# Generalized Techniques in Numerical Integration


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# The plan

- Introduction and Motivation
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# Introduction & Motivation

Integration by parts is one of the most popular techniques in the analysis of integrals and is one of the simplest method to generate asymptotic expansions of integrals.

The product of the technique is usually a divergent series formed from evaluating boundary terms and a remaining integral:

$$\begin{aligned} \text{Initial Integral} &= \sum \text{Boundary Terms} \\ &\pm \text{A Transformed Integral.} \end{aligned}$$

Due to the successive differentiation and anti-differentiation required to form the series or the remaining integral, the technique is difficult to apply to problems more complicated than the simplest.

In this contribution, we explore a generalized and formalized integration by parts to create equivalent representations to some challenging integrals.

Integrating by parts the Euler integral $\mathrm{Ei}(x)$ where $x$ is real and positive, leads to:

$$\begin{aligned}\int_x^\infty \frac{e^{-t}}{t}\,\mathrm{d}t &= \frac{e^{-x}}{x}\sum_{n=0}^{N}(-1)^n\,\frac{n!}{x^n} + (-1)^N\,N!\int_x^\infty \frac{e^{-t}}{t^{N+1}}\,\mathrm{d}t \\ &= S_N(x) + R_N(x).\end{aligned}$$

We set $S_n(x)$ to be the partial sum of the first $n$ terms:

$$S_n(x) = e^{-x}\left(\frac{1}{x} - \frac{1}{x^2} + \ldots + \frac{(-1)^{n-1}\,(n-1)!}{x^n}\right),$$

For large $n$, the magnitude of the $n^{\mathrm{th}}$ term of $S_n(x)$ increases as $n$ increases. The infinite series for which $S_n(x)$ is the partial sum is then divergent for any fixed $x$.

$R_n(x)$ which we set to be the remainder after $n$ terms:

$$R_n(x) = (-1)^n \, n! \int_x^\infty \frac{e^{-t}}{t^{n+1}} \, dt \qquad \text{is unbounded as} \quad n \to \infty.$$

If we let $x$ become large and consider $N$ fixed, then:

$$|R_N(x)| = \left| (-1)^N \, N! \int_x^\infty \frac{e^{-t}}{t^{N+1}} \, dt \right| < \frac{N!}{x^{N+1}} e^{-x} \to 0 \quad \text{as} \quad x \to \infty.$$

Note that $\dfrac{N!}{x^{N+1}} e^{-x}$ is the $(N+1)^{\text{th}}$ term of the series $S_n(x)$.

Note also that the ratio of $R_N(x)$ to the last term in $S_N(x)$ is:

$$\left| \frac{R_N(x)}{(-1)^{N-1} \, e^{-x} \, (N-1)!/x^{-N}} \right| < \frac{N}{x} \to 0 \quad \text{as} \quad x \to \infty.$$

# Asymptotic Series / Divergent Series

Integrating by parts the Euler integral leads to the Euler series:

$$\int_x^{\infty} \frac{e^{-t}}{t} \mathrm{d}t \quad \sim \quad \frac{e^{-x}}{x} \sum_{n=0}^{\infty} (-1)^n \frac{n!}{x^n} \quad \text{as} \quad x \to \infty.$$

The key distinction here is the order in which the limits are taken:

- The series would be convergent if $\lim_{n\to\infty} R_n(x) = 0$ for fixed $x > 1$.
- The series is asymptotic since $\lim_{x\to\infty} R_N(x) = 0$ for fixed $N$.

From a computational or numerical point of view asymptotic/divergent expansions are preferred over convergent series.

