Generalized Techniques in Numerical Integration

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Approximation and Extrapolation of Convergent and Divergent Sequences and Series

CIRM Luminy

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The Plan

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- **A Mathematical Tool**
  - Formulae for Higher Order Derivatives

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Introduction

The Euler series arising from integrating the Euler integral by parts:

$$\int_x^\infty \frac{e^{-t}}{t}\,\mathrm{d}t = \frac{e^{-x}}{x}\sum_{l=0}^{\infty}(-1)^l\,\frac{l!}{x^l} + (-1)^n\,n!\int_x^\infty \frac{e^{-t}}{t^{n+1}}\,\mathrm{d}t$$

$$\sim \frac{e^{-x}}{x}\sum_{l=0}^{\infty}(-1)^l\,\frac{l!}{x^l}, \qquad x \to \infty.$$

Integration by parts by $\underline{x\mathrm{d}x}$ led to:

$$\int_0^\infty g(x)\,\underline{j_\lambda(x)}\,\mathrm{d}x = \int_0^\infty g(x)\,\underline{(-1)^\lambda\,x^\lambda\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^\lambda\left(\frac{\sin(x)}{x}\right)}\,\mathrm{d}x$$

$$= (-1)^\lambda\int_0^\infty \left[x^{\lambda-1}\,g(x)\right]\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^\lambda\left(\frac{\sin(x)}{x}\right)\,\underline{x\mathrm{d}x}.$$

Introduction

$$\begin{aligned} &= (-1)^{\lambda} \left[x^{\lambda-1}\, g(x)\right] \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^{\lambda-1} \left(\frac{\sin(x)}{x}\right)\Bigg|_{0}^{\infty} \\ &\quad + (-1)^{\lambda-1} \int_0^{\infty} \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right) \left[x^{\lambda-1}\, g(x)\right] \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^{\lambda-1} \left(\frac{\sin(x)}{x}\right) x\mathrm{d}x \\ &= \sum_{l=0}^{\lambda-1} (-1)^{\lambda+l} \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^{l} \left[x^{\lambda-1}\, g(x)\right] \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^{\lambda-1-l} \left(\frac{\sin(x)}{x}\right)\Bigg|_{0}^{\infty} \\ &\quad + \int_0^{\infty} \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^{\lambda} \left[x^{\lambda-1}\, g(x)\right] \left(\frac{\sin(x)}{x}\right) x\mathrm{d}x. \end{aligned}$$

Leading at:

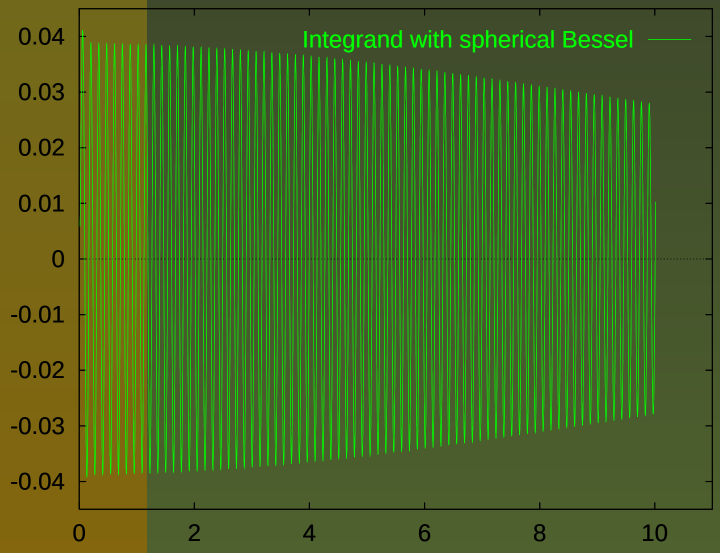
$$\int_0^{\infty} g(x)\, \boxed{j_{\lambda}(v\, x)}\, \mathrm{d}x = \frac{1}{v^{\lambda+1}} \int_0^{\infty} \left[\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^{\lambda} \left(x^{\lambda-1}\, g(x)\right)\right] \boxed{\sin(v\, x)}\, \mathrm{d}x.$$

