Towards a General Error Theory of the Trapezoidal Rule

Jörg Waldvogel, ETH Zürich

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1. Introduction

For numerically approximating the integral

$$I = \int_a^b f(x)\,dx$$

the classical trapezoidal rule uses the $n+1 \geq 2$ equally spaced points

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

The trapezoidal sum $T(h)$ is then defined as

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

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

General Error law

The discretization error of a trapezoidal sum follows from the Euler-Maclaurin summation formula,

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

where B_N is the Bernoulli number of the even order $N \geq 2$, and R_N is the remainder term, f having at least $N - 1$ continuous derivatives.

In general, the trapezoidal rule converges very slowly with respect to step refinement: 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.

2. Analytic integrands and exponential convergence

We restrict ourselves to integrands f analytic in the open interval of integration.

Of particular interest are three cases with the property that all terms of the Euler-Maclaurin series vanish, except for the remainder R_N:

1. f is periodic, $[a, b]$ a full period (or an integer number of periods)
2. f is a flat function at both boundaries, i.e. all derivatives of f at $x = a$ and $x = b$ vanish.
3. I is an integral over the real line $\mathbb{R}$, i.e. f is integrable over $\mathbb{R}$ and $a = -\infty,\ b = \infty$.

In all three cases convergence with respect to step refinement is faster than any finite order, referred to as exponential convergence.

Case 3: Integrals over the real line $\mathbb{R}$

Let f be such that its integral over $\mathbb{R}$ exists,

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

Trapezoidal sum, step h, offset s :

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

Periodicity:

$$T(h,s) = T(h, s+h)$$

Refinement:

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

Truncation of infinite trapezoidal sums

$$\tilde{T}(h, s) = h \sum_{j=n_0}^{n_1} f(s + jh).$$

Desirable truncation rule: Truncate if $|f(x)| < \varepsilon$, where $x := s + jh$, and $\varepsilon > 0$ is a given tolerance reflecting the working precision.

A (moderately) robust implementation:

- Choose an interior point x_0 and accumulate two separate sums upwards from $x_0 + h$ and downwards from x_0
- Truncate each sum if two (or three) consecutive terms do not contribute to the sum

The truncation error

Remainder for the truncation limit X:

$$R_X := \int_X^\infty f(x)\,dx, \quad \text{where} \quad f(X) = \varepsilon$$

(i) Algebraic decay:

$$f(x) = x^{-\alpha-1}, \quad (\alpha > 0), \qquad R_X = \frac{X^{-\alpha}}{\alpha} = \frac{\varepsilon^{\alpha/(1+\alpha)}}{\alpha}$$

No good! Remainder may be $>> \varepsilon$. E. g. $R_X = O(\sqrt{\varepsilon})$ for $\alpha = 1$.

(ii) Exponential decay:

$$f(x) = e^{-\alpha\, x}, \quad (\alpha > 0), \qquad R_X = \frac{1}{\alpha}\, e^{-\alpha\, X} = \frac{\varepsilon}{\alpha}$$

Better, but dangerous if $\alpha << 1$.

(iii) Doubly exponential decay:

$$\begin{aligned} f(x) &= \exp(-e^{\alpha x}), \quad (\alpha > 0), \\ R_X &= \frac{1}{\alpha} \exp(-e^{\alpha X}) \left(e^{-\alpha X} - e^{-2\alpha X} + 2!\, e^{-3\alpha X} + \dots\right) \end{aligned}$$

Truncation limit:

$$f(X) = \varepsilon \implies X = \frac{1}{\alpha} \log\log\frac{1}{\varepsilon} \, ,$$

therefore

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

Truncation is safe even for $\alpha << 1$ if ε is sufficiently small.

3. Simple error formulas

Let f be analytic in the symmetric strip $\left|\mathrm{Im}\ x\right| < \gamma,\ \gamma > 0$ containing $\mathbb{R}$.

Case 1 (of Slide 5) For simplicity: $a = 0,\ b = 2\pi$

$$I := \int_0^{2\pi} f(x)\,dx \qquad f:\ 2\pi - \text{periodic}$$

Fourier series:

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

We have $I = 2\pi\, c_0$. For the trapezoidal sum with $h := \frac{2\pi}{n}$ we obtain

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

Therefore

$$T(h) - I = 2\pi \left(c_n + c_{-n} + c_{2\,n} + c_{-2\,n} + \ldots \right).$$

Theorem. The error of the trapezoidal sum $T(h)$ with n equal subintervals for the integral I of an analytic 2π-periodic function f over a full period is asymptotically $(n \to \infty)$ given by $T(h) - I \sim 2\pi \left(c_n + c_{-n} \right)$, where c_n is the nth Fourier coefficient of f.

