although the higher-level estimates are never far behind.

For the pathological problem f4, which features highly oscillatory behavior near -1, the estimates are not nearly as accurate. But even here they are accurate to within a factor of three for all $h \le 1/8$, which is more than sufficient to determine the order of magnitude of error in a practical computation.

5 Two Illustrative Examples

Example I. We first illustrate the usage of these techniques with a computational proof of a recent problem from the *MAA Monthly*[1]. In equivalent form, it requests a proof of

$$\int_{-\infty}^{\infty} \frac{t^2}{1+4t+3t^2-4t^3-2t^4+2t^5+t^6}\,dt \quad = \quad \pi. \tag{15}$$

The actual integrand in the problem was

$$\frac{x^8 - 4\,x^6 + 9\,x^4 - 5\,x^2 + 1}{x^{12} - 10\,x^{10} + 37\,x^8 - 42\,x^6 + 26\,x^4 - 8\,x^2 + 1}.$$

However, a partial fraction expansion reduces this to (15). This reduction also dramatically reduces the degree and length estimates needed below.

[1]This is Problem *M11148* posed in the April 2005 issue of the *American Mathematical Monthly.*

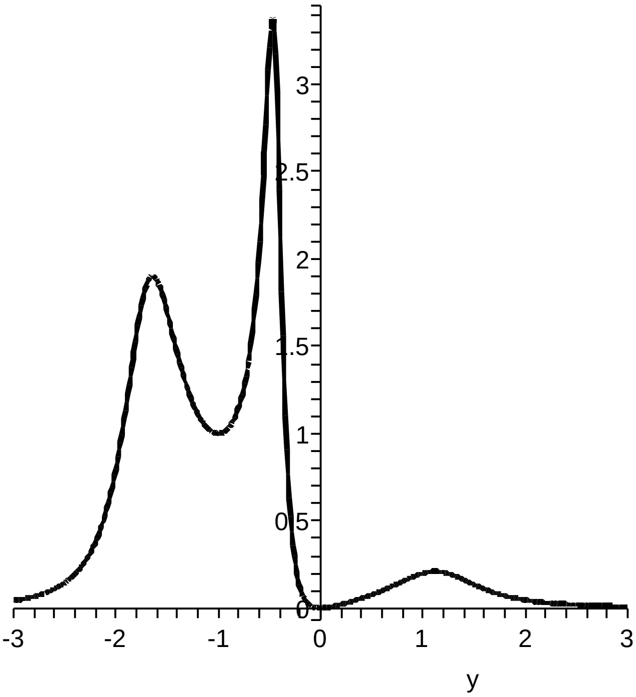

Figure 4: Plot of $F_5(t) = t^2/(1 + 4t + 3t^2 - 4t^3 - 2t^4 + 2t^5 + t^6)$

A plot of the above integrand function is shown in Figure 3. A purely qualitative analysis with partial fractions and arctangents shows the integral is of the form $\beta\,\pi$ where β is an algebraic number of degree at most six with length ℓ (the length ℓ of an algebraic number is the absolute sum of the coefficients of the minimal polynomial) much less than 10^{25}. It follows from well-known results in irrational number theory that

$$|\beta - 1| \leq \frac{\pi}{32\,\ell} \quad \text{implies} \quad \beta = 1.$$

See, for example, [5, Exercise 8, pg 358] with $P(x) = x - 1, D = 1, L = 2, d = 6, \ell = 10^{25}$. All this means that confirming identity (15) to 25-digit accuracy, with a certificate, completes a proof of the identity.

