Towards a general error theory of the trapezoidal rule

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Dedicated to the 60th birthday of Gradimir V. Milovanović

Abstract The trapezoidal rule is the method of choice for numerical quadrature of analytic functions over the real line $\mathbb{R}$. Other intervals and slowly decaying integrands may elegantly be handled by means of simple analytic transformations of the integration variable. In the case of an integrand analytic in an open strip containing $\mathbb{R}$ the discretization error is exponentially small in the reciprocal step size. If the integrand has singularities arbitrarily close to $\mathbb{R}$, the discretization error is larger and its theory is more complicated. We present examples illustrating possible error laws of the trapezoidal rule.

1 Introduction

The (composite) trapezoidal rule, being the simplest and probably oldest algorithm for numerical quadrature, is often dismissed as insufficient for the purpose of high-precision quadrature, mainly due to its low order of precision for integrating generic integrands over a finite interval. However, for integrals over the real line $\mathbb{R}$ of functions analytic in an open strip containing $\mathbb{R}$ the discretization error of the trapezoidal rule has been proven to be exponentially small in the reciprocal step size. Hence in some cases the trapezoidal rule is among the most powerful algorithms for numerical quadrature of analytic functions.

By means of appropriate analytic transformations of the integration variable general intervals may be mapped to the real line, and the decay rate of the integrand may be enhanced, which is desirable in order to reduce the number of terms in infinite trapezoidal sums. Since such transformations may generate new singularities in the

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complex plane, no strip of analyticity may exist for the transformed integrand. To the knowledge of this author, no general theory of the discretization error of the trapezoidal rule in the absence of a strip of analyticity exists.

The trapezoidal rule in connection with quadrature of analytic functions has already been studied 1949 by Goodwin [7], 1969 by Schwartz [12] and later by Stenger [14]. The idea of using transformations of the integration variable has been mentioned in [12] as well as 1973 by Takahasy and Mori [16]; see also [13], Chapter 8 for a summary. The entire topic is comprehensively treated in the textbooks [4] and [15].

Here we will first summarize the well-known error theory of the classical trapezoidal rule. We then consider the particular cases with an exponentially small discretization error, mainly using integrals over the real line $\mathbb{R}$. Finally, we will present examples of integrals with singularities arbitrarily cose to $\mathbb{R}$, where the trapezoidal rule still yields powerful high-precision integrators of somewhat slower convergence, still with an exponentially small discretization error.

2 The Classical Trapezoidal Rule

In its classical form the (composite) trapezoidal rule is stated as an algorithm for numerically approximating the integral I of the integrable function f over the interval $a \le x \le b$,

$$I := \int_a^b f(x)\,dx, \tag{1}$$

using the $n+1 \ge 2$ equally spaced points

$$x_j := a + jh, \quad j = 0,\ldots,n, \quad h := \frac{b-a}{n}, \tag{2}$$

where h is the step size. The trapezoidal sum $T(h)$ is then defined as

$$T(h) := h \sum_{j=0}^n w_j f(x_j), \tag{3}$$

where the weights w_j are $w_0 = w_n = \frac{1}{2}$, $w_1 = w_2 = \cdots = w_{n-1} = 1$.

If f has at least $2N - 1 > 0$ continuous derivatives, the *discretization error* of a trapezoidal sum is given by the Euler-Maclaurin summation formula (for a good account see, e.g., [8]) as

$$\begin{aligned} T(h) - I = {} & \frac{h^2}{12}\Big(f'(b) - f'(a)\Big) - \frac{h^4}{720}\Big(f'''(b) - f'''(a)\Big) + \ldots \\ & + \frac{h^{2N}B_{2N}}{(2N)!}\big(f^{(2N-1)}(b) - f^{(2N-1)}(a)\big) + R_{2N}, \end{aligned} \tag{4}$$

where B_{2N} is the Bernoulli number of the even order $2N$,

$$B_0 = 1, \ B_2 = \frac{1}{6}, \ B_4 = -\frac{1}{30}, \ B_6 = \frac{1}{42}, \ B_8 = -\frac{1}{30}, \ B_{10} = \frac{5}{66}, \ \dots \ ,$$

and R_{2N} is the remainder term. R_{2N} can be specified [8], but this is rather involved. Since the above series is usually divergent for any fixed step $h > 0$, it must be truncated at a finite value of N.

In general, the trapezoidal rule converges very slowly with respect to step refinement. Convergence is of *second* order: Halving of the step (i.e. doubling the computational effort) reduces the discretization error by a factor of 4, i.e. merely yields 0.6 additional digits of accuracy. This does not allow to obtain more than a few digits of accuracy.

In the following we restrict ourselves to integrands f *analytic* in the *open* interval of integration, i.e. integrable boundary singularities are permitted, and x will be understood as a *complex* variable. Of particular interest are the cases with the property that the terms of the series (4) vanish up to arbitrary values of N. Then the discretization error is given by the remainder R_{2N} as $N \to \infty$. We distinguish three cases:

1. f is periodic with no singularities on the real line $\mathbb{R}$; the interval $[a,b]$ is a full period (or an integer number of periods).
2. f is integrable over the real line $\mathbb{R}$, and I is its integral over $\mathbb{R}$, i.e. $a = -\infty$, $b = \infty$.
3. f is a flat function at both boundaries, i.e. all derivatives of f at $x = a$ and $x = b$ vanish.