Remark. From the theory of Fourier series:

$$c_n = O\left(e^{-(\gamma-\varepsilon)\,|n|}\right) \quad \text{for any} \quad \varepsilon > 0.$$

Case 3 (of Slide 5) $a = -\infty,\ b = \infty$

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

Fourier Transform: $\hat{f}(\omega) := \int_{-\infty}^{\infty} e^{-i\,\omega\,x}\ f(x)\ dx\,, \quad I = \hat{f}(0)$

Trapezoidal sum with offset: $T(h,s) := h\ \sum_{j=-\infty}^{\infty} f(j\,h + s)$

Poisson summation formula: $T(h,s) = PV \sum_{k=-\infty}^{\infty} \hat{f}\left(k\,\frac{2\pi}{h}\right)\ e^{i\,s\,k\cdot 2\pi/h}$

For offset $s = 0$ we obtain the error formula

$$T(h,0) - I = \hat{f}\left(\frac{2\pi}{h}\right) + \hat{f}\left(-\frac{2\pi}{h}\right) + \hat{f}\left(\frac{4\pi}{h}\right) + \hat{f}\left(-\frac{4\pi}{h}\right) + \ldots$$

Theorem. The error of the infinite trapezoidal sum for a small step $h > 0$ is asymptotic to the sum of the Fourier transform values of the integrand at $\pm 2\pi/h$.

Particular cases

(i) Integrand analytic in a strip of the complex plane

Let $f(x)$ be analytic in $\left|\mathrm{Im}(x)\right| < \gamma,\ \gamma > 0$. Then

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

and the discretization error for $h \to 0$ is

$$T(h,0) - I = O(e^{-(\gamma-\varepsilon)\,\omega}) \quad \text{with} \quad \omega := 2\,\pi/h.$$

(ii) Proliferation of singularities due to sinh transformations

Convergence may be slower, such as (with some $\gamma > 0$)

$$T(h,0) - I = O(e^{-\gamma\,\omega/\log(\omega)}) \quad \text{or} \quad T(h,0) - I = O(e^{-\gamma\sqrt{\omega}}).$$

4. Transformations

Use an appropriate transformation $x = \phi(t),\ t \in \mathbb{R}$ in order to transform the integral under consideration,

$$I = \int_a^b f(x)\,dx\,,$$

to the integral of a quickly decaying analytic function over $\mathbb{R}$.

Desired properties of ϕ:

- analytic, monotonic
- quickly and accurately computable, e.g. a combination of elementary functions

Result:

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

Examples

Interval	Transformation
1. Finite interval, e.g. $(-1,1)$:	$x=\phi(t)=\tanh(t)$
2. Semi-infinite interval, $(0,\infty)$:	$x=\phi(t)=\exp(t)$
3. Real line $\mathbb{R}$, enhance the decay:	$x=\phi(t)=\sinh(t)$
4. Real line $\mathbb{R}$, enhance decay as $t\to+\infty$:	$x=\phi(t)=t+\exp(t)$
5. Real line $\mathbb{R}$, enhance decay as $t\to-\infty$:	$x=\phi(t)=t-\exp(-t)$

Remark. In the case of finite boundaries integrable boundary singularities are allowed.

Implementation

Goal: Avoid cancellation near the boundaries of finite intervals.

Example:

$$I = \int_0^b \frac{dx}{\sqrt{x\,(b-x)}}$$

Integrand:

$$f(x) = \frac{1}{\sqrt{x\,(1-x)}} = \frac{1}{\sqrt{x\;x_1}}, \quad x_1 = b - x$$

Transformation: The tanh transformation becomes

$$\begin{aligned} x &= \frac{b}{1+e^{-t}}, \quad x_1 = \frac{b}{1+e^{t}} \\ dx &= \frac{b\;e^{-t}}{(1+e^{-t})^2}\,dt \end{aligned}$$

Implementation of the transformed integrand:

Transmit both distances from the interval boundaries, although this seems to be (but isn't!) redundant.

With

$$f(x, x_1) := \frac{1}{\sqrt{x\ x_1}}\,, \quad x_1 = b - x$$

find

$$I := \int_0^b f(x, x_1)\ dx = \int_{-\infty}^{\infty} g(t)\ dt.$$

Algorithm for accurately evaluating $g(t),\ t \in \mathbb{R}$:

$$x = \frac{b}{1 + e^{-t}}; \quad x_1 = \frac{b}{1 + e^{t}}; \quad dx = x^2 \cdot e^{-t}/b; \quad g = f(x, x_1) \cdot dx$$

All computations are done with numerical values; no symbolic manipulations necessary!

Test integrals

$$L(x) := \log(\tfrac{1}{x})$$

$$I_1 = \int_0^1 dx, \qquad I_2 = \int_0^1 e^x \, dx,$$

$$I_3 = \int_0^1 x^{63} \, dx, \qquad I_4 = \int_0^1 \sin(8\pi \, x^2) \, dx,$$

$$I_5 = \int_0^1 \frac{1}{1+\exp(x)} \, dx, \qquad I_6 = \int_0^1 \frac{1}{x+0.5} \, dx,$$

$$I_7 = \int_0^1 \sqrt{12.25 - (5\,x-3)^2} \, dx, \qquad I_8 = \int_0^1 \frac{10}{1+(10\,x-4)^2} \, dx,$$

$$I_9 = \int_0^1 \frac{1}{\sqrt{x\,(1-x)}} \, dx, \qquad I_{10} = \int_0^1 \frac{\cos(2\pi x)}{\sqrt{1-x}} \, dx,$$

$$I_{11} = \int_0^1 x^{-3/4}\,(1-x)^{1/4}\,(3-2\,x)^{-1} \, dx, \qquad I_{12} = \int_0^1 x^{-3/4}\,L(x)^{-3/4} \, dx,$$

$$I_{13} = \int_0^1 x^{0.21} \sqrt{L(x)}\, dx, \qquad I_{14} = \int_0^1 L(x)^{\sqrt{L(x)}}\, dx,$$

