Computing Integrals of Analytic Functions: A Universal Algorithm with Exponential Convergence

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Applied Mathematics

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New Methods for Quadrature

Third Scopes Meeting

Zürich, December 9, 2006

The Problem

Evaluate to arbitrary precision

$$I = \int_D f(x)dx, \quad D = \begin{cases} (-\infty, \infty) \\ (0, \infty) \\ (0, b), \quad b > 0 \end{cases}$$

f: analytic in D

integrable boundary singularities allowed

not highly oscillatory

1. Sequence of mappings

$$t \in \mathbb{R} \stackrel{E}{\longmapsto} u \in \mathbb{R} \stackrel{F}{\longmapsto} v \in \mathbb{R} \stackrel{G}{\longmapsto} x \in D$$

to transform I into

$$I = \int_{\mathbb{R}} g(t)\, dt$$

where g decays doubly exponentially as $t \to \pm\infty$

Transformations

First step: Let

$$\begin{aligned} G_0(v) &= v+\sqrt{1+v^2} = \frac{1}{-v+\sqrt{1+v^2}} \\ G_1(v) &= \frac{G_0(v)}{1+G_0(v)} \end{aligned}$$

then

$$x = G(v) := \begin{cases} v & \text{if } D=(-\infty,\infty) \\ G_0(v) & \text{if } D=(0,\infty) \\ b\,G_1(v) & \text{if } D=(0,b); \quad b-x = b\,G_1(-v) \end{cases}$$

Second step: iterate

$$u \mapsto v = F(u) := \sinh(u)$$

until doubly exponential decay is reached on one side

Third step: iterate

$$t \mapsto u = E_0(t) := t + e^t \quad \text{or} \quad t \mapsto u = E_1(t) := -E_0(-t) = t - e^{-t}$$

until equal decay rates on both sides are reached

The exponential type, n

Model integrands $f_n(x), g_n(t)$, integrable for $\alpha > 0$:

n	$f_n(x)$ as $x \to +\infty$	$g_n(t)$ as $t := \dfrac{1}{x} \to +0$
-1	$f_{-1}(x) = x^{-1}\,(\log x)^{-\alpha-1}$	$g_{-1}(t) = t^{-1}\,(\log \frac{1}{t})^{-\alpha-1}$
0	$f_0(x) = x^{-\alpha-1}$	$g_0(t) = t^{\alpha-1}$
1	$f_1(x) = e^{-\alpha\, x}$	$g_1(t) = t^{-2}\, e^{-\alpha/t}$
2	$f_2(x) = \exp(x - \alpha\, e^x)$	$g_2(t) = t^{-2}\, \exp\left(\frac{1}{t} - \alpha\, e^{1/t}\right)$
$n+1$	$f_{n+1}(x) = e^x\, f_n(e^x)$	$g_{n+1}(t) = t^{-2}\, f_n(\frac{1}{t})$

2. Trapezoidal Rule

$$I = \int_{-\infty}^{\infty} g(t)\, dt$$

Trapezoidal sum, step h, offset s :

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

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 the trapezoidal sums

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

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

A (moderately) robust implementation:

- Start at an interior point and accumulate two separate sums upwards and downwards
- Truncate each sum if two (or three) consecutive terms do not contribute to the sum

The truncation error

Remainder for the truncation limit T:

$$R_T := \int_T^\infty g(t)\, dt, \quad \text{where} \quad g(T) = \varepsilon$$

(i) Algebraic decay:

$$g(t) = t^{-\alpha-1}, \quad (\alpha > 0), \qquad R_T = \frac{T^{-\alpha}}{\alpha} = \frac{\varepsilon^{\alpha/(1+\alpha)}}{\alpha}$$

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

(ii) Exponential decay:

$$g(t) = e^{-\alpha\, t}, \quad (\alpha > 0), \qquad R_T = \frac{1}{\alpha}\, e^{-\alpha\, T} = \frac{\varepsilon}{\alpha}$$

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

(iii) Doubly exponential decay:

$$\begin{aligned} g(t) &= \exp(-e^{\alpha\, t}), \quad (\alpha > 0), \\ R_T &= \frac{1}{\alpha}\, \exp(-e^{\alpha\, T})\, \left(e^{-\alpha\, T} - e^{-2\,\alpha\, T} + 2!\; e^{-3\,\alpha\, T} + \ldots\right) \end{aligned}$$

Truncation limit:

$$g(T) = \varepsilon \implies T = \frac{1}{\alpha}\, \log\log\frac{1}{\varepsilon}\;,$$

therefore

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

Truncation is safe for sufficiently small ε.

Theory of the discretization error

Let g be analytic on $\mathbb{R}$, and let $I := \int_{-\infty}^{\infty} g(t)\, dt$

Fourier Transform: $\hat{g}(\omega) := \int_{-\infty}^{\infty} e^{-i\,\omega\,t}\; g(t)\; dt\,, \quad I = \hat{g}(0)$

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

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

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

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

The error of the trapezoidal sum for a small step h approximately equals 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 $g(t)$ be analytic in $|\mathrm{Im}(t)| < \gamma,\ \gamma > 0$. Then

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

and the discretization error is

$$T(h,0) - I = O(e^{-(\gamma-\epsilon)\,2\pi/h}) \quad \text{as} \quad h \to 0.$$

(ii) Proliferation of singularities due to sinh transformations

Convergence may be slower, such as

$$T(h,0) - I = O(e^{-1/h^{\alpha}}) \quad \text{with} \quad \frac{1}{2} < \alpha < 1.$$

3. Implementation

Avoiding 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:

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

Implementation of the transformed integrand:

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!

4. The test integrals

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Closed forms

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

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

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

$S(z), C(z)$: Fresnel integrals; $K_1(z)$: Modified Bessel function;
agm: arithmetic-geometric mean

Remarks

- 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} 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_{25}, the convergence rate is $O(\exp(-c/h)),\ c > 0$.