In all three cases convergence with respect to step refinement is faster than any finite order, referred to as *exponential convergence*. Case 3 corresponds to using the *IMT rule* proposed in 1969 by Iri, Moriguti and Takasawa (see, e.g. [10]). Case 2 may be considered as a particular instance of Case 3; however, integration over the entire real line is more fundamental and often leads to more efficient algorithms. We will mainly concentrate on integrals over $\mathbb{R}$, but we begin with a short discussion of Case 1.

3 The Periodic Case

With no loss of generality we assume $a = 0$, $b = 2\pi$. Let f be 2π-periodic and analytic on the entire real axis, and consider the integral

$$I := \int_0^{2\pi} f(x)\,dx. \tag{5}$$

With $n \geq 1$ subintervals of equal length $h = \frac{2\pi}{n}$ the trapezoidal sum (3) becomes

$$T(h) = h \sum_{l=0}^{n-1} f(lh). \tag{6}$$

The Fourier series of f (in a somewhat unconventional notation),

$$f(x) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} c_k e^{ikx} \quad \text{with} \quad c_k = \int_0^{2\pi} f(x) e^{-ikx} dx, \tag{7}$$

implies $I = c_0$. Hence the trapezoidal sum (6) becomes

$$T(h) = \frac{1}{n} \sum_{k=-\infty}^{\infty} c_k \sum_{l=0}^{n-1} \exp(i\frac{2\pi}{n} kl) = \sum_{j=-\infty}^{\infty} c_{jn}, \tag{8}$$

and we obtain the discretization error $E_n := T(h) - I$ with $n = 2\pi/h$ as

$$\boxed{E_n = c_n + c_{-n} + c_{2n} + c_{-2n} + \dots} \tag{9}$$

Therefore the discretization error of the trapezoidal rule for small steps is governed by the deacy rate of the Fourier coefficients c_n of the integrand for large absolute values of the index n.

A more informative statement may be formulated if f is analytic in the symmetric strip $|\text{Im}\, x| < \gamma$, $\gamma > 0$. Then the theory of Fourier series [11], [4] states

$$c_n = O\!\left(e^{-(\gamma-\varepsilon)|n|}\right) \quad \text{for any} \quad \varepsilon \in (0, \gamma) \quad \text{as} \quad n \to \pm\infty. \tag{10}$$

Combining this with the error formula (9) yields the following result:

Theorem 1. *Let f be a 2π-periodic function, analytic in the strip $|\text{Im}\, x| < \gamma$, $\gamma > 0$, and let I be the integral of f over a full period. Then the discretization error $E_n := T(h) - I$ of the trapezoidal sum $T(h)$, with $n \geq 1$ subintervals of equal length $h = 2\pi/n$, decays as $O\!\left(e^{-(\gamma-\varepsilon)|n|}\right)$ as $n \to \pm\infty$ for any $\varepsilon \in (0, \gamma)$.*

4 Integrals over the Real Line

We now consider Case 2 of Section 2, i.e. Equ. (1) is specialized to

$$I := \int_{-\infty}^{\infty} f(x)\, dx, \tag{11}$$

where f is analytic on $\mathbb{R}$ and integrable over $\mathbb{R}$. By slightly generalizing the definition (3) we will approximate I by the *shifted* trapezoidal sum with step h and offset s,

$$T(h,s) = h \sum_{j=-\infty}^{\infty} f(s + jh), \tag{12}$$

where the doubly infinite sum converges as a consequence of the integrability of f. As a function of s, $T(h,s)$ is periodic with period h, $T(h,s) = T(h,s+h)$, and the relation

$$T(\frac{h}{2},s) = \frac{1}{2}\left(T(h,s) + T(h,s+\frac{h}{2})\right) \tag{13}$$

may be used for an efficient transition from step h to step $h/2$.

Aside from the approximation of I, the evaluation of the infinite sum (12) may be a problem in itself. Here we will not discuss this aspect; instead, we assume a sufficiently fast decay of $|f(x)|$ as $x \to \pm\infty$, such that simple truncation rules for the infinite sum (12) may be used. In the next section we will motivate this approach by discussing transformations of the integration variable in order to obtain quickly decaying integrands.

As in the periodic case of Section 3, the discretization error may be obtained by Fourier theory. The basic tool is the Poisson summation formula (see, e.g., [9]),

$$T(h,s) = PV \sum_{k=-\infty}^{\infty} \hat{f}(k\,r)\,e^{iskr} \qquad \text{with} \qquad r := \frac{2\pi}{h}, \tag{14}$$

which expresses the shifted trapezoidal sum (12) of f with step h again as a (weighted) trapezoidal sum, but of the Fourier transform $\hat{f}$, and with step $r := 2\pi/h$. Here PV stands for the Cauchy principal value of the sum, i.e. the sum over all integers k must be taken as the limit of the symmetric sum from $-K$ to K as $K \to \infty$. The Fourier transform $\hat{f}$ of f is defined as

$$\hat{f}(\omega) := \int_{-\infty}^{\infty} e^{-i\omega x}\,f(x)\,dx, \quad \omega \in \mathbb{R}, \tag{15}$$

which immediately yields $I = \hat{f}(0)$.

