A comparative study of extrapolation methods, sequence transformations and steepest descent methods

Computing infinite-range integrals

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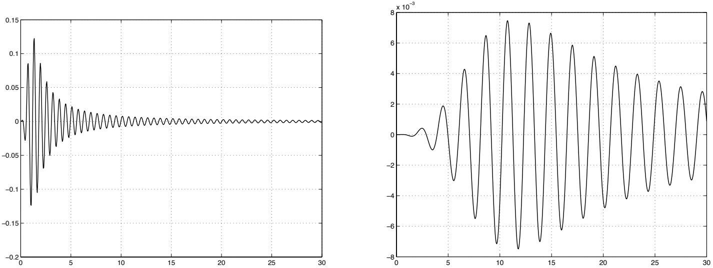
Oscillatory integrals: A numerical challenge



- Classical quadrature deteriorates rapidly as the oscillations become strong.
- New methods / New oscillatory quadrature methods were developed.

The plan

- **The three most popular methods**:
  - **Extrapolation methods**
  - **Sequence transformations**
  - **Numerical steepest descent**
- **Applications & Comparison**:
  - **We computed four integrals using the three methods**
  - **We introduced some refinements to the algorithms**
  - **We performed comparisons with regard to efficiency**
- **Conclusion**

Extrapolation methods

Let $f(x)$ satisfy:

$$f(x) = \sum_{k=1}^{m} p_k(x) f^{(k)}(x) \quad \text{where} \quad p_k(x) \sim x^k \sum_{i=0}^{\infty} \frac{\alpha_i}{x^i} \text{ as } x \to \infty.$$

Then [**Levin & Sidi 1981**]:

$$\int_x^\infty f(t)\,\mathrm{d}t \sim \sum_{k=0}^{m-1} x^{k+1} f^{(k)}(x) \sum_{i=0}^{\infty} \frac{\beta_{k,i}}{x^i} \quad \text{as} \quad x \to \infty.$$

Let $D_n^{(m)}$ represent approximations to $\int_0^\infty f(t)\,\mathrm{d}t$ [**Levin & Sidi**]:

$$D_n^{(m)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=0}^{m-1} x_l^{k+1} f^{(k)}(x_l) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x_l^i},$$

where $\{x_l\}_{l=0}^{mn+1}$ is an increasing sequence.

In general, m is equal or can be reduced to 1 or 2.

Extrapolation methods

When $m = 2$, we use the $\bar{D}_n^{(2)}$ approximation [**Sidi 1982**]:

$$\bar{D}_n^{(2)} = F(x_l) + x_l^2 f'(x_l) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i} \quad \text{where} \quad F(x) = \int_0^x f(t)\,\mathrm{d}t,$$

where $\{x_l\}_{l=0}^{n+1}$ are the successive positive zeros of $f(x)$.

To compute $D_n^{(1)}$ or $\bar{D}_n^{(2)}$, we use the W algorithm [**Sidi 1982**]:

$$WD_n^{(1)} = \frac{M_n^{(1)}}{N_n^{(1)}} \qquad \text{or} \qquad W\bar{D}_n^{(2)} = \frac{M_n^{(2)}}{N_n^{(2)}}.$$

$M_n^{(j)}$ and $N_n^{(j)}$ for $n, j = 1, 2, \ldots,$ are computed recursively by:

$$M_0^{(j)} = \frac{F(x_j)}{x_j^2 f'(x_j)} \quad \text{and} \quad N_0^{(j)} = \frac{1}{x_j^2 f'(x_j)}$$

$$M_n^{(j)} = \frac{M_{n-1}^{(j+1)} - M_{n-1}^{(j)}}{x_{j+n}^{-1} - x_j^{-1}} \quad \text{and} \quad N_n^{(j)} = \frac{N_{n-1}^{(j+1)} - N_{n-1}^{(j)}}{x_{j+n}^{-1} - x_j^{-1}}.$$

Sequence transformations

Let us consider $I(\lambda)$:

$$I(\lambda) = \int_0^{\infty} f(x;\lambda)\,\mathrm{d}x \sim \sum_{k=0}^{\infty} a_k(\lambda).$$

$$S[a] - S_n[a] \sim R_n[a] \quad \Rightarrow \quad S[a] \approx S_n[a] + R_n[a].$$