Introduction

Semi-infinite spherical Bessel integrals in molecular integrals:

$$g(x) \;=\; x^{n_x}\,\frac{\hat{k}_{n+\frac{1}{2}}[R\,\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}, \qquad \hat{k}_{n+\frac{1}{2}}(z) = \frac{z^n}{e^z}\sum_{j=0}^{n}\frac{(n+j)!}{j!(n-j)!}\,\frac{1}{(2\,z)^j}$$

$$\gamma(s,x) = \sqrt{(1-s)\zeta_i^2 + s\zeta_j^2 + s(1-s)\,x^2}. \quad s \in [0,1].$$



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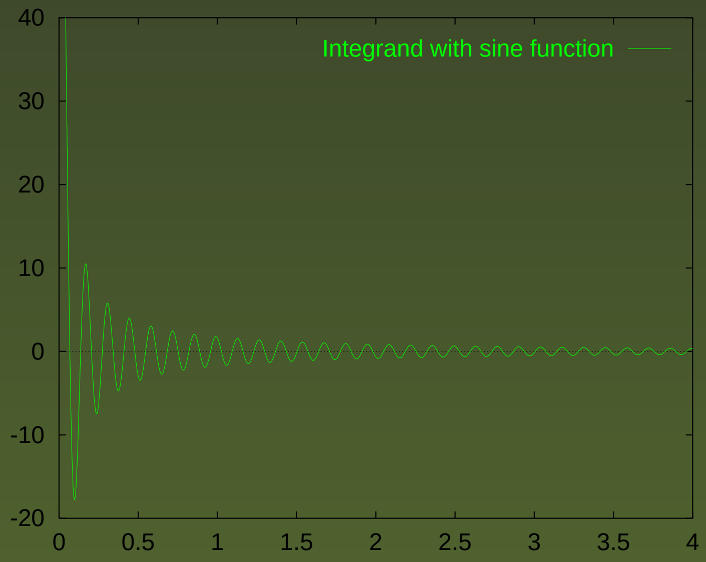

How can we use this technique for any $\int_a^b f(x)\,\mathrm{d}x$?

Higher Order Derivatives

Let us determine the k$^{\text{th}}$ derivatives of $G_1(x) = x^3\, f(x^2)$:

$$\left(\frac{\mathrm{d}}{\mathrm{d}x}\right) G_1(x) = 3\,x^2\, f(x^2) + 2\,x^4\, f'(x^2).$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 G_1(x) = 6\,x\, f(x^2) + (6\,x^3 + 8\,x^3) f'(x^2) + 4\,x^5\, f''(x^2).$$

How about this:

$$\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)(x^{-3}G_1(x)) = 2\, f'(x^2) \Longrightarrow \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^k (x^{-3}G_1(x)) = 2^k\, f^{(k)}(x^2).$$

For $G_2(x) = x^2\, f\,(\ln(x))$: $\left(\frac{\mathrm{d}}{x^{-1}\mathrm{d}x}\right)^k (x^{-2}G_2(x)) = f^{(k)}\,(\ln(x)).$

Can we express $\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^k G(x)$ in terms of $\left(\frac{\mathrm{d}}{x^m\mathrm{d}x}\right)^i (x^{-n}G(x))$ for $i = 0, 1, \ldots, k$?

Higher Order Derivatives

The Slevinsky-Safouhi formulae [Slevinsky and Safouhi, 2009]:

Theorem Let $G(x)$ be kth differentiable with $\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^k (x^{-n}\, G(x))$ well-defined. The Slevinsky-Safouhi formula I for (α, β, m, n) is given by:

$$\left(\frac{\mathrm{d}}{x^\alpha \mathrm{d}x}\right)^k (x^{-\beta} G(x)) = \sum_{i=0}^{k} A_k^i \, x^{n-\beta+i(m+1)-k(\alpha+1)} \left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n} G(x)),$$

with coefficients [$N = (n - \beta - (k-1)(\alpha+1))$]:

$$A_k^i = \begin{cases} 1 & \text{for} \quad i = k \\ N\, A_{k-1}^0 & \text{for} \quad i = 0,\ k > 0 \\ (N + i(m+1))A_{k-1}^i + A_{k-1}^{i-1} & \text{for} \quad 0 < i < k. \end{cases}$$

$$A_k^i = \sum_{j=0}^{i} \frac{(-1)^{i-j}\, (n - \beta + j(m+1) - (k-1)(\alpha+1))_{k,\alpha+1}}{(m+1)^i\, j!\, (i-j)!}, \quad m \neq -1.$$