In the following we restrict ourselves to the particular case of vanishing offset, $s = 0$, using the notation $T(h) := T(h,0)$. In view of the definition $r := 2\pi/h$ in Equ. (14) we introduce the discretization errror $E(r)$ as a function of r,

$$E(r) := T(h) - I, \quad h := \frac{2\pi}{r}. \tag{16}$$

Equ. (14) now yields the *error formula*

$$\boxed{E(r) = \hat{f}(r) + \hat{f}(-r) + \hat{f}(2r) + \hat{f}(-2r) + \dots} \tag{17}$$

Therefore, in complete analogy with Equ. (9), with r taking the role of the index n, the discretization error of the trapezoidal rule for small steps h is governed by the deacy rate of the Fourier transform $\hat{f}$ of the integrand for large values of $\omega = \pm r := \pm 2\pi/h$.

A more informative statement may be formulated if f is analytic in the symmetric strip $|\text{Im}\,x| < \gamma$, $\gamma > 0$ and integrable along any path $\text{Im}\,x = \gamma_0 = \text{const}$ with $|\gamma_0| < \gamma$. Then we have

$$\hat{f}(\omega) = O\!\left(e^{-(\gamma-\varepsilon)|\omega|}\right) \quad \text{for any} \quad \varepsilon \in (0,\, \gamma) \quad \text{as} \quad \omega \to \pm\infty \qquad (18)$$

([3] Chapter 3, [11] Thm. IX.14, or [4]). Combining (17), (18) yields the following theorem:

Theorem 2. *Let f be analytic in the strip $\left|\operatorname{Im} x\right| < \gamma$, $\gamma > 0$ and integrable along any path $\operatorname{Im} x = \gamma_0 = \mathrm{const}$ with $|\gamma_0| < \gamma$, and let I be the integral of f over $\mathbb{R}$. Then the discretization error $E_n := T(h) - I$ of the trapezoidal sum $T(h)$ with step $h = 2\pi/r$ and decays as $O\!\left(e^{-(\gamma-\varepsilon)|r|}\right)$ as $r \to \pm\infty$ for any $\varepsilon \in (0,\, \gamma)$.*

5 Transforming the Integration Variable

The trapezoidal rule for integrals over $\mathbb{R}$ is particularly attractive for quickly decaying integrands (at least exponential decay). Then the truncation of the infinite trapezoidal sums can be easily handled. A simple truncation rule for an infinite sum is *truncation if the contribution of the current term is below a given tolerance $\varepsilon > 0$.* If necessary, this simple rule can be made more robust by truncating only if two (or three) consecutive terms do not contribute. Accumulation of doubly infinite sums has to be done upwards and downwards from an interior point.

   To validate such a truncation procedure the tail of the truncated sum needs to be estimated. Ideally, the contribution of the truncated tail should be $< \varepsilon$. We will use the the function

$$f(x) := \exp(-e^{\alpha x}), \quad \alpha > 0 \qquad (19)$$

as a simple model of a doubly exponentially decaying integrand as $x \to +\infty$. The tail of the sum, truncated at $x = X > 0$, will be modeled by the integral

$$R_X := \int_X^\infty f(x)\, dx.$$

For the integrand (19) we obtain

$$R_X = \frac{1}{\alpha}\, \exp(-e^{\alpha X})\, \left(e^{-\alpha X} - e^{-2\alpha X} + 2!\, e^{-3\alpha X} + \dots\right).$$

The suggested truncation limit X, given by $f(X) = \varepsilon$, is found to be

$$X = \frac{1}{\alpha}\, \log\log\frac{1}{\varepsilon}\,;$$

therefore

$$R_X = -\frac{\varepsilon}{\alpha}\left(\frac{1}{\log \varepsilon} + O((\log \varepsilon)^{-2})\right).$$

Truncation is safe even for $\alpha \ll 1$, since $|R_X| < \varepsilon$ if ε is sufficiently small.

Our strategy is to use the simple tool of transformations of the integration variable in order to transform a given integral into one over $\mathbb{R}$ with a quickly decaying integrand. Beginning with the integral I of Equ. (1), we use an appropriate transformation

$$x = \phi(t), \quad t \in \mathbb{R}, \tag{20}$$

where ϕ is a monotonically increasing, differentiable function $\phi : t \in \mathbb{R} \mapsto x = \phi(t) \in (a,b)$. The result is

$$I = \int_{-\infty}^{\infty} F(t)\,dt \quad \text{with} \quad F(t) := f\big(\phi(t)\big)\,\phi'(t). \tag{21}$$

There is a wide range for the choice of ϕ. Since we are working with analytic integrands we only consider analytic transformation functions. In view of numerical applications we will choose ϕ as a combination of elementary functions, for which reliable implementations in arbitrary precision are readily available.

In the following table we list a few standard intervals $[a,b]$ for the integral (1), together with suggested elementary transformations $x = \phi(t)$. Possibly, a composition of several of the suggested mappings may have to be used in order to achieve doubly exponential decay of the transformed integrand $F(t)$ as $t \to \pm\infty$. In all cases (including the cases with finite boundaries) integrable boundary singularities are allowed. However, in the case of finite intervals care must be taken to accurately transmit the distances to both interval boundaries.