Consider the case where the remainder is given by:

$$S[a] - S_n[a] \sim \omega_n \sum_{j=0}^{\infty} \frac{c_j}{(n+\beta)^j} \qquad \text{as} \qquad n \to \infty.$$

A Levin transformation [**Levin 1973**]:

$$L_k^{(n)}(\beta) = \frac{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+\beta+j)^{k-1}}{(n+\beta+k)^{k-1}} \frac{S_{n+j}[a]}{\omega_{n+j}}}{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+\beta+j)^{k-1}}{(n+\beta+k)^{k-1}} \frac{1}{\omega_{n+j}}}.$$

Sequence transformations

A recursive algorithm [**Fessler et al. 1983**] to compute $L_k^{(n)}(\beta)$:

1. For $n = 0, 1, \ldots$, set:

$$P_0^{(n)} = \frac{S_n[a]}{\omega_n} \qquad \text{and} \qquad Q_0^{(n)} = \frac{1}{\omega_n}.$$

2. For $n = 0, 1, \ldots$, $k = 1, 2, \ldots$, compute $P_k^{(n)}$ and $Q_k^{(n)}$ from:

$$U_k^{(n)} = U_{k-1}^{(n+1)} - \frac{\beta + n}{\beta + n + k} \left(\frac{\beta + n + k - 1}{\beta + n + k} \right)^{k-2} U_{k-1}^{(n)},$$

   where the $U_k^{(n)}$ stand for either $P_k^{(n)}$ or $Q_k^{(n)}$.

3. For all n and k, set:

$$L_k^{(n)} = \frac{P_k^{(n)}}{Q_k^{(n)}}.$$

We choose $\omega_n = a_n$, which gives rise to the $t_k^{(n)}(\beta)$ transformation.

Numerical steepest descent

Huybrechs and Vandewalle 2006. Consider the integral:

$$\mathcal{I} = \int_a^b f(x)\, e^{i\, w\, g(x)}\, \mathrm{d}x, \quad e^{i\, w\, g(x)} = e^{-w\, \Im g(x)}\, e^{i\, w\, \Re g(x)}.$$

The steepest descent is based on:

1. $e^{i\, w\, g(x)}$ decays exponentially fast if $\Im g(x) > 0$.
2. $e^{i\, w\, g(x)}$ does not oscillate if $\Re g(x)$ is fixed.
3. The value of $\mathcal{I}$ does not depend on the exact path taken (Cauchy theorem).

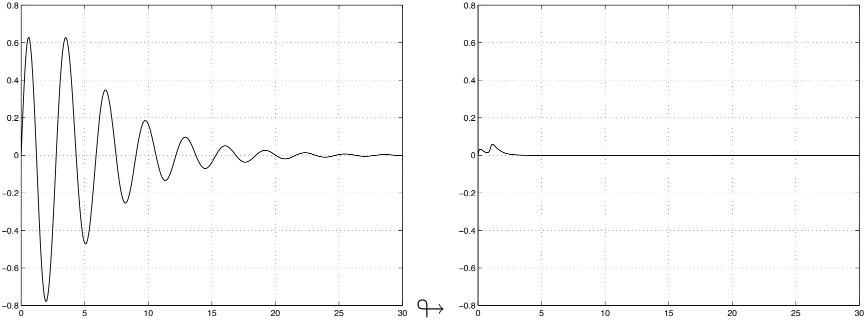
A new path is defined at a [**Huybrechs & Vandewalle 2006**]:

$$g(h_a(\kappa)) = g(a) + \kappa\, i \quad \text{with} \quad \kappa \geq 0.$$

The integral is then equivalent to:

$$\mathcal{I} = F(a) - F(b) \text{ where } F(t) = e^{i\, w\, g(a)} \int_0^\infty f(a + \kappa\, i)\, e^{-w\, \kappa}\, i\, \mathrm{d}\kappa.$$

Numerical steepest descent



The first integral

$$\mathcal{I}_1(\beta) = \int_0^\infty \frac{e^{-x}}{x+\beta}\,\mathrm{d}x = -e^\beta\,\mathrm{Ei}(-\beta).$$

No substitution is required to apply Gauss-Laguerre quadrature.
The integrand satisfies a first order linear differential equation:

$$f_1(x) = -\frac{x+\beta}{x+\beta+1} f_1'(x).$$

The integral has the asymptotic expansion:

$$\mathcal{I}_1(\beta) \sim \frac{1}{\beta}\sum_{k=0}^\infty \frac{k!}{(-\beta)^k} \quad \text{as} \quad \beta \to \infty.$$

The first integral

Table: Numerical valuation of $\mathcal{I}_1(\beta)$.