The Slevinsky-Safouhi formula II: $(\alpha, \beta, m, n) = (0, 0, 1, 0)$.

Part I

The Generalized

S_n Transformation

&

The Staircase Algorithm

The generalized S_n

Let $f(x)$ be integrable on $[a,b]$, i.e. $\int_a^b f(x)\,\mathrm{d}x$ exists. We write:

$$\int_a^b f(x)\,\mathrm{d}x = \int_a^b G_0(x)\,H_0(x)\,\underline{w(x)\,\mathrm{d}x},$$

for some weight function $w(x)$, whose choice depends on $f(x)$.

If $f(x) \in \mathcal{C}^n[a,b]$, then $\int_a^b f(x)\,\mathrm{d}x$ has the equivalent representation, which we obtain after $\underline{n \text{ integration by parts by } w(x)\,\mathrm{d}x}$:

$$\boxed{\int_a^b f(x)\,\mathrm{d}x = \sum_{l=0}^{n-1} G_l(x)\,H_{l+1}(x)\Big|_a^b + \int_a^b G_n(x)\,H_n(x)\,w(x)\,\mathrm{d}x}$$

where:

$$G_l(x) = (-1)^l \left(\frac{\mathrm{d}}{w(x)\,\mathrm{d}x}\right)^l g(x) \quad \text{and} \quad H_l(x) = \left(\frac{\mathrm{d}}{w(x)\,\mathrm{d}x}\right)^{-l} h(x).$$

The Staircase Algorithm

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Approximations to $\displaystyle\int_a^b f(x)\,\mathrm{d}x$ take the following form:

- For $a < x_0 < b$, initialize: $\displaystyle S_0 = \int_a^{x_0} G_0(x)\,H_0(x)\,w(x)\,\mathrm{d}x,$

$$\int_{x_0}^{b} G_0(x)\,H_0(x)\,w(x)\,\mathrm{d}x = G_0(x)\,H_1(x)\Big|_{x_0}^{b} + \int_{x_0}^{b} G_1(x)\,H_1(x)\,w(x)\,\mathrm{d}x.$$

$$S_1 \;=\; S_0 + G_0(x)\,H_1(x)\Big|_{x_0}^{b} + \int_{x_0}^{x_1} G_1(x)\,H_1(x)\,w(x)\,\mathrm{d}x, \quad x_0 < x_1 < b.$$

- For the sequence $\{x_l\}_{l=1}^{n}$ satisfying $a < x_{l-1} < x_l < b$, define:

$$S_l \;=\; S_{l-1} + G_{l-1}(x)\,H_l(x)\Big|_{x_{l-1}}^{b} + \int_{x_{l-1}}^{x_l} G_l(x)\,H_l(x)\,w(x)\,\mathrm{d}x.$$

The approximations to $\displaystyle\int_a^b f(x)\,\mathrm{d}x$ form the sequence $\{S_l\}_{l=0}^{n}$.

Bessel Integral

The integral that follows appeared in Numerical Recipes:

$$\mathcal{I}_1 = \int_0^b \frac{x}{x^2+1}\, J_0(x)\, \mathrm{d}x = K_0(1).$$

By choosing $w(x) = x$, we have $G_0(x) = \dfrac{1}{x^2+1}$ and $H_0(x) = J_0(x)$.

$$\hookrightarrow \quad G_l(x) = \frac{2^l\, l!}{(x^2+1)^{l+1}} \quad \text{and} \quad H_l(x) = x^l\, J_l(x).$$