Interval: $x \in (a,\ b)$	Transformation: $x = \phi(t) =$
1. Finite interval $(-1,1)$:	$\tanh(t/2)$
2. Finite interval $(0,1)$:	$1/\big(1 + \exp(-t)\big)$
3. Semi-infinite interval $(0,\infty)$:	$\exp(t)$
4. Real line $\mathbb{R}$, accelerate decay as $x \to \pm\infty$	$\sinh(t)$
5. Real line $\mathbb{R}$, accelerate decay as $x \to +\infty$	$t + \exp(t)$
6. Real line $\mathbb{R}$, accelerate decay as $x \to -\infty$	$t - \exp(-t)$

6 Error Theory of Integrals over $\mathbb{R}$

In the remaining sections we will go back to the problem of Section 4, the integral I over $\mathbb{R}$ of (11), to be approximated by the infinite trapezoidal sum of Equ. (12), $T(h) = T(h,0)$ with step h. In the case of f being analytic in a symmetric strip of half-width $\gamma > 0$ containing $\mathbb{R}$ the discretization error of $T(h)$ is exponentially small in h according to Theorem 2, more precisely

$$E(r) = O\big(e^{-(\gamma-\varepsilon)|r|}\big) \quad \text{as} \quad r := \pm 2\pi/h \to \pm\infty \quad \forall\ \varepsilon \in (0,\ \gamma). \tag{22}$$

This also applies to integrals one would hardly attempt to directly approximate by the trapezoidal rule, e.g. $I = \int_{-\infty}^{\infty} dx/(1+x^2) = \pi$. In such cases it is advisable to

enhance the decay of the integrand according to Section 5 before invoking the trapezoidal rule. However, transformations enhancing the decay of the integrand may bear the danger of generating new singularities in the complex plane (possibly closing in on the real line), such that Theorem 2 is no longer applicable. We will consider this situation in more detail in Section 7.

The essential ingredient for an error theory of the infinite trapezoidal sum is the Fourier transform $\hat{f}(\omega)$ of the integrand, defined in Equ. (15); then the discretization error is given by the error formula (17). We will now develop an error formula for transformed integrals. Consider the integral I over $\mathbb{R}$ of Equ. (11), and assume $\phi : t \in \mathbb{R} \mapsto x = \phi(t) \in \mathbb{R}$ to be used in order to modify the decay rate of the integrand; the transformed integral is given by Equ. (21). The Fourier transform $\hat{F}(\omega)$ of $F(t)$ becomes

$$\hat{F}(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} f(\phi(t)) \phi'(t) \, dt. \tag{23}$$

Going back to the original variable x by using the *inverse* transformation $\phi^{[-1]} : x \in \mathbb{R} \mapsto t = \phi^{[-1]}(x) \in \mathbb{R}$ and the relation $\phi'(t) \, dt = dx$ yields

$$\hat{F}(\omega) = \int_{-\infty}^{\infty} e^{-i\omega \phi^{[-1]}(x)} f(x) \, dx, \tag{24}$$

a *modified "Fourier" transform* of f, where the factor x in the exponent of Equ. (15) is replaced by $\phi^{[-1]}(x)$. Combining this with the error formula (17) yields the following result:

Theorem 3. *Let $\tilde{T}(h)$ be the infinite trapezoidal sum with step h, obtained from the integral $I = \int_{-\infty}^{\infty} f(x) \, dx$ after having transformed the integration variable by means of the isomorphism $\phi : t \in \mathbb{R} \mapsto x = \phi(t) \in \mathbb{R}$,*

$$\tilde{T}(h) = h \sum_{k=-\infty}^{\infty} f(\phi(kh)) \phi'(kh).$$

Then the discretization error $\tilde{E}(r) := \tilde{T}(h) - I$ of $\tilde{T}(h)$ is given by

$$\tilde{E}(r) = \sum_{k \neq 0} \hat{F}(kr), \quad r = \frac{2\pi}{h},$$

where $\hat{F}(\omega)$ is given by Equ. (24).

7 Asymptotics

According to the error formula (17) the discretization error of the infinite trapezoidal rule for small steps h is governed by the Fourier transform $\hat{f}(r)$ of the integrand at large arguments $r = \pm 2\pi/h$. Therefore, an error theory of the trapezoidal rule

amounts to an asymptotic theory of the Fourier transform of the integrand. Such a theory is complicated and has not been fully developed so far.

In the simple case of a strip of analyticity (of half-width γ) with the symmetry axis $\mathbb{R}$, Theorem 2 establishes the discretization error to be of order $O\big(\exp((\varepsilon - \gamma)r)\big)$. However, if a transformation $x = \phi(t)$ is necessary in order to achieve a sufficient decay rate of the integrand, the strip of analyticity may be lost (i.e. the sigularities may fill the area outside a "funnel" closing in on the real axis, see Figure 1). Then Theorem 2 is no longer applicable, and an asymptotic theory of the modified Fourier transform (24) is needed. In several examples conjectured decay rates of order $O\big(\exp(-\gamma\omega/\log(c\,\omega))\big)$ or $O\big(\exp(-\gamma\sqrt{\omega})\big)$ with $\gamma > 0$, $c > 0$ were observed.