We calculated $Q(h)$, the numerical approximation of the integral of this function, using the sinh-sinh rule (i.e., using the transformation function $g(t) = \tanh(\sinh t)$), with $h = 10^{-4}$ and 220-digit arithmetic, and found that $|\pi - Q(h)| \leq 10^{-200}$. We also calculated the error estimates $E_2(h,1)$ through $E_2(h,5)$, using formula (11), and found that each is less than 10^{-200}. In fact, we found that $|\pi - Q(h)| \leq 10^{-200}$ and $|E_2(h,m)| \leq 10^{-200}$ for $m = 1, 2, \cdots, 5$, even when $h = 10^{-3}$. As part of the computation of the error bound $E_2(h,5)$, we determined that the function $|D^{10}f(t)|$ never exceeds 2.6×10^{17} within the interval $[-0.5, -0.3]$, never exceeds 1.6×10^{17} within the interval $[-1.2, -1.0]$, and has relatively negligible values outside these two intervals. This fact was confirmed by symbolic computation using *Mathematica*. Using this information, and applying formulas (12) and (13) on a hand calculator, we find that the $|E(h) - E_2(h,5)| \leq 2.13 \times 10^{-38}$.

Thus 2.13×10^{-38}*, is a "certificate"* on the accuracy of our evaluation of the above integral. Hence, this calculation confirms the identity (15). □

Example II. We next addressed the integral

$$I \;:=\; \frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \;\stackrel{?}{=}\; L_{-7}(2), \tag{16}$$

which we mentioned in the introduction. In [4], we applied a highly parallel implementation of the tanh-sinh quadrature algorithm to calculate the numerical value of this integral to 20,000-digit precision, and found that it agreed precisely with a 20,000-digit evaluation of the right-hand side. Our integral evaluation employed only an ad-hoc error estimation procedure, so some colleagues have challenged us to find a more modest but rigorous "certificate" on the accuracy of this result.

To that end, we note that (16) can be written as

$$I \;=\; \frac{24}{7\sqrt{7}} \left(b_1 \int_{-1}^{1} w_1(t)\, dt - b_2 \int_{-1}^{1} w_2(t)\, dt + b_3 \int_{-1}^{1} w_3(t)\, dt - b_4 \int_{-1}^{1} w_4(t)\, dt \right),$$

where

$$\begin{aligned} w_1(t) &= \log\left[\tan(a_1 + b_1 t) + c_1\right] \\ w_2(t) &= \log\left[-\tan(a_2 + b_2 t) + c_2\right] \\ w_3(t) &= \log\left[\tan(a_3 + b_3 t) + c_3\right] \\ w_4(t) &= \log\left[\tan(a_4 + b_3 t) + c_4\right] \end{aligned}$$

and where

$$\begin{array}{lll} a_1 = (\arctan(\sqrt{7}) + \pi/3)/2, & b_1 = (\arctan(\sqrt{7}) - \pi/3)/2, & c_1 = \sqrt{7} \\ a_2 = (\arctan(\sqrt{7}) + \pi/3)/2, & b_2 = (\arctan(\sqrt{7}) - \pi/3)/2, & c_2 = \sqrt{7} \\ a_3 = (\arctan(\sqrt{7}) + \pi/2)/2, & b_3 = (-\arctan(\sqrt{7}) + \pi/2)/2, & c_3 = \sqrt{7} \\ a_4 = (\arctan(\sqrt{7}) + \pi/2)/2, & b_4 = (-\arctan(\sqrt{7}) - \pi/2)/2, & c_4 = -\sqrt{7}. \end{array}$$

In a similar manner as in the *Monthly* problem, we calculated the estimated errors $E_1(h,1)$ through $E_1(h,5)$, for each of the four component integrals, using the tanh-sinh rule, with $h = 10^{-4}$ and 220-digit arithmetic. We found that each of these 20 errors is less than 10^{-200} (in fact, this is true even when $h = 10^{-2}$). As part of the computation of the error bound $E_2(h,5)$, we determined that $|D^{10} f(t)|$, where $f(t) = w_4(g(t))g'(t)$, is bounded by 10^6 within the interval $[-3,3]$, and has relatively negligible values outside this interval. This fact was confirmed by symbolic computation using *Mathematica*. Applying formulas (12) and (13) on a hand calculator, we obtain a bound of 3.82×10^{-49} for this integral. The other three integrals yield slightly smaller bounds. *Hence,* 3.82×10^{-49} *is a certificate for the integral (16).* □

Of course, this is all premised on: (1) correct implementations of the algorithms, (2) faithful implementation of the underlying arithmetic (performed using the ARPREC software), (3) correct symbolic differentiation (performed using *Mathematica*), and (4) correct location of the maximum of the tenth-order derivatives (performed using ARPREC and confirmed using *Mathematica*). Nonetheless, by means of validity checks that we have employed, we are confident that these operations have been done correctly.