$$I_{15} = \int_0^1 x^{0.6}\, L(x)^{-0.7} \cos(2\,L(x))\, dx, \qquad I_{16} = \int_0^\infty \frac{1}{x^2 + \exp(4\,x)}\, dx,$$

$$I_{17} = \int_0^\infty \frac{1}{1 + x^2 + \frac{x^4}{1+\exp(-x)}}\, dx, \qquad I_{18} = \int_0^\infty \frac{1}{x^{2/3} + x^{3/2}}\, dx,$$

$$I_{19} = \int_0^\infty e^{-\sqrt{x}}\, dx, \qquad I_{20} = \int_0^\infty \mathrm{Re}\, \frac{e^{-x}}{\log(1 + i\,x)}\, dx,$$

$$I_{21} = \int_{-\infty}^\infty \frac{1}{1 + x^2 + \frac{x^4}{1+\exp(-x)}}\, dx, \qquad I_{22} = \int_{-\infty}^\infty \frac{1}{x^2 + \exp(4\,x)}\, dx,$$

$$I_{23} = \int_{-\infty}^\infty (1 + x^2)^{-5/4}\, dx, \qquad I_{24} = \int_{-\infty}^\infty \exp(-\sqrt{1 + x^2})\, dx,$$

$$I_{25} = \int_{-\infty}^\infty \frac{1}{x^2 + \frac{1}{\cosh(x)}}\, dx\ .$$

Closed forms

$$\begin{array}{llllllllll}
I_1 & = & 1, & I_2 & = & e-1, & I_3 & = & \frac{1}{64}, \\
I_4 & = & \frac{S(4)}{4}, & I_5 & = & \frac{1}{2}-\log\cosh(\frac{1}{2}), & I_6 & = & \log 3, \\
I_8 & = & \pi-\arctan\frac{10}{23}, & I_9 & = & \pi, & I_{10} & = & C(2), \\
I_{11} & = & \pi\, 2^{1/2}\, 3^{-3/4}, & I_{12} & = & \sqrt{2}\;\Gamma(\frac{1}{4}), & I_{13} & = & \dfrac{\sqrt{\pi}}{2.662},
\end{array}$$

$$I_7 = \frac{1}{20}\,(\sqrt{132}+\sqrt{117})+\frac{49}{40}\,(\arcsin\frac{4}{7}+\arcsin\frac{6}{7}), \quad I_{15} = \Gamma(0.3)\,\mathsf{Re}\,(1.6+2\,i)^{-0.3},$$

$$I_{18} = 1.2\,\pi\sqrt{2-\frac{2}{\sqrt{5}}}, \quad I_{19} = 2, \quad I_{23} = 2\,\mathsf{agm}(1,\sqrt{2}), \quad I_{24} = 2\,K_1(1).$$

$S(z), C(z)$: Fresnel integrals; $K_1(z)$: Modified Bessel function;

agm: arithmetic-geometric mean

Remarks concerning the test integrals

- No closed forms could be found for the remaining integrals.
- Maple could not find the closed forms for I_{11}, I_{15}, I_{24}.
- Mathematica found I_{15}, did not find I_{24} either, and returned I_{11} erroneously, with a superfluous factor $-i$.
- The Inverse Symbolic Calculator (see URL below) correctly identified 8 among the 16 non-integer closed forms, based on 16-digit approximations alone.

  http://oldweb.cecm.sfu.ca/projects/ISC/ISCmain.html

- Except for I_{17}, I_{21}, I_{25}, the convergence rate is $O(\exp(-\gamma/h)),\ \gamma > 0$.

Case	Corr.digits per stage	# of function evaluations	Entire test suite
1	2,6,14,31,66	15,29,53, 97,183	in 67-digit
2	2,6,13,29,62,65	15,29,53, 97,183,349	working precision
3	0,1, 4,13,37,66	11,21,37, 66,121,227	1.6 MHz processor:
4	0,0, 1,10,33,66	13,25,46, 84,155,294	4.1 seconds,
5	2,6,14,31,67	15,29,53, 97,183	65 ... 66
6	2,5,12,24,50,65	15,29,53, 97,183,349	correct digits
7	2,5,11,20,40,65	15,29,53, 97,183,349	
8	1,0, 2, 4, 8,17,35,65	15,29,53, 97,181,347,674,1323	
9	4,7,15,32,66	15,31,59,109,205	
10	0,5,12,26,58,65	15,30,56,103,194,371	
11	2,6,12,25,50,65	16,31,59,110,209,402	
12	4,7,15,32,66	17,33,63,119,226	
13	3,6,14,31,65	13,27,50, 93,173	
14	2,5,11,26,56,65	15,30,55,101,190,363	
15	1,3, 7,15,30,59,65	15,30,56,103,194,371,721	
16	2,4,10,22,43,65	13,26,47, 86,160,304	
17	3,5, 9,14,23,38,65	14,29,54,100,187,357,694	slower convergence
18	3,7,16,33,66	17,34,65,122,233	
19	4,8,18,35,65	20,39,73,138,263	
20	3,6,12,23,45,65	15,29,53, 97,182,348	
21	1,2, 5, 8,15,28,51,65	14,29,54,100,187,358,695,1373	slower convergence
22	0,0, 2, 4, 8,18,36,65	14,27,50, 92,171,325,629,1242	
23	3,7,15,32,65	15,29,55,101,191	
24	3,7,16,32,66	15,31,59,109,205	
25	1,4, 7,12,20,35,58	15,31,59,109,205,393,765	slower convergence

Conjectured convergence rates of I_{17}, I_{21}, I_{25}

Let $\quad \omega := \dfrac{2\,\pi}{h} \quad$ where $\quad h > 0 \quad$ is the step size.