7.1 An Introductory Example

We begin with the discussion of the explicit example mentioned in connection with Equ. (22), subjected to repeated sinh transformations of the integration variable. Adapting the notation by using $t_0 := x$, $I_0 := I$, consider

$$I_k = \int_{-\infty}^{\infty} f_k(t_k)\, dt_k = \pi, \; k = 0,1,2,3 \quad \text{with} \quad f_0(t) := \frac{1}{1+t^2}. \tag{25}$$

and the transformations

$$t_k = \sinh(t_{k+1}), \quad f_{k+1}(t) = f_k\big(\sinh(t)\big)\cosh(t), \quad k = 0,1,2. \tag{26}$$

Hence the integrands

$$f_1(t) = \frac{1}{\cosh(t)}, \; f_2(t) = \frac{\cosh(t)}{\cosh\big(\sinh(t)\big)}, \; f_3(t) = \frac{\cosh\big(\sinh(t)\big)}{\cosh\big(\sinh(\sinh(t))\big)}$$

show single, double, or triple exponential decay. The singularities (poles) t_0, t_1, t_2 of f_0, f_1, f_2, respectively, are given by

$$t_0 = \pm i$$
$$t_1 = iu\frac{\pi}{2}, \quad u \text{ odd}$$
$$t_2 = \text{sign}(u)\,\text{Acosh}\big(|u|\frac{\pi}{2}\big) + iv\frac{\pi}{2}, \quad u,v \text{ odd}.$$

The poles t_2 of f_2 still leave a strip of analyticity $|\text{Im}\,t| < \pi/2$, whereas the poles of f_3 close in on the real axis as $t \to \pm\infty$, see Figure 1.

In the cases $k = 0$ and $k = 1$ the Fourier transforms $\hat{f}_k(\omega)$ and the discretization errors $E_k(r)$, see (15, 17), may be expressed explicitly as
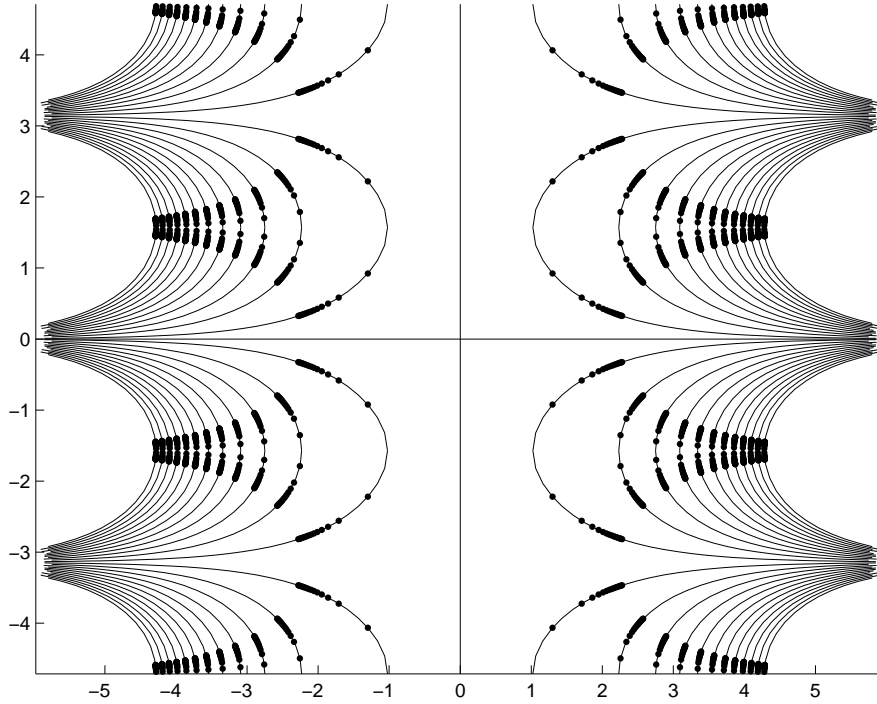
Fig. 1 Singularities of the integrand f_3 of $\int_{-\infty}^{\infty} dx/(1+x^2)$ after 3 sinh transformations. The dots on the curves, to be continued in increasing density, mark singularities. The arc-shaped areas to the left and to the right are densely filled with singularities not marked in the figure.

$$\hat{f}_0(\omega) = \pi \, e^{-|\omega|}\,, \qquad E_0(r) = \frac{2\pi}{e^r - 1}\,, \quad r = 2\pi/h$$

$$\hat{f}_1(\omega) = \frac{\pi}{\cosh(\omega \, \pi/2)}\,, \, E_1(r) = \sum_{j=1}^{\infty} \frac{2\pi}{\cosh(j \, r \, \pi/2)}\,.$$

In the case $k = 2$ Theorem 3 yields the Fourier transform $\hat{f}_2(\omega)$ as the integral

$$\hat{f}_2(\omega) = \int_{-\infty}^{\infty} \frac{e^{-i\,\omega\,\mathrm{Asinh}(t)}}{\cosh(t)} \, dt \tag{27}$$

which does not have an obvious closed form. However, according to Theorem 2 we have

$$\hat{f}_2(\omega) = O\big(e^{(\varepsilon-\pi/2)\,|\omega|}\big) \quad \text{as} \quad \omega \to \pm\infty \quad \text{for any} \quad \varepsilon \in (0, \frac{\pi}{2})\,. \tag{28}$$

Evaluation of the integral (27) by a branch cut integral along the imaginary axis or by the saddle point method ([5]; [6] for a worked example) corroborates (28). In Figure 2 the exponentially amplified discretization error, $\exp(r\,\pi/2)\,E_2(r)$, is plotted versus