We add that for each of the four component integrals of Example II, for instance, 200-digit values can be produced in less than one second runtime, using tanh-sinh quadrature with $h = 1/64$. If we count the computation of abscissas and weights for tanh-sinh quadrature, the total is still only three seconds. Computing the error estimates $E_2(h, m)$ to the same accuracy (which also uses $h = 1/64$) is somewhat more expensive, mainly due to the cost of evaluating $D^{10} f(t)$. In contrast, obtaining a certificate for one of these integrals to, say, 50-digit accuracy, requires computing $E_2(h, 5)$ with $h = 10^{-4}$, which multiplies the runtime by a factor of more than 150. Some savings are doubtless possible in these computations, but in general our experience here is similar to the experience in other arenas of computational mathematics—it is much easier to produce practical high-precision numerical values than to produce rigorous certificates. Nonetheless, certificates do carry a measure of "proof" that is not available with more informal computations.

6 The Fourier Connection

One central question remains unresolved: *why, for many functions of interest, do the quadrature results exhibit quadratic convergence*, namely a near-doubling of the number of correct digits with each halving of the interval h. Evidently this is related to behavior of the Fourier coefficients (or coefficients based on other orthonormal basis sets) of higher derivatives of the transformed function.

Assume, as we may, that we are working on $[0, 1]$ and consider the periodic extension of a real function f which vanishes at 0 and at 1. Write

$$f(x) \quad = \quad c_0 + \sum_{k \neq 0} c_k \exp(ik2\pi x).$$

Then, $c_{-k} = \overline{c}_k$, and normalized appropriately, $c_0 = \int_0^1 f$. Thus, writing $c_k = a_k + ib_k$, for each $N > 0$, we have

$$\begin{aligned} E(1/N) \;:=\; \left| \int_0^1 f(t)\, dt - \frac{1}{N} \sum_{n=1}^{N} f\left(\frac{n}{N}\right) \right| \quad &= \quad \left| \sum_{k \neq 0} c_k \frac{1}{N} \sum_{n=1}^{N} \exp\left(\left(2\pi\, i\, \frac{k}{N} \right) n \right) \right| \\ &= \quad \left| \sum_{j \neq 0} c_{jN} \right| \;=\; 2 \left| \sum_{j=1}^{\infty} a_{jN} \right|, \end{aligned}$$

since for non-zero integer k, the exponential sum, $\frac{1}{N} \sum_{n=1}^{N} \exp\left(\left(2\pi\, i\, \frac{k}{N}\right) n\right)$, is zero unless N divides k, in which case the sum is unity. The convergence of the Fourier series and the interchange of sums is certainly justified when $\sum_k |c_k| < \infty$, as is true in the sequel.

Now, assuming that f is infinitely differentiable and periodic, on integrating by parts, we see that for all $k, n > 0$,

$$c_k = \frac{i^n}{(2k\pi)^n} \int_0^1 f^{(n)}(x) \exp(2k\pi\, ix)\, dx$$

so that for all $N, k, n > 0$,

$$|a_k| \;\leq\; |c_k| \;\leq\; \frac{C_1(n)}{k^n} \quad \text{and so} \quad |E(1/N)| \;\leq\; \frac{C_2(n)}{N^n},$$

for constants C_1, C_2 depending only on n. In particular we have proven:

Theorem 4 *For a p-times differentiable periodic function on* $[a, b]$*, one has*

$$|E(1/N)| \;=\; \left|\sum_{j=1}^{\infty} 2\, a_{jN}\right| \;=\; o\left(\frac{1}{N^p}\right),$$

as N *tends to infinity. In particular, if the function is infinitely differentiable*

$$|E(1/N)| \;=\; o\left(\frac{1}{N^\alpha}\right),$$

for all $\alpha > 0$*, as* N *tends to infinity.*

Moreover, at least informally, for most ‘regular’ expansions—say with c_{n+1} being $o(c_n)$,

$$E(1/N) \;\sim\; 2|a_N|,$$

which suggests why we see the observed performance, since $\{a_j\}$ will then decay at least super-linearly.