Observed error of the trapezoidal sum $T(h)$ in the range of Slide 22:

$$\boxed{T(h) - I = O(e^{-\gamma\,\omega/\log(c\,\omega)})}$$

where for

$$I = I_{17}: \quad \gamma \doteq 2.35, \quad c \doteq 1.0$$

$$I = I_{21}: \quad \gamma \doteq 2.21, \quad c \doteq 5.0$$

$$I = I_{25}: \quad \gamma \doteq 1.57, \quad c \doteq 0.28$$

5. Evaluating the Fourier transforms

Error formula for transformed integrals

From Slides 14 and 12 with transformation $x = \phi(t),\ t = \phi^{[-1]}(x)$:

$$I = \int_{-\infty}^{\infty} f_0(x)\,dx \ = \int_{-\infty}^{\infty} f_1(t)\,dt \quad \text{with} \quad f_1(t) := f_0\big(\phi(t)\big)\,\phi'(t)\,.$$

Error of the trapezoidal sums of f_1:

$$T_{f_1}(h) - I = \sum_{k\neq 0} \hat{f}_1\left(k\,\frac{2\pi}{h}\right)\,,$$

where

$$\hat{f}_1(\omega) = \int_{-\infty}^{\infty} f_0\big(\phi(t)\big)\,e^{-i\,\omega\,t}\,\phi'(t)\,dt = \int_{-\infty}^{\infty} f_0(x)\ e^{-i\,\omega\,\phi^{[-1]}(x)}\ dx\,.$$

The asinh function in the complex plane

The principal value, $\mathrm{Asinh}(z)$, is defined in the cut plane, cut along $\mathrm{Re}(z) = 0,\ |\mathrm{Im}(z)| > 1$. Values on the branch cut:

$$\lim_{\varepsilon \to \pm 0} \mathrm{Asinh}(\varepsilon + i\,y) = \begin{cases} i \arcsin(y), & |y| \le 1 \\ \mathrm{sign}(\varepsilon)\,\mathrm{Acosh}(|y|) + i\,\mathrm{sign}(y)\,\dfrac{\pi}{2}, & |y| \ge 1 \end{cases}$$

All values: $\mathrm{asinh}(z) = (-1)^k\,\mathrm{Asinh}(z) + i\,k\,\pi\,, \quad k \in \mathbb{Z}$

Series expansions: Use $\mathrm{Asinh}(-z) = -\mathrm{Asinh}(z)$ and

$$\mathrm{Asinh}(z) = \sum_{l=0}^{\infty} \binom{-1/2}{l} \frac{z^{2\,l+1}}{2\,l+1}\,, \quad |z| < 1$$

$$\mathrm{Asinh}(z) = \mathrm{Log}(2\,z) - \sum_{l=1}^{\infty} \binom{-1/2}{l} \frac{z^{-2\,l}}{2\,l}\,, \quad |z| > 1,\ \mathrm{Re}(z) > 0$$

Example

$$I = \int_{-\infty}^{\infty} \frac{dz}{1+z^2} = \int_{-\infty}^{\infty} \frac{dx}{\cosh(x)} = \int_{-\infty}^{\infty} \frac{\cosh(t)\ dt}{\cosh(\sinh(t))} = \pi$$