$r \in (0.5, 70)$, where $E_2(r) \approx 2\,\mathrm{Re}\,\hat{f}_2(r)$ according to the error formula (17). The complicated irregular behavior seen in Figure 2 reflects the fact that infinitely many singularities or saddles contribute to the integral (27). The slow (sub-exponential) growth of the amplitude in Figure 2 exemplifies the necessity of the parameter ε in Theorem 2.
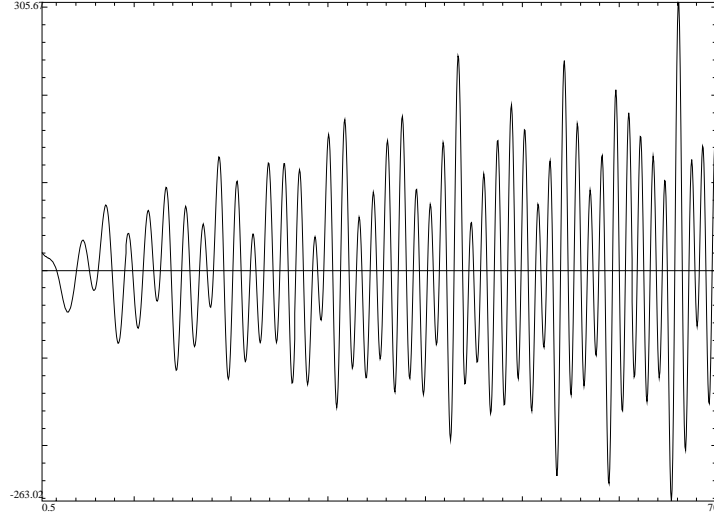

Fig. 2 Exponentially amplified discretization error, $e^{r\pi/2} E_2(r)$, versus $r = 2\pi/h$, $0.5 \le r \le 70$. High-precision computations done with the software package PARI [2].

The case $k = 3$ is even more complicated. In spite of a "mine field" of singularities, the real axis does not hit a single one, and the integrand on $\mathbb{R}$ becomes exceedingly small. Nevertheless, in the range of Figure 3 the discretization error seems to be exponentially small of the conjectured order

$$E_2(r) \approx O\big(e^{-\gamma r/\log(cr)}\big) \quad \text{with} \quad \gamma \doteq 2.285\,, \; c \doteq 6.05\,. \tag{29}$$

Figure 3 shows a plot of $\log_{10}(|E_2(r)|)$, i.e. a plot of minus the number of correct digits, versus $r = 2\pi/h$, together with the empirical envelope

$$\log_{10}\big(9\exp(-\gamma r/\log(cr))\big)$$

with γ, c from (29). In spite of the singularities, halving the step size almost doubles the number of correct digits, at least up to an accuracy of 45 digits.

As a summary, Figure 4 shows $\log_{10}\big(|E_k(r)|\big)$ for $k = 1, 2, 0, 3$ (bottom to top) versus $r = 2\pi/h$ in the interval $5.5 \le r \le 70$. The algorithm with $k = 0$ is impractical due to the slow decay of the integrand (very long trapezoidal sums). $k = 3$ works with short trapezoidal sums but, as a consequence of the small slope in Figure 4, requires a much smaller step size for reaching the same accuracy. The best perfor-
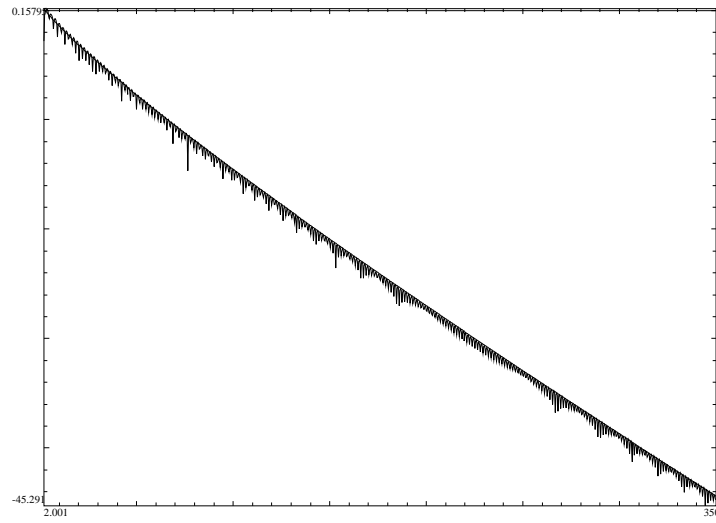
Fig. 3 The integral $\int_{-\infty}^{\infty} dx/(1+x^2)$ with 3 sinh transformations. Plot of $\log_{10}\left(|E_2(r)|\right) \in (-45.3, 0.2)$ versus $r \in (2, 350)$, including an empirical upper envelope.