For illustration, consider $H(x) := (2\cos(x) - 1)/(5 - 4\cos x + 5)$ on $[0, 2\pi]$. Then $H(x) = \sum_{k=1}^{\infty} 2^{-k}\cos(kx)$ is infinitely differentiable and $E(1/N) = 1/(2^N - 1)$, so that $\log|E(1/(2N))|/\log|E(1/N)| \to 2$, showing quadratic convergence. It also appears that $H(x)$ exhibits quadratic convergence when the function is scaled linearly to $[-1, 1]$—yielding $\bar{H}(x) = (2\cos(\pi x) + 1)/(4\cos(\pi x) + 5)$—and tanh-sinh quadrature is applied, see Table 6.

Perchance the techniques introduced in this paper will further elucidate the underlying reasons for this phenomenon, and help determine the precise conditions under which quadratic convergence occurs. This is perhaps best understood and analyzed in the case for the tanh-rule, see [7].

7 Conclusion

We have derived two estimates of the error in Euler-Maclaurin-based quadrature, one of which is particularly simple to implement, since it only involves summation of derivatives of the transformed function, at the same equi-spaced arguments as the quadrature calculation itself. It appears, from our results in several test problems, that the simplest instance of these estimates, namely $E_2(h, 1)$, is not only easy to compute, but in fact very accurate once h is even modestly small. What is more, the difference between these estimates and the actual error can be bounded with an easily computed formula, thus permitting "certificates" of quadrature values computed using Euler-Maclaurin-based schemes. Finally, the uses of *automatic differentiation methods* in this setting certainly merits further study, since it might in many cases considerably facilitate the various derivative computations needed in our estimates.

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h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$	$\lvert E(h)-E_2(h,2)\rvert$	$\lvert E(h)-E_2(h,3)\rvert$	$\lvert E(h)-E_2(h,4)\rvert$
1/1	5.34967×10^{-3}	9.81980×10^{-4}	4.77454×10^{-3}	1.87712×10^{-2}	6.48879×10^{-2}
1/2	-3.36641×10^{-4}	1.12000×10^{-7}	5.60084×10^{-7}	2.35316×10^{-6}	9.53208×10^{-6}
1/4	-3.73280×10^{-8}	1.67517×10^{-16}	8.37583×10^{-16}	3.51785×10^{-15}	1.42389×10^{-14}
1/8	5.58389×10^{-17}	2.29357×10^{-32}	1.14679×10^{-31}	4.81651×10^{-31}	1.94954×10^{-30}
1/16	-7.64525×10^{-33}	2.07256×10^{-64}	1.03628×10^{-63}	4.35237×10^{-63}	1.76167×10^{-62}
1/32	-6.90852×10^{-65}	7.23441×10^{-129}	3.61721×10^{-128}	1.51923×10^{-127}	6.14925×10^{-127}
1/64	$-2.41147 \times 10^{-129}$	9.08805×10^{-259}	4.54403×10^{-258}	1.90849×10^{-257}	7.72485×10^{-257}

Table 2: Results for $F_1(t) = 1/(1+t^2+t^4+t^6)$ on $[-1,1]$.