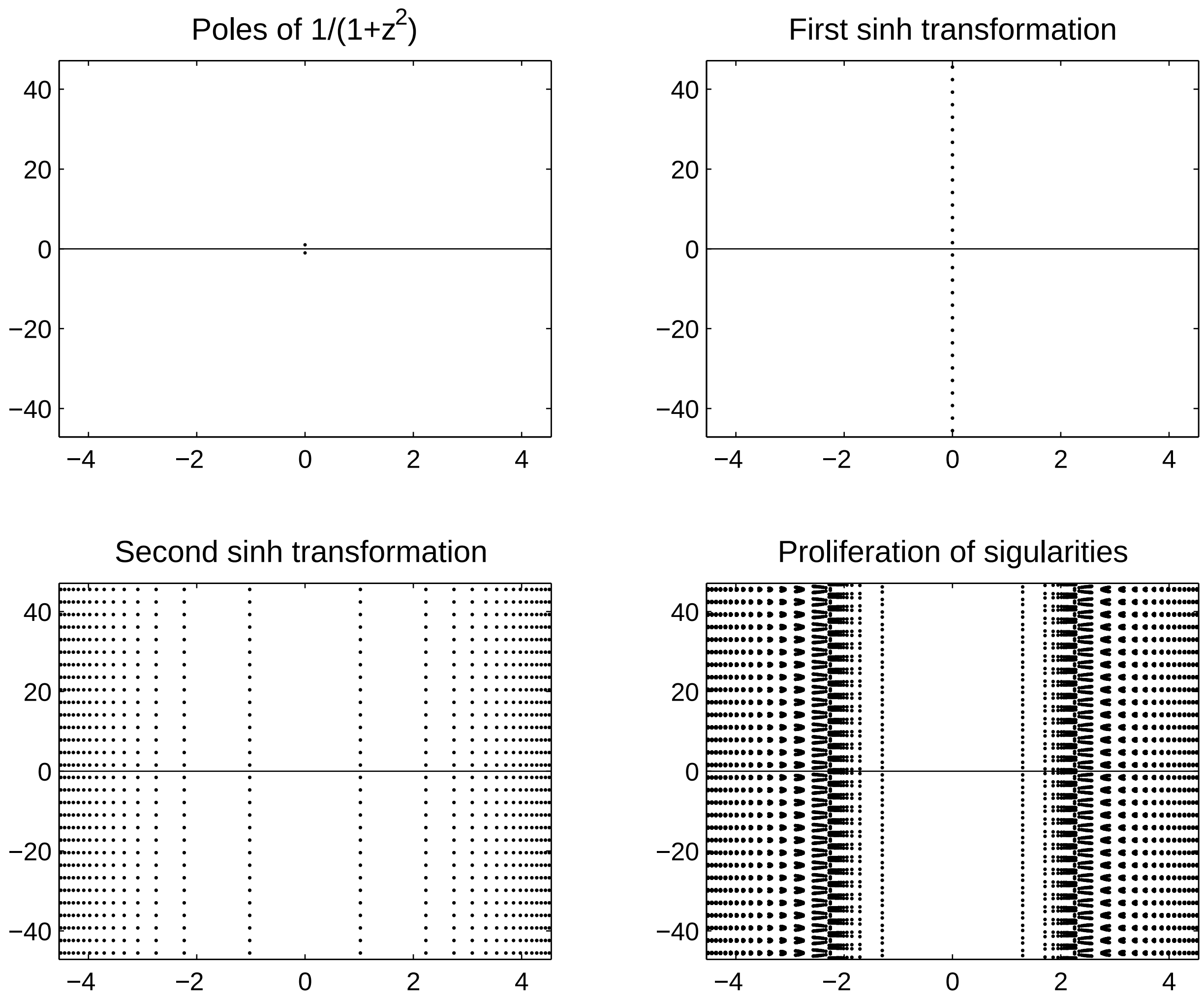
Integrands:

$$f_0(z) = \frac{1}{1+z^2}, \quad f_1(x) = \frac{1}{\cosh(x)}, \quad f_2(t) = \frac{\cosh(t)}{\cosh(\sinh(t))}$$

Transformations: $z = \sinh(x) \qquad x = \sinh(t)$

Singularities: $z = \pm i,\ \ x = i\,u\,\frac{\pi}{2},\ \ t = \pm \mathrm{Acosh}(|u\,\frac{\pi}{2}|) + i\,v\,\frac{\pi}{2},\ \ u, v$ odd

Breeding singularities by sinh transformations, $\int_{-\infty}^{\infty} \frac{dz}{1+z^2}$



Error formulas

Error: $$E_l(h) = T_l(h,0) - \pi = \sum_{k \neq 0} \hat{f}_l(k\,\omega),\ l = 0, 1, 2, \qquad \omega = \frac{2\pi}{h}$$

Fourier transforms:

$$\hat{f}_0(\omega) = \pi\ e^{-|\omega|}, \quad \hat{f}_1(\omega) = \frac{\pi}{\cosh(\omega\ \pi/2)},$$