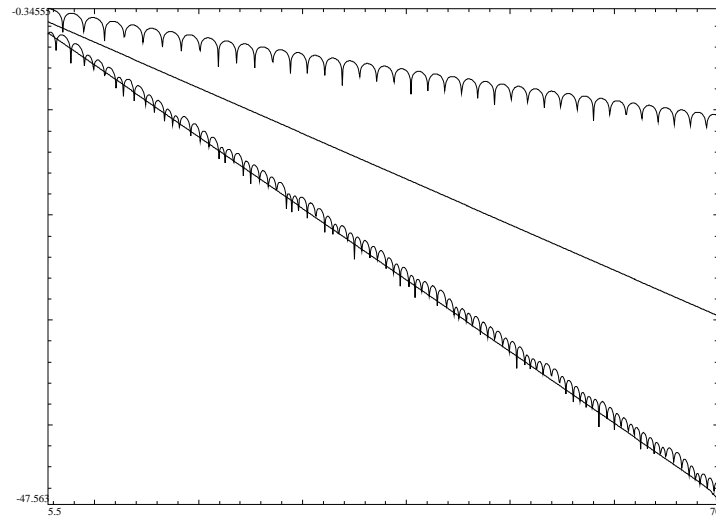mance results from $k = 2$, featuring an integrand of doubly exponential decay in a strip of analyticity.

Fig. 4 Plots of $\log_{10}\left(|E_k(r)|\right) \in (-47,\ 0)$ for $k = 1, 2, 0, 3$ (bottom to top) versus $r = 2\pi/h \in (5.5, 70)$.

7.2 A Difficult Integral

Slowly decaying analytic functions with many singularities may be difficult to integrate over $\mathbb{R}$ by the algorithms discussed here. Transformations to accelerate the decay of the integrand (Section 5) may breed more singularities (Figure 1) and slow down the decay rate of the discretization error with respect to step refinement. Consider, e.g., the integral

$$I(a) := \int_{-\infty}^{\infty} \frac{dx}{\cosh(x)\,\big(\cosh(a) + \cos(x)\big)}\,. \tag{30}$$

Explicit values may be obtained from calculus of residues using the poles $x_1 = iu\frac{\pi}{2}$, $x_2 = v\pi \pm ia$, u,v odd:

$$I(a) = 2\pi \left(\sum_{k=0}^{\infty} \frac{(-1)^k}{\cosh(a) + \cosh(k+\frac{1}{2})\pi} + \frac{2\cos(a)}{\sinh(a)} \sum_{u=1,3,\ldots} \frac{\cosh(u\pi)}{\cosh^2(u\pi) - \sin^2(a)} \right)$$

For $a = 1$ the quickly convergent series easily yields the 50D approximation

$$I(1) = 1.9473499863\,38691\,95445\,99206\,53366\,23422\,62265\,42793\,65329$$

to be used as a reference value.

For a numerical high-precision evaluation by the trapezoidal rule with step h an integrand of doubly exponential decay may be desirable; therefore we transform the integration variable by means of $x = \sinh(t)$.

The behaviour of the discretization error $E(r)$ of the transformed integral as function of $r := 2\pi/h$ turns out to be complicated. Here we formulate a conjecture concerning the decay rate of $E(r)$:

Conjecture.

$$E(r) = O\big((ar)^{1/4}\,e^{-2\sqrt{ar}}\big), \quad r := \frac{2\pi}{h}\,. \tag{31}$$

In the following we give a heuristic derivation of the above conjecture. In view of the error formula (17), $E(r) \sim \hat{F}(r) + \hat{F}(-r)$ and Theorem 3 it suffices to investigate the modified Fourier transform

$$\hat{F}(\omega) = \int_{-\infty}^{\infty} \frac{e^{-i\omega\,\mathrm{Asinh}(z)}}{\cosh(z)\,\big(\cosh(a) + \cos(z)\big)}\,dz \tag{32}$$

for large $|\omega|$. For this purpose we deform ("pull down") the path of integration $\mathbb{R}$ and consider the following contributions F_k, $k = 1,2,3,4$ to the integral $\hat{F}(\omega)$:

1. Lower semi-circle of radius R: $F_1 \to 0$ as $R \to \infty$
2. Branch cut along the imaginary axis, Im $z < -1$: $F_2 = O(e^{-|\omega|\pi/2})$, negligible as $\omega \to \pm\infty$
3. Poles on branch cut, $z_v := i\frac{\pi}{2}v$, $v < 0$, odd: $F_3 = O(e^{-|\omega|\pi/2})$, negligible as $\omega \to \pm\infty$

4. Poles $z_u := u\pi - ia$, u odd: the *dominant* contributions, F_4:

Summation over the poles z_u yields

$$F_4 = \frac{4\pi}{\sinh(a)} \sum_{u=1,3,\dots} \mathrm{Re}\ \frac{e^{-i\omega\,\mathrm{Asinh}(u\pi-ia)}}{\cosh(u\pi-ia)}. \tag{33}$$
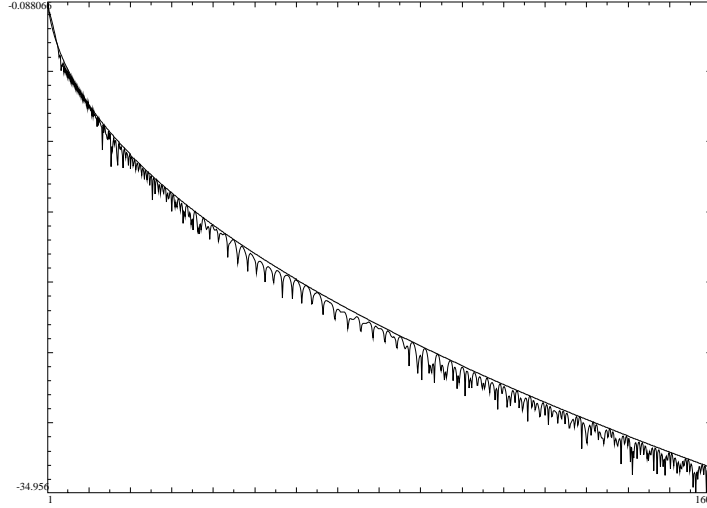

Fig. 5 Plot of $\log_{10}(\frac{1}{2}|E(r)|) \in (-35,\ 0)$ versus $r = 2\pi/h \in (1,\ 1600)$ for the inegral (30) with one sinh transformation, together with the conjectured upper bound from (36).