The integral then has the equivalent representations:

$$\boxed{\mathcal{I}_1 = \sum_{l=0}^{n-1} \frac{-2^l\, l!\, x^{l+1}}{(x^2+1)^{l+1}}\, J_{l+1}(x) \Big|_0^\infty + 2^n\, n! \int_a^\infty \frac{x^{n+1}}{(x^2+1)^{n+1}}\, J_n(x)\, \mathrm{d}x}$$

All the boundary terms vanish and consequently:

$$\int_0^\infty \frac{x}{x^2+1} J_0(x)\, \mathrm{d}x = 2^n\, n! \int_0^\infty \frac{x^{n+1}}{(x^2+1)^{n+1}}\, J_n(x)\, \mathrm{d}x = K_0(1).$$

Bessel Integral - Results

Table 1: $\mathcal{I}_1 = 0.421024438240708$. $x_l = 2\pi(l+1)$.

l	$\bar{S}_l$	l	$\bar{S}_l$
0	0.414 193 276 771 795	7	0.421 024 438 053 642
1	0.421 696 746 593 657	8	0.421 024 438 183 915
2	0.421 072 353 906 909	9	0.421 024 438 241 771
3	0.421 020 653 966 770	10	0.421 024 438 241 364
4	0.421 023 974 243 269	11	0.421 024 438 240 707
5	0.421 024 464 857 404	12	0.421 024 438 240 700
6	0.421 024 443 256 394	13	0.421 024 438 240 708

Fresnel Integrals

The integrals are given by:

$$\mathcal{I}_2(a,v) = \int_a^\infty \sin(v\,x^2)\,\mathrm{d}x \quad \text{and} \quad \tilde{\mathcal{I}}_2(a,v) = \int_a^\infty \cos(v\,x^2)\,\mathrm{d}x.$$

By choosing $w(x) = x$, we have $G_0(x) = \dfrac{1}{x}$ and $H_0(x) = \sin(v\,x^2)$.

$$\hookrightarrow \qquad G_l(x) = \frac{(2l)!}{2^l\,l!\,x^{2l+1}} \quad \text{and} \quad H_l(x) = \frac{\sin(v\,x^2 - l\pi/2)}{(2\,v)^l}.$$

The integral $\mathcal{I}_2(a,v)$ then has the equivalent representations:

$$\boxed{\sum_{l=0}^{n-1} \frac{-2(2l)!}{(4v)^{l+1}\,l!}\,\frac{\sin\left(vx^2 - \frac{(l+1)\pi}{2}\right)}{x^{2l+1}}\Bigg|_a + \frac{(2n)!}{(4v)^n\,n!}\int_a^\infty \frac{\sin\left(vx^2 - \frac{n\pi}{2}\right)}{x^{2n}}\mathrm{d}x}$$

Fresnel Integrals - Results

Table 2: $\mathcal{I}_2(0,1) = .6266570686577750.$ $x_l = \sqrt{2\pi(l+1)/v}.$

l	$\bar{S}_l$	l	$\bar{S}_l$
0	0.629 878 864 869 732	7	0.626 657 068 644 466
1	0.627 294 419 199 049	8	0.626 657 068 657 872
2	0.626 651 451 723 302	9	0.626 657 068 657 790
3	0.626 655 488 072 699	10	0.626 657 068 657 749
4	0.626 657 083 038 776	11	0.626 657 068 657 749
5	0.626 657 073 115 469	12	0.626 657 068 657 750
6	0.626 657 068 616 796		

The integral $\tilde{\mathcal{I}}_2(a,v)$ then has the equivalent representations:

$$\boxed{\sum_{l=0}^{n-1} \frac{-2\,(2l)!}{(4v)^{l+1}\,l!}\,\frac{\cos\left(v\,x^2 - \frac{(l+1)\pi}{2}\right)}{x^{2l+1}}\Bigg|_a + \frac{(2n)!}{(4v)^n\,n!}\int_a^\infty \frac{\cos\left(vx^2 - \frac{n\pi}{2}\right)}{x^{2n}}\,\mathrm{d}x}$$