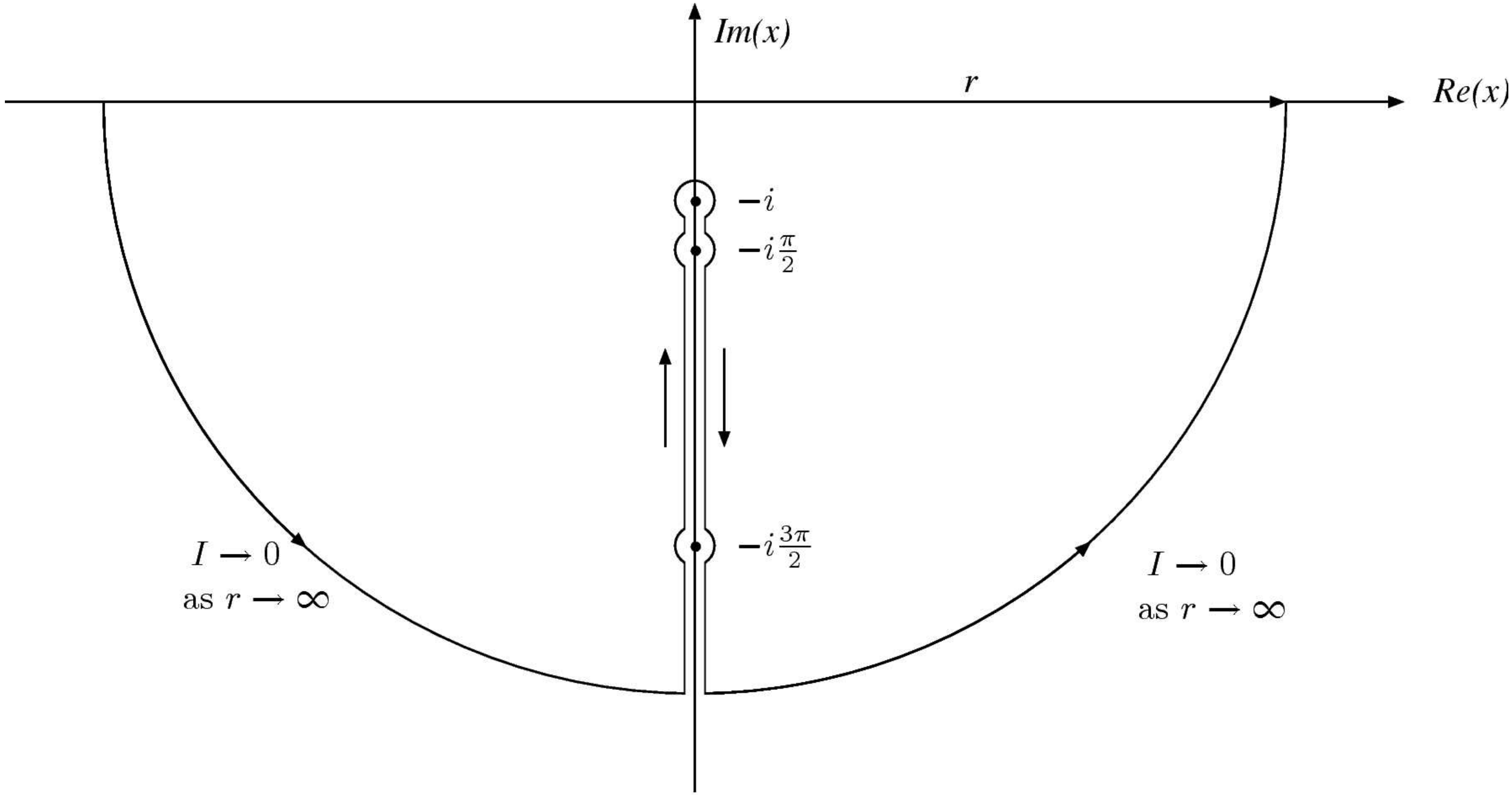
$$\hat{f}_2(\omega) = \int_{-\infty}^{\infty} \frac{e^{-i\,\omega\,\mathrm{Asinh}(x)}}{\cosh(x)}\, dx$$

Evaluate $\hat{f}_2(\omega)$ by a branch cut integral along the imaginary axis. Infinitely many singularities contribute. Irregular behavior!

Explicit error formulas for $l = 0, 1$:

$$T_0(h,0) = \frac{\pi}{\tanh(\pi/h)}, \quad E_0(h) = \frac{2\pi}{e^{2\pi/h} - 1}, \qquad E_1(h) = \sum_{k=1}^{\infty} \frac{2\pi}{\cosh(k\ \pi^2/h)}$$

Deformation of the path of integration for the integral $\hat{f}_2(\omega)$



A complicated error curve

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

with the transformation $x = \sinh(t)$.

Closed form using the poles $x_1 = i\,u\,\frac{\pi}{2},\ x_2 = v\,\pi \pm i\,a, \quad u, v \text{ odd}$:

$$\begin{aligned} I &= 2\pi \left(\sum_{k=0}^{\infty} \frac{(-1)^k}{\cosh(a)+\cosh(k+\frac{1}{2})\pi} + \frac{2\ \cos(a)}{\sinh(a)} \sum_{u=1,3,..} \frac{\cosh(u\,\pi)}{\cosh^2(u\pi)-\sin^2(a)} \right) \\ &= 1.94734\,99863\,38691\,95445\,99206\,53366 \qquad \text{for} \qquad a = 1 \end{aligned}$$

The error $T(h) - I$ as a function of $\omega := \frac{2\pi}{h}$ is very complicated, nevertheless it decreases exponentially.

Conjecture: $\quad T(h) - I = O\Big((a\,\omega)^{1/4}\ e^{-2\sqrt{a\,\omega}}\Big)\,, \quad \omega = \frac{2\pi}{h}$

A (sketchy) derivation of the asymptotic error $\hat{f}_1(\omega) + \hat{f}_1(-\omega)$

Consider the integral I of Slide 30 with the transformation $x = \phi(t) := \sinh(t)$, and find the Fourier transform $\hat{f}_1(\omega)$ according to Slide 24:

$$\hat{f}_1(\omega) = \int_{-\infty}^{\infty} \frac{e^{-i\,\omega\,\mathrm{Asinh}(z)}}{\cosh(z)\,\big(\cosh(a) + \cos(z)\big)}\,dz.$$

Deform ("pull down") the path of integration (the real axis).