β	n	Error^{GL_n}	n	$\text{Error}^{WD_n^{(1)}}$	n	$\text{Error}^{LT_n^{(0)}}$
0.03	124	.87(-03)	17	.22(-12)	16	.32(-01)
0.10	124	.25(-05)	17	.84(-12)	17	.11(-02)
0.30	124	.16(-09)	17	.71(-14)	17	.14(-05)
1.00	124	.13(-13)	12	.56(-15)	21	.18(-07)
3.00	34	.36(-14)	8	.13(-14)	20	.21(-12)
4.00	34	.40(-14)	7	.22(-14)	19	.40(-15)
5.00	22	.65(-15)	6	.31(-14)	18	.16(-15)
10.00	15	.61(-15)	3	.30(-14)	16	.30(-15)
30.00	9	.17(-14)	3	.47(-14)	13	.00(00)
100.00	6	.18(-15)	2	.21(-14)	9	.18(-15)

$$\frac{\text{Calculation time } WD_n^{(1)}}{\text{Calculation time } GL_n} = 0.49 \quad \text{and} \quad \frac{\text{Calculation time } LT_n^{(0)}}{\text{Calculation time } GL_n} = 0.075.$$

Refinement – The first integral

For the sequence transformation:

As the values of the governing parameter(s) tend to 0^+, we resort to using a series representation of the integrals:

$$\mathcal{I}_1(\beta) = -e^{\beta}\left(\mathbf{C} + \ln\beta + \sum_{k=1}^{\infty}\frac{(-\beta)^k}{k\cdot k!}\right) \quad \text{as} \quad \beta \to 0^+.$$

For the Steepest descent:

$$\int_0^{\infty} f(x)\, e^{-x}\, \mathrm{d}x = \int_0^{x_n} e^{-x}\, \mathrm{d}x + e^{-x_n}\int_0^{\infty} f(x+x_n)\, e^{-x}\, \mathrm{d}x$$

- Compute $\displaystyle\int_0^{x_n} e^{-x}\, \mathrm{d}x = \sum_{i=1}^{n}\int_{x_{i-1}}^{x_i} f(x)\, e^{-x}\, \mathrm{d}x.$
- n is determined by:

$$\left|\int_{x_{n-1}}^{x_n} f(x)e^{-x}\,\mathrm{d}x\right| < \frac{1}{2}\left|\int_{x_{n-2}}^{x_{n-1}} f(x)e^{-x}\,\mathrm{d}x\right|.$$

Refinement – The first integral

Table: Numerical valuation of $\mathcal{I}_1(\beta)$ with the refinement.

β	n	Error^{GL_n}	n	$\text{Error}^{WD_n^{(1)}}$	n	$\text{Error}^{LT_n^{(0)}}$
0.03	70	.10(-12)	17	.22(-12)	7	.15(-15)
0.10	53	.18(-14)	17	.84(-12)	9	.00(00)
0.30	41	.13(-14)	17	.71(-14)	12	.18(-15)
1.00	22	.13(-14)	12	.56(-15)	17	.00(00)
3.00	12	.17(-14)	8	.13(-14)	28	.47(-14)
4.00	12	.17(-14)	7	.22(-14)	19	.40(-15)
5.00	12	.28(-14)	6	.31(-14)	18	.16(-15)
10.00	8	.33(-14)	3	.30(-14)	16	.30(-15)
30.00	6	.47(-14)	3	.47(-14)	13	.00(00)
100.00	5	.19(-14)	2	.21(-14)	9	.18(-15)

$$\frac{\text{Calculation time } WD_n^{(1)}}{\text{Calculation time } GL_n} = 2.2 \quad \text{and} \quad \frac{\text{Calculation time } LT_n^{(0)}}{\text{Calculation time } GL_n} = 0.27.$$