The Twisted Tail

The integral is proposed in the book "*The SIAM 100-Digit Challenge*":

$$\mathcal{I}_3 = \int_0^1 t^{-1} \cos\left(t^{-1} \ln(t)\right) \,\mathrm{d}t = \int_0^{\infty} \cos(x\, e^x)\,\mathrm{d}x, \quad (x = -\ln(t)).$$

$$w(x) = (1+x)e^x \;\hookrightarrow\; G_0(x) = \frac{1}{(1+x)\,e^x} \text{ and } H_0(x) = \cos(x\,e^x).$$

$$\hookrightarrow\; G_l(x) = \left(\frac{-\mathrm{d}}{(1+x)\,e^x \mathrm{d}x}\right)^l \frac{1}{(1+x)\,e^x} \text{ and } H_l(x) = \cos\left(x\,e^x - \frac{l\pi}{2}\right).$$

The general form of $G_l(x)$ is:

$$G_l(x) = \frac{e^{-(l+1)\,x}}{(1+x)^{2l+1}}\, p_l(x) \qquad \left\{ \begin{array}{lcl} p_0(x) & = & 1 \\ p_1(x) & = & 2+x \\ p_2(x) & = & 9+8x+2x^2 \\ p_3(x) & = & 64+79x+36x^2+6x^3 \\ \vdots & \vdots & \vdots \end{array} \right.$$

The Twisted Tail

The integral $\mathcal{I}_3$ then has the equivalent representations:

$$\boxed{\sum_{l=0}^{n-1} \frac{-p_l(x)\,e^{-(l+1)x}\cos\left(x\,e^x - \frac{(l+1)\pi}{2}\right)}{(1+x)^{2l+1}}\Bigg|_0 + \int_0^\infty \frac{p_n(x)\,e^{-nx}\cos\left(xe^x - \frac{n\pi}{2}\right)}{(1+x)^{2n}}\,\mathrm{d}x}$$

As a specific case, the generalized S_1 yields the equivalent representation:

$$\boxed{\int_0^\infty \cos(x\,e^x)\,\mathrm{d}x = \int_0^\infty e^{-x}\,\frac{2+x}{(1+x)^2}\,\sin(x\,e^x)\,\mathrm{d}x}$$

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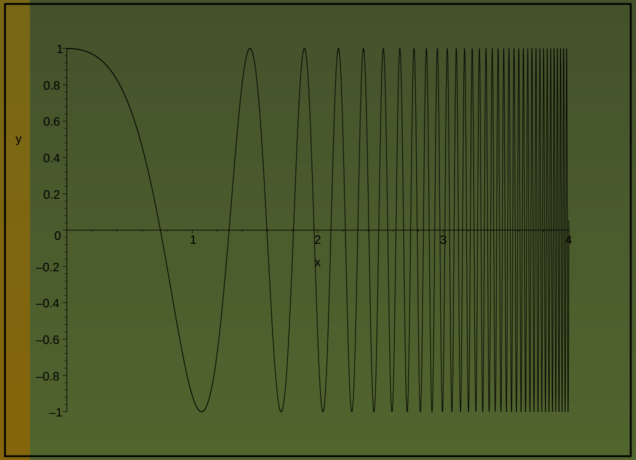

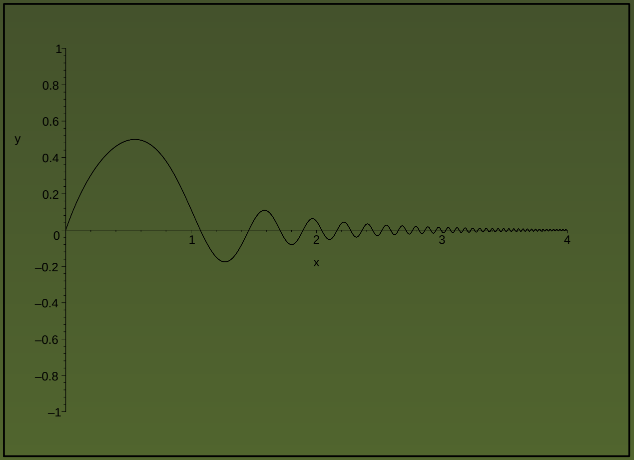

Twisted Tail - Results

Table 3: $\mathcal{I}_3 = 0.323367431677778.$

l	$\bar{S}_l$	l	$\bar{S}_l$
0	0.322 927 888 336 864	6	0.323 367 431 645 417
1	0.323 237 526 926 992	7	0.323 367 431 679 447
2	0.323 365 916 051 665	8	0.323 367 431 677 892
3	0.323 367 727 513 215	9	0.323 367 431 677 774
4	0.323 367 440 006 498	10	0.323 367 431 677 778
5	0.323 367 430 974 309		