Contributions F_k to $\hat{f}_1(\omega)$:

- Lower semi-circle of radius R: $F_1 \to 0$ as $R \to \infty$
- Branch cut, $\mathrm{Im}\, z < -1$: $F_2 = O(e^{-\omega\,\pi/2})$, small as $\omega \to \infty$
- Poles on branch cut, $z_v := i\,\frac{\pi}{2}\,v,\ \ v < 0$, odd: $F_3 = O(e^{-\omega\,\pi/2})$, small as $\omega \to \infty$
- Poles $z_u := u\,\pi - i\,a,\ \ u$ odd: the dominant contributions, F_4:

Error law, continued

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

For $u \to \infty$ the terms of the sum are approximated by

$$2\ \mathrm{Re}\ \exp\Big(-i\,\omega\,\big(\log(2\,u\,\pi) - \frac{i\,a}{u\,\pi}\big) + i\,a - u\,\pi\Big)\ .$$

By further approximating the sum by the corresponding integral we obtain

$$F_4 \approx \frac{4}{\sinh(a)} \int_0^\infty \exp(-\frac{a\,\omega}{u} - u)\ \cos(\omega\ \log(2\,u) - a)\ du\ .$$

Estimate: $\quad |F_4| \dot{<} \frac{4}{\sinh(a)} \int_0^\infty \exp(-\frac{a\,\omega}{u} - u)\ du$

Error law, final

The substitution $u = \sqrt{a\,\omega}\; e^t$ and Equ. 9.6.24 of Abramowitz/Stegun yields the following closed form in terms of a modified Bessel function:

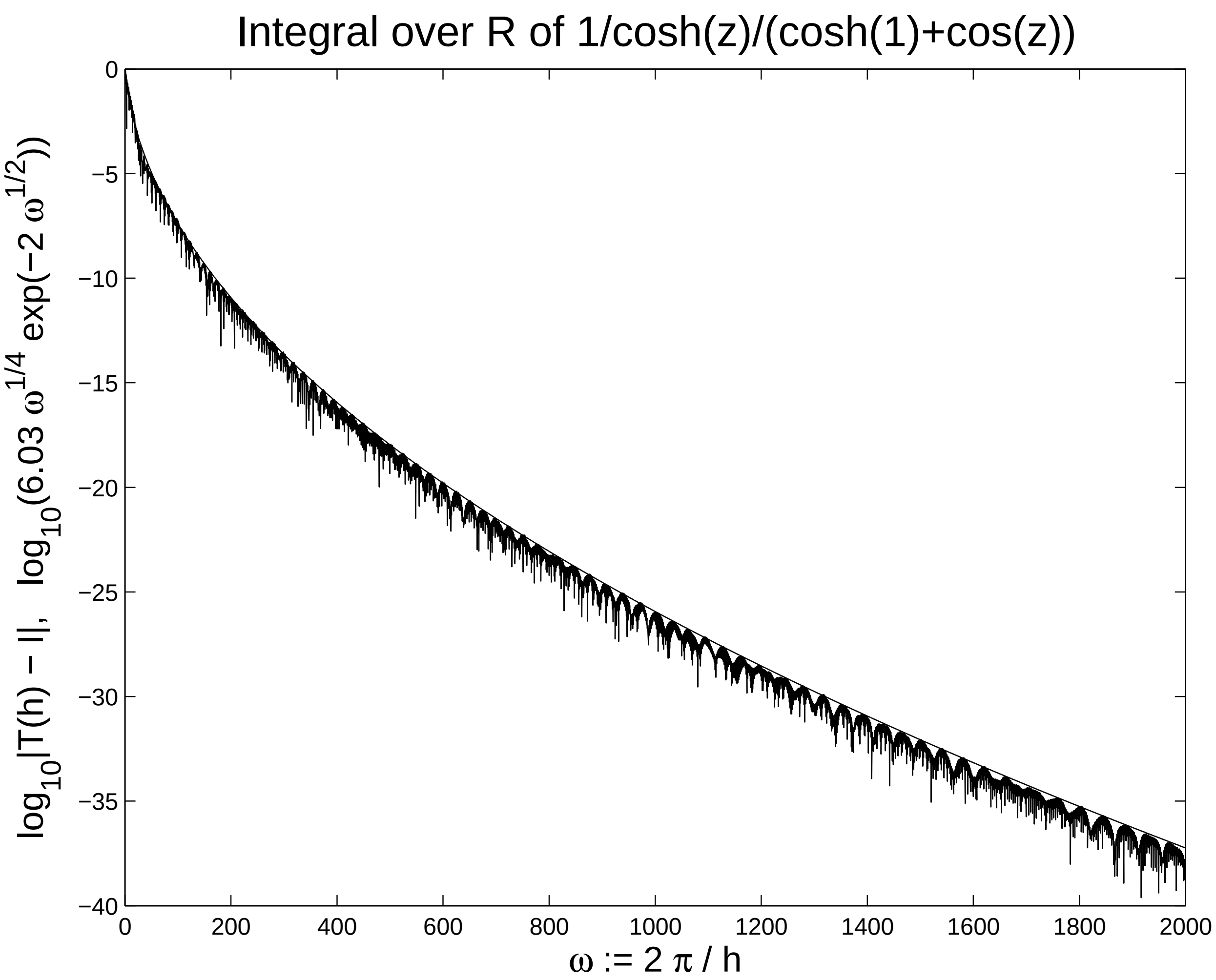
$$\int_0^\infty \exp(-\frac{a\,\omega}{u} - u)\; du = 2\sqrt{a\,\omega}\; \mathrm{K}_1(2\sqrt{a\,\omega})$$

Asymptotics of K_1 (Abramowitz/Stegun 9.7.2) yields the approximate inequality

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

The plot on the next slide shows this bound in comparison with half the error of the trapezoidal sum with step $h = 2\,\pi/\omega$. The agreement is striking!