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$	$\lvert E(h)-E_2(h,2)\rvert$	$\lvert E(h)-E_2(h,3)\rvert$	$\lvert E(h)-E_2(h,4)\rvert$
1/1	2.92136×10^{-2}	4.12347×10^{-5}	2.06449×10^{-4}	8.69796×10^{-4}	3.54584×10^{-3}
1/2	1.37266×10^{-5}	3.40342×10^{-11}	1.70174×10^{-10}	7.14758×10^{-10}	2.89332×10^{-9}
1/4	1.13445×10^{-11}	1.60476×10^{-21}	8.02380×10^{-21}	3.36999×10^{-20}	1.36405×10^{-19}
1/8	5.34920×10^{-22}	1.06920×10^{-41}	5.34599×10^{-41}	2.24532×10^{-40}	9.08818×10^{-40}
1/16	3.56399×10^{-42}	1.36460×10^{-81}	6.82298×10^{-81}	2.86565×10^{-80}	1.15991×10^{-79}
1/32	4.54865×10^{-82}	6.34476×10^{-161}	3.17238×10^{-160}	1.33240×10^{-159}	5.39305×10^{-159}
1/64	2.11492×10^{-161}	3.89818×10^{-319}	1.94909×10^{-318}	8.18618×10^{-318}	3.31345×10^{-317}

Table 3: Results for $F_2(t) = (1-t^4)^{1/2}$ on $[-1,1]$.

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$	$\lvert E(h)-E_2(h,2)\rvert$	$\lvert E(h)-E_2(h,3)\rvert$	$\lvert E(h)-E_2(h,4)\rvert$
1/1	-9.38039×10^{-5}	2.00740×10^{-7}	1.00302×10^{-6}	4.20595×10^{-6}	1.69621×10^{-5}
1/2	6.69591×10^{-8}	1.17622×10^{-15}	5.88109×10^{-15}	2.47006×10^{-14}	9.99785×10^{-14}
1/4	-3.92072×10^{-16}	2.48852×10^{-32}	1.24426×10^{-31}	5.22589×10^{-31}	2.11524×10^{-30}
1/8	-8.29506×10^{-33}	2.17847×10^{-66}	1.08924×10^{-65}	4.57479×10^{-65}	1.85170×10^{-64}
1/16	-7.26158×10^{-67}	4.51319×10^{-135}	2.25659×10^{-134}	9.47769×10^{-134}	3.83621×10^{-133}
1/32	$-1.50440 \times 10^{-135}$	3.19951×10^{-272}	1.59976×10^{-271}	6.71897×10^{-271}	2.71958×10^{-270}
1/64	1.06650×10^{-272}	4.25792×10^{-546}	2.12896×10^{-545}	8.94163×10^{-545}	3.61923×10^{-544}

Table 4: Results for $F_3(t) = (1-t^2)^{-1/2}$ on $[-1,1]$.

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$
1/1	-6.45859×10^{-1}	3.54091×10^{0}
1/2	2.54145×10^{-2}	7.23759×10^{-1}
1/4	-1.69389×10^{-2}	1.00104×10^{-1}
1/8	-8.84080×10^{-3}	1.37392×10^{-2}
1/16	1.08078×10^{-3}	8.85166×10^{-4}
1/32	-2.39628×10^{-4}	8.44565×10^{-5}
1/64	-4.87134×10^{-5}	3.42934×10^{-5}

Table 5: Results for $F_4(t) = (1+t)^2 \sin(2\pi/(1+t))$ on $[-1,1]$.

h	$E(h)$	$\frac{\log \lvert E(h) \rvert}{\log \lvert E(2h) \rvert}$
$1/2$	1.49277×10^{-2}	
$1/4$	-4.28430×10^{-5}	2.39217
$1/8$	2.78529×10^{-10}	2.18747
$1/16$	3.18995×10^{-19}	1.93574
$1/32$	-1.88766×10^{-38}	2.03956
$1/64$	7.78764×10^{-77}	2.01751
$1/128$	1.33566×10^{-152}	1.99549
$1/256$	$-2.20499 \times 10^{-305}$	2.00598
$1/512$	8.84172×10^{-610}	1.99915
$1/1024$	$-7.31953 \times 10^{-1220}$	2.00169
$1/2048$	$2.25521 \times 10^{-2438}$	1.99949
$1/4096$	$-9.51498 \times 10^{-4877}$	2.00030

Table 6: Errors and log ratios using tanh-sinh quadrature for $\bar{H}(x) = (2\cos(\pi t) + 1)/(4\cos(\pi t) + 5)$ on $[-1, 1]$.