$$\{x_l\}_{l=0}^{n} = \left\{ \ln(2\pi(l+2)) - \ln(\ln(2\pi(l+2))) + \frac{\ln(\ln(2\pi(l+2)))}{\ln(2\pi(l+2))} \right\}_{l=0}^{n}.$$

This sequence is derived from the asymptotic expansion of the Lambert W function defined implicitly by $w(x)\, e^{w(x)} = x$.

Airy Functions

The Airy functions $\pi\,\mathrm{Ai}(z)$ are given by:

$$\mathcal{I}_4(a,z) = \int_a^\infty \cos\left(\frac{x^3}{3} + zx\right)\,\mathrm{d}x.$$

$$w(x) = x^2 + z \;\hookrightarrow\; G_0(x) = \frac{1}{x^2+z} \quad \text{and} \quad H_0(x) = \cos\left(\tfrac{x^3}{3} + z\,x\right).$$

$$\hookrightarrow\; G_l(x) = \left(\frac{-\mathrm{d}}{(x^2+z)\,\mathrm{d}x}\right)^l \frac{1}{x^2+z} \text{ and } H_l(x) = \cos\left(\frac{x^3}{3} + zx - \frac{l\pi}{2}\right).$$

$$G_l(x) = \frac{p_l(x)}{(x^2+z)^{2l+1}} \quad \text{where} \quad p_l(x) \text{ are polynomials.}$$

It can be shown that $p_{2k+1}(0) = 0$ and $p_{2k}(0)$ exist and since $H_l(0) = 0$, the boundary terms vanish at $a = 0$ for $z \neq 0$.

Airy Functions

The integral $\mathcal{I}_4(0,z)$ then has the equivalent representations:

$$\boxed{\mathcal{I}_4(0,z) = \int_0^\infty \frac{p_n(x)}{(x^2+z)^{2n}} \cos\left(\frac{x^3}{3} + z\,x - \frac{n\,\pi}{2}\right) \mathrm{d}x}$$

How to determine the functionals $G_l(x)$ explicitly?

We can decompose $\mathcal{I}_4(a,z)$ as follows:

$$\mathcal{I}_4(a,z) = \int_a^\infty \left[\cos(zx)\cos\left(x^3/3\right) - \sin(zx)\sin\left(x^3/3\right)\right] \mathrm{d}x.$$

By choosing the weight function $w(x) = x^2$, we obtain:

$$G_l(x) = (-1)^l \left(\frac{\mathrm{d}}{x^2\,\mathrm{d}x}\right)^l x^{-2} \begin{matrix}\cos\\ \sin\end{matrix} (zx) \text{ and } H_l(x) = \begin{matrix}\cos\\ \sin\end{matrix} \left(\frac{x^3}{3} - \frac{l\pi}{2}\right).$$

The Slevinsky-Safouhi formula I with $(\alpha,\beta,m,n) = (2,2,0,0)$:

$$G_l(x) = \frac{(-1)^l}{x^{3l+2}} \sum_{i=0}^{l} A_l^i\,(z\,x)^i \begin{matrix}\cos\\ \sin\end{matrix} \left(zx + \frac{i\pi}{2}\right).$$