Error and asymptotics (Case Slide 30) as a function of ω



An example by Tanaka, Sugihara, Murota, and Mori

Submitted to Numerische Mathematik, 2007

$$I = \int_{-1}^{1} \frac{2\,(1-z^2)\;dz}{\cosh(2)+\cos\big(4\;\mathrm{Atanh}(z)\big)} = \int_{-\infty}^{\infty} \frac{2\;dx}{\cosh^4(x)\;\big(\cosh(2)+\cos(4\;x)\big)}$$

transforming $z = \tanh(x)$. Difficult for double-exponential formulas!

Unexpected "closed" form by residues, using the poles

$$x_1 = i\,u\,\frac{\pi}{2},\;\; x_2 = v\,\frac{\pi}{4} \pm \frac{i}{2}, \quad u, v \text{ odd}:$$

$$I = \frac{8/3}{\sinh(2)} \left(1 + 4\,\pi \sum_{k=1}^{\infty} (-1)^k\; e^{-2\,k}\; \frac{k + 4\,k^3}{\sinh(2k\pi)} \right) = 0.71194\,38229\,70598\,27888$$

21 terms yield 67 digits in 1.4 ms (1.6 GHz processor).

6. Saddle point asymptotics

Richard Varga's example

$$I = \alpha! = \int_0^\infty e^{-z}\, z^\alpha\, dz = \int_{-\infty}^\infty f(x)\, dx \quad \text{with} \quad f(x) = \exp\big((\alpha+1)\,x - e^x\big)\,,$$

using the transformation $z = e^x$.

Fourier transform:

$$\begin{aligned} \hat{f}(\omega) &= \int_{-\infty}^\infty f(x)\, e^{-i\,\omega\,x}\, dx = \int_0^\infty e^{-z}\, z^{\alpha - i\,\omega}\, dz = (\alpha - i\,\omega)! \\ (*) \qquad &= \int_{-\infty}^\infty \exp\big(g(x)\big)\, dx \quad \text{with} \quad g(x) := (\alpha + 1 - i\,\omega)\,x - e^x \end{aligned}$$

Saddle points in x: $\frac{d}{dx} g(x) = 0$,

$$\Longrightarrow \qquad x = x_k := \mathrm{Log}(\alpha + 1 - i\,\omega) + 2k\pi\, i\,, \quad k \in \mathbb{Z}$$

Consider the particular case $\alpha = 0$. Dominant saddle: $k = 0$.

The saddle point technique

Step 1: Expand g in the dominant saddle x_0,

$$g(x_0 + \xi) = (x_0 - 1)\,(1 - i\,\omega) + s$$

where

$$s = c^2\,(\xi^2 + \frac{\xi^3}{3} + \frac{\xi^4}{12} + \dots) \quad \text{with} \quad c^2 := \frac{1}{2} g''(x_0) = -\frac{1}{2}(1 - i\,\omega)$$

Step 2: Write the integral $(*)$ in terms of s; expand in powers of $s^{1/2}$,

$$\frac{\sqrt{s}}{c} = \xi + \frac{\xi^2}{6} + \frac{\xi^3}{36} + \dots, \quad \xi = \frac{s^{1/2}}{c} - \frac{1}{6}\,\frac{s}{c^2} + \frac{1}{36}\,\frac{s^{3/2}}{c^3} + \dots,$$

$$d\xi = \left(\frac{s^{-1/2}}{2c} - \frac{1}{6c^2} + \frac{1}{24}\,\frac{s^{1/2}}{c^3} + \dots \right) ds$$

Step 3: Deform the path of integration into a saddle path and further into loops along the branch cut. The integral (*) becomes

$$\hat{f}(\omega) = (1 - i\,\omega)^{1-i\,\omega}\; e^{-(1-i\,\omega)} \int_\Gamma e^s \left(\text{last parenthesis of Slide 37}\right) ds\,,$$

where the path Γ encircles the negative-real axis counterclockwise.

Using $\int_\Gamma e^s\, s^\nu\, ds = -2\,i\,\sin(\nu\,\pi)\,\nu!$ finally yields

$$\hat{f}(\omega) = \sqrt{2\pi}\,(1 - i\,\omega)^{\frac{1}{2}-i\,\omega}\; \exp\left(-\,(1 - i\,\omega)\; + \frac{1}{12}\,(1 - i\,\omega)^{-1} - \ldots\right),$$

which is exactly the Stirling series for the closed form of Slide 36.

Exercise: Find the convergence rate of the trapezoidel rule $T(h)$ applied to the integral I of Slide 36.

Conclusions

- In general, for a finite interval the trapezoidal rule with step h has a discretization error of $O(h^2)$. Practically, this is rarely good enough.
- In two exceptional cases of analytic integrands the trapezoidal rule has an exponentially small error of order $O\big(\exp(-\gamma\, 2\pi/h)\big),\ \gamma > 0$:
  1. A periodic function integrated over a full period.
  2. All derivatives of the integrand vanish at both integration limits, which includes integrable functions to be integrated over $\mathbb{R}$.
- Transformations such as $x = \sinh(t)$ in integrals over $\mathbb{R}$ enhance the decay rate of the integrand, thus simplifying truncation of the infinite trapezoidal sums, but bear the danger of “breeding“ singularities.
- Asymptotics of the Fourier transform of the integrand yields the discretization error. Well understood for functions analytic in a strip. Otherwise, trapezoidal rule may still be useful, error theory difficult.