The second integral

$$\mathcal{I}_2(a,b) = \int_0^\infty \sin\left(\frac{a}{x}\right)\sin(b\,x)\,\mathrm{d}x = \frac{\pi}{2}\sqrt{\frac{a}{b}}J_1(2\sqrt{a\,b}).$$

Asymptotic expansion as $a\,b \to \infty$:

$$\begin{aligned}\mathcal{I}_2(a,b) \quad &\sim \quad \sqrt{\frac{\pi\,a}{2\,b}}\frac{1}{\sqrt{2\sqrt{a\,b}}}\left\{\cos(2\sqrt{a\,b} - 3\pi/4)\right.\\ &\times \quad \sum_{k=0}^{\infty}\frac{(-1)^k}{(16\,a\,b)^k}\frac{\Gamma(3/2+2k)}{(2k)!\,\Gamma(3/2-2k)}\\ &- \left.\frac{\sin(2\sqrt{a\,b} - 3\pi/4)}{4\sqrt{a\,b}}\sum_{k=0}^{\infty}\frac{(-1)^k}{(16\,a\,b)^k}\frac{\Gamma(5/2+2k)}{(2k+1)!\,\Gamma(1/2-2k)}\right\}.\end{aligned}$$

The second integral

Splitting the integration interval with respect to $x_0 = \sqrt{\frac{a}{b}}$:

$$\begin{aligned}
\mathcal{I}_2(a,b) &= \int_0^{x_0} \sin\left(\frac{a}{x}\right) \sin(b\,x)\,\mathrm{d}x + \int_{x_0}^{\infty} \sin\left(\frac{a}{x}\right) \sin(b\,x)\,\mathrm{d}x \\
&= \int_{x_0^{-1}}^{\infty} \sin\left(\frac{b}{x}\right) \frac{\sin(a\,x)}{x^2}\,\mathrm{d}x + \int_{x_0}^{\infty} \sin\left(\frac{a}{x}\right) \sin(b\,x)\,\mathrm{d}x \\
&= \mathrm{Im}\left\{\int_{x_0^{-1}}^{\infty} \sin\left(\frac{b}{x}\right) \frac{e^{\mathrm{i}a\,x}}{x^2}\,\mathrm{d}x\right\} + \mathrm{Im}\left\{\int_{x_0}^{\infty} \sin\left(\frac{a}{x}\right) e^{\mathrm{i}b\,x}\,\mathrm{d}x\right\}.
\end{aligned}$$

The substitutions $x_{\mathrm{new}} = \mathrm{i}\,a(x_0^{-1} - x_{\mathrm{old}})$ and $x_{\mathrm{new}} = \mathrm{i}\,b(x_0 - x_{\mathrm{old}})$ lead to:

$$\begin{aligned}
\mathcal{I}_2(a,b) &= \mathrm{Im}\left\{\frac{\mathrm{i}}{a}\int_0^{\infty} \sin\left(\frac{b}{x_0^{-1} + \mathrm{i}x/a}\right) \frac{e^{\mathrm{i}a\,x_0^{-1}} e^{-x}}{(x_0^{-1} + \mathrm{i}x/a)^2}\,\mathrm{d}x\right\} \\
&+ \mathrm{Im}\left\{\frac{\mathrm{i}}{b}\int_0^{\infty} \sin\left(\frac{a}{x_0 + \mathrm{i}x/b}\right) e^{\mathrm{i}b\,x_0} e^{-x}\,\mathrm{d}x\right\}.
\end{aligned}$$

The second integral

Table: Numerical valuation of $\mathcal{I}_2(a, b)$.