Airy Functions - Results

Ultimately, we derive the explicit form of the transformed integrals as:

$$\begin{aligned}\mathcal{I}_4(a,z) \;=\; & \sum_{l=0}^{n-1} \frac{(-1)^{l+1}}{x^{3l+2}} \sum_{i=0}^{l} A_l^i (zx)^i \cos\left(\frac{x^3}{3} + zx - (l+1-i)\pi/2\right)\Bigg|_a \\ & + (-1)^n \int_a^\infty \sum_{i=0}^{n} \frac{A_n^i (zx)^i}{x^{3n}} \cos\left(\frac{x^3}{3} + zx - (n-i)\pi/2\right) \mathrm{d}x.\end{aligned}$$

Table 4: $\mathcal{I}_4(0,1) \;=\; 0.425033661174960$. $x_l = \sqrt[3]{6\pi(l+1)}$.

l	$\bar{S}_l$	l	$\bar{S}_l$
0	0.432 683 511 614 577	6	0.425 033 661 201 175
1	0.425 050 712 855 878	7	0.425 033 661 169 297
2	0.425 018 211 967 205	8	0.425 033 661 174 750
3	0.425 032 964 456 715	9	0.425 033 661 174 971
4	0.425 033 674 972 581	10	0.425 033 661 174 961
5	0.425 033 663 440 207	11	0.425 033 661 174 960

Part II

An Algorithm for
The $G_n^{(1)}$ Transformation
&
Computation of
Incomplete Bessel Functions

The $G_n^{(m)}$ Transformation

Let $f(x)$ be integrable on $[0,\infty)$ and if:

$$f(x) = \sum_{k=1}^{m} p_k(x)\, f^{(k)}(x) \;\; \text{where} \;\; p_k(x) \sim x^{i_k} \sum_{i=0}^{\infty} \frac{a_i}{x^i} \text{ as } x \to \infty, \;\; i_k \le k.$$

Levin and Sidi, 1981:

$$\int_0^\infty f(t)\mathrm{d}t \approx \int_0^x f(t)dt + \sum_{k=0}^{m-1} f^{(k)}(x) x^{\sigma_k} \sum_{i=0}^{n-1} \frac{\beta_{i,k}}{x^i}.$$

The approximation $G_n^{(m)}$ of $\int_0^\infty f(t)\mathrm{d}t$ is given by [Gray and Wang, 1992]:

$$\frac{\mathrm{d}^l}{\mathrm{d}x^l}\left\{ G_n^{(m)} = \int_0^x f(t)\,\mathrm{d}t + \sum_{k=0}^{m-1} x^{\sigma_k} f^{(k)}(x) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x^i} \right\}, \; 0 \le l \le mn,$$

where it is assumed that $\frac{\mathrm{d}^l}{\mathrm{d}x^l} G_n^{(m)} \equiv 0, \forall l > 0.$

The $G_n^{(1)}$ Transformation

By considering the equation with $l = 0$:

$$G_n^{(1)} = F(x) + x^{\sigma_0} f(x) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{0,i}}{x^i}, \qquad F(x) = \int_0^x f(t)\,\mathrm{d}t,$$

and by isolating the summation on the RHS, we obtain:

$$\frac{G_n^{(1)} - F(x)}{x^{\sigma_0} f(x)} = \sum_{i=0}^{n-1} \frac{\bar{\beta}_{0,i}}{x^i} \implies \left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)\left(\frac{G_n^{(1)} - F(x)}{x^{\sigma_0} f(x)}\right) = \sum_{i=1}^{n-1} \frac{-i\,\bar{\beta}_{0,i}}{x^{i-1}}.$$

If we apply $\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n$, we obtain:

$$\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{G_n^{(1)} - F(x)}{x^{\sigma_0} f(x)}\right) = 0 \implies G_n^{(1)} = \frac{\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{F(x)}{x^{\sigma_0} f(x)}\right)}{\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{1}{x^{\sigma_0} f(x)}\right)} = \frac{\mathcal{N}_n(x)}{\mathcal{D}_n(x)}.$$