This is simplified by approximating the sum by the corresponding integral and replacing the terms of the sum by the expressions

$$2\,\mathrm{Re}\ \exp\left(-i\omega\left(\log(2u\pi) - \frac{ia}{u\pi}\right) + ia - u\pi\right),$$

which are asymptotic to the terms of the sum as $u \to \infty$. The result is

$$F_4 \approx \frac{4}{\sinh(a)} \int_0^\infty \exp\left(-\frac{a\omega}{v} - v\right)\ \cos(\omega\log(2v) - a)\ dv, \tag{34}$$

where $v = u\pi$. A crude upper bound for $|F_4|$ is therefore

$$|F_4| \mathrel{\dot{<}} \frac{4}{\sinh(a)} \int_0^\infty \exp\left(-\frac{a\omega}{v} - v\right)\ dv. \tag{35}$$

The substitution $v = \sqrt{a\omega}\,e^t$ and Equ. 9.6.24 of [1] results in the following closed form of the integral in (35) in terms of a *modified Bessel* function:

$$\int_0^\infty \exp(-\frac{a\,\omega}{v} - v)\, dv = 2\sqrt{a\,\omega}\, K_1(2\sqrt{a\,\omega}).$$

Asymptotics of K_1 ([1], Equ. 9.7.2) yields the approximate inequality

$$|\hat{F}(\omega)| \mathrel{\dot{<}} c\,(a\,\omega)^{1/4}\, e^{-2\sqrt{a\,\omega}}, \quad c = \frac{4\sqrt{\pi}}{\sinh(a)}. \tag{36}$$

Figures 5 and 6 show this bound in comparison with half the error of the trapezoidal sum with step $h = 2\pi/\omega$. The agreement is striking!
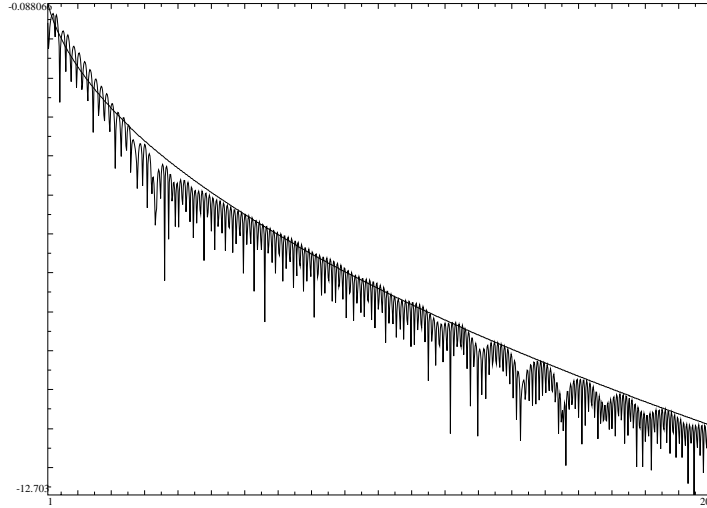

Fig. 6 Detail of Figure 5 in the range $r \in (1,\ 200)$ in higher resolution. As expected, Equ. (36) does not give a strict bound.

The error law (31) implies that doubling the accuracy requires quartering the step; this is still exponential convergence, but at a slower rate. For this reason the trapezoidal rule applied to the original integral (30) turns out to be more efficient, in spite of the longer trapezoidal sums. With the software package PARI [2] and a working precision of 57 digits (resulting in about 54 correct digits), the computation time for the direct approach is 45 % of the time taken for the transformed integral.

8 Conclusions

We have proposed to use the trapezoidal rule on the entire real line $\mathbb{R}$ as the standard algorithm for numerical quadrature of analytic functions. Finite and semi-infinite intervals as well as boundary singularities may be handled by using a new integration variable t, thus transforming the original variable x as $x = \phi(t)$, where in practice ϕ

may be chosen as an appropriate combination of elementary functions. Slow decay at infinity may be accelerated by the transformation $x = \sinh(t)$.

If the transformed integrand is analytic in a strip containing $\mathbb{R}$ the discretization error is known to be exponentially small in $r := 2\pi/h$, h being the step size. If the integrand has singularities arbitrarily close to $\mathbb{R}$, as it often happens in integrands transformed with sinh, the behaviour of the discretization error may be very complicated; no general theory is known. Decay rates $O\big(\exp(-\gamma r/\log(c\,r))\big)$ and $O\big(\exp(-\gamma\sqrt{r})\big)$ with $\gamma > 0$, $c > 0$ have been observed; in both cases the trapezoidal rule is still a powerful algorithm.

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