a	b	n	Error^{GL_n}	n	Error$^{W\bar{D}_n^{(2)}}$	n	Error$^{LT_n^{(0)}}$
1.0	1.0	124	.19(-09)	16	.86(-15)	23	.29(-08)
2.0	1.0	124	.60(-11)	17	.12(-14)	24	.34(-10)
2.0	2.0	124	.72(-12)	17	.17(-14)	24	.33(-12)
3.0	1.0	124	.12(-11)	18	.27(-15)	23	.10(-11)
3.0	2.0	124	.75(-14)	17	.55(-15)	25	.17(-14)
3.0	3.0	117	.68(-14)	17	.51(-15)	18	.13(-15)
10.0	1.0	124	.29(-14)	19	.16(-14)	20	.44(-15)
100.0	1.0	124	.76(-14)	10	.91(-01)	8	.21(-14)
10.0	10.0	124	.59(-14)	7	.79(-02)	8	.20(-14)
100.0	10.0	69	.20(-14)	8	.26(01)	5	.16(-14)

$$\frac{\text{Calculation time } W\bar{D}_n^{(2)}}{\text{Calculation time } GL_n} = 0.096 \quad \text{and} \quad \frac{\text{Calculation time } LT_n^{(0)}}{\text{Calculation time } GL_n} = 0.011.$$

Refinement – The second integral

Table: Numerical evaluation of $\mathcal{I}_2(a,b)$ with the refinement.

a	b	n	Error^{GL_n}	n	$\text{Error}^{W\bar{D}_n^{(2)}}$	n	$\text{Error}^{LT_n^{(0)}}$
1.0	1.0	53	.86(-15)	16	.16(-14)	10	.37(-15)
2.0	1.0	53	.75(-15)	18	.12(-14)	12	.12(-15)
2.0	2.0	53	.24(-14)	18	.36(-14)	15	.15(-14)
3.0	1.0	53	.13(-14)	18	.54(-15)	14	.00(00)
3.0	2.0	70	.92(-15)	17	.15(-14)	25	.17(-14)
3.0	3.0	53	.77(-15)	17	.64(-15)	18	.13(-15)
10.0	1.0	56	.11(-14)	19	.44(-14)	20	.44(-15)
100.0	1.0	34	.38(-14)	26	.12(-12)	8	.21(-14)
10.0	10.0	56	.12(-14)	29	.98(-13)	8	.20(-14)
100.0	10.0	53	.39(-14)	35	.17(-11)	5	.16(-14)

$$\frac{\text{Calculation time } W\bar{D}_n^{(2)}}{\text{Calculation time } GL_n} = 100.0 \quad \text{and} \quad \frac{\text{Calculation time } LT_n^{(0)}}{\text{Calculation time } GL_n} = 0.022.$$

The third integral

$$\mathcal{I}_3(\mu,\alpha,\beta) = \int_0^\infty x^\mu e^{-\alpha x^2} K_0(\beta x)\,\mathrm{d}x, = \frac{\left\{\Gamma\left(\frac{\mu+1}{2}\right)\right\}^2}{2\alpha^{\mu/2}\beta} \exp\left(\frac{\beta^2}{8\alpha}\right) W_{-\frac{\mu}{2},0}\left(\frac{\beta^2}{4\alpha}\right).$$

The integral has the asymptotic expansion as $\dfrac{\beta^2}{4\,\alpha} \to \infty$:

$$\mathcal{I}_3(\mu,\alpha,\beta) \sim \frac{\left\{\Gamma\left(\frac{\mu+1}{2}\right)\right\}^2}{2^{1-\mu}\beta^{\mu+1}} \sum_{k=0}^{\infty} \frac{\left\{\left(\frac{\mu+1}{2}\right)_k\right\}^2}{k!} \left(-\frac{4\,\alpha}{\beta^2}\right)^k.$$

$\mathcal{I}_3(\mu,\alpha,\beta)$ also has the series representation as $\dfrac{\beta^2}{4\,\alpha} \to 0^+$:

$$\mathcal{I}_3(\mu,\alpha,\beta) = \frac{1}{4\,\alpha^{\frac{\mu+1}{2}}} \sum_{k=0}^{\infty} \frac{\Gamma\left(k+\frac{\mu+1}{2}\right)}{(k!)^2} \left(\frac{\beta^2}{4\,\alpha}\right)^k \times \left[2\,\psi(k+1) - \psi\left(k+\frac{\mu+1}{2}\right) - \ln\left(\frac{\beta^2}{4\,\alpha}\right)\right].$$