Incomplete Bessel functions

We begin with:

$$K_\nu(x,y) = x^\nu \int_x^\infty \frac{e^{-t-xy/t}}{t^{\nu+1}}\,\mathrm{d}t.$$

The integrands $f_{x,y,\nu}(t) = f(t) = \dfrac{e^{-t-xy/t}}{t^{\nu+1}}$. We have:

$$f(t) = \frac{-t^2}{t^2 - x\,y + (\nu+1)\,t}\,f'(t).$$

Programming the approximation $G_1^{(1)}$ of $\displaystyle\int_0^\infty \frac{e^{-t-xy/t}}{t^{\nu+1}}\,\mathrm{d}t$, we obtain:

$$G_1^{(1)} = x^\nu \frac{\mathcal{N}_1(x)}{\mathcal{D}_1(x)} = \frac{x\,e^{-x-y}}{x^2 - x\,y + (\nu+1)\,x} \underline{+ x^\nu \int_0^x \frac{e^{-t-xy/t}}{t^{\nu+1}}\mathrm{d}t.}$$

We then extract the approximation to the functions $K_\nu(x,y)$:

$$\tilde{G}_1^{(1)} = \frac{x\,e^{-x-y}}{x^2 - x\,y + (\nu+1)\,x}.$$

Incomplete Bessel functions

The approximations to $K_\nu(x,y)$ take the form:

$$\tilde{G}_n^{(1)} = x^\nu \, \frac{\widetilde{\mathcal{N}}_n(x)}{\mathcal{D}_n(x)}.$$

The Leibniz product rule and the Slevinsky-Safouhi formula I with $(\alpha, \beta, m, n) = (-2, -\nu - 1, 0, 0)$ lead at:

$$\begin{aligned}
\mathcal{D}_n(x) &= \left(t^2 \frac{\mathrm{d}}{\mathrm{d}t} \right)^n \left(t^{\nu+1} e^{t+xy/t} \right) \Big|_{t=x} \\
&= (-x\,y)^n \, x^{\nu+1} \, e^{x+y} \sum_{r=0}^{n} \binom{n}{r} (-y)^{-r} \sum_{i=0}^{r} A_r^i \, x^i. \\
\widetilde{\mathcal{N}}_n(x) &= \frac{e^{-x-y}}{x^\nu \, y} \sum_{r=1}^{n} \binom{n}{r} D_{n-r}(x, y, \nu) \, (x\,y)^r \\
&\qquad \times \sum_{s=0}^{r-1} \binom{r-1}{s} y^{-s} \sum_{i=0}^{s} A_s^i (-x)^i.
\end{aligned}$$

Numerical Results

Table 5: Numerical Results.

x	y	ν	$K_\nu(x,y)$	n	Error	n	Error
.01	4	0	.222531076126646(1)	10	.57(-10)	21	.88(-15)
.01	4	1	.213894166822940(0)	7	.96(-10)	17	.36(-15)
.01	4	2	.545034697997010(-1)	5	.78(-10)	13	.31(-15)
.01	4	3	.232531215077077(-1)	6	.21(-11)	9	.75(-15)
.01	4	4	.130427509960796(-1)	7	.21(-11)	9	.13(-16)
.01	4	5	.856753499064864(-2)	8	.31(-11)	10	.52(-17)
.01	4	6	.620867680660073(-2)	9	.66(-11)	11	.10(-16)
.01	4	7	.480108523817746(-2)	10	.19(-10)	12	.34(-16)
.01	4	8	.388407204962680(-2)	11	.72(-10)	13	.11(-15)
.01	4	9	.324679800314839(-2)	13	.62(-12)	14	.58(-15)
4.95	5	2	.122499879970633(-4)	16	.27(-10)	22	.63(-15)
10.00	2	6	.415004594191625(-6)	4	.29(-10)	10	.17(-15)
3.10	2.6	5	.528504325243644(-3)	12	.62(-10)	27	.49(-15)

Some Conclusions

- Part I – Generalized S_n transformation:
  - Expansions of some challenging integrals.
  - Integrals representations with better convergence properties.
  - Generally applicable to a wide class of integrals.
  - The staircase algorithm allow for accurate numerical evaluation.

- Part II – The $G_n^{(1)}$ transformation:
  - The Slevinsky-Safouhi formula I for higher order derivatives allows for rapid evaluation of high-order $G_n^{(1)}$ transformations.
  - Accurate computation of the challenging incomplete Bessel functions.

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