The third integral

The substitutions $x_{\rm new} = \alpha\, x_{\rm old}^2 + \beta\, x_{\rm old}$ leads to:

$$\begin{aligned}
\mathcal{I}_3(\mu,\alpha,\beta) &= \int_0^\infty \left(\frac{-\beta + \sqrt{\beta^2 + 4\,\alpha\,x}}{2\,\alpha}\right)^\mu \\
&\times \exp\left(\frac{-\beta^2 + \beta\sqrt{\beta^2 + 4\,\alpha\,x}}{2\,\alpha}\right) \\
&\times K_0\left(\frac{-\beta^2 + \beta\sqrt{\beta^2 + 4\,\alpha\,x}}{2\,\alpha}\right) \frac{e^{-x}\,\mathrm{d}x}{\sqrt{\beta^2 + 4\,\alpha\,x}}.
\end{aligned}$$

The third integral

Table: Numerical valuation of $\mathcal{I}_3(\mu, \alpha, \beta)$.

μ	α	β	n	Error^{GL_n}	n	$\text{Error}^{W\bar{D}_n^{(2)}}$	n	$\text{Error}^{LT_n^{(0)}}$
0	3.0	1.0	124	.59(-02)	16	.30(-03)	18	.57(-03)
0	1.0	1.0	124	.46(-02)	15	.33(-03)	18	.80(-06)
0	3.0	3.0	124	.39(-02)	20	.36(-03)	19	.25(-08)
0	1.0	3.0	124	.35(-02)	19	.38(-03)	21	.11(-12)
1	4.0	1.0	124	.13(-03)	17	.23(-06)	17	.11(-01)
1	1.0	4.0	124	.20(-04)	17	.24(-06)	19	.40(-15)
1	1.0	8.0	124	.17(-04)	18	.23(-06)	15	.12(-15)
2	5.0	1.0	124	.90(-05)	18	.32(-09)	16	.41(-01)
2	1.0	5.0	124	.15(-06)	17	.21(-09)	19	.73(-15)
2	1.0	10.0	124	.12(-06)	19	.19(-09)	15	.15(-15)

$$\frac{\text{Calculation time } W\bar{D}_n^{(2)}}{\text{Calculation time } GL_n} = 0.089 \quad \text{and} \quad \frac{\text{Calculation time } LT_n^{(0)}}{\text{Calculation time } GL_n} = 0.000\,22.$$

Refinement – The third integral

Table: Numerical evaluation of $\mathcal{I}_3(\mu, \alpha, \beta)$ with the refinement.

μ	α	β	n	Error^{GL_n}	n	$\text{Error}^{W\bar{D}_n^{(2)}}$	n	$\text{Error}^{LT_n^{(0)}}$
0	3.0	1.0	123	.14(-03)	18	.30(-06)	9	.38(-15)
0	1.0	1.0	123	.11(-03)	18	.33(-06)	12	.00(00)
0	3.0	3.0	123	.91(-04)	16	.36(-06)	16	.51(-15)
0	1.0	3.0	123	.83(-04)	16	.38(-06)	24	.12(-14)
1	4.0	1.0	81	.24(-06)	17	.97(-12)	9	.00(00)
1	1.0	4.0	85	.44(-07)	17	.95(-12)	19	.40(-15)
1	1.0	8.0	87	.38(-07)	19	.87(-12)	15	.12(-15)
2	5.0	1.0	56	.15(-08)	20	.14(-12)	9	.00(00)
2	1.0	5.0	61	.51(-10)	17	.72(-13)	19	.73(-15)
2	1.0	10.0	63	.42(-10)	20	.25(-13)	15	.15(-15)

$$\frac{\text{Calculation time } W\bar{D}_n^{(2)}}{\text{Calculation time } GL_n} = 1.7 \quad \text{and} \quad \frac{\text{Calculation time } LT_n^{(0)}}{\text{Calculation time } GL_n} = 0.000\,42.$$

Conclusion

- The three methods are capable of reaching high pre-determined accuracies.
- The sequence transformation methods applied to the asymptotic expansions of the integrals provide an extremely accurate and efficient algorithm.
- Further research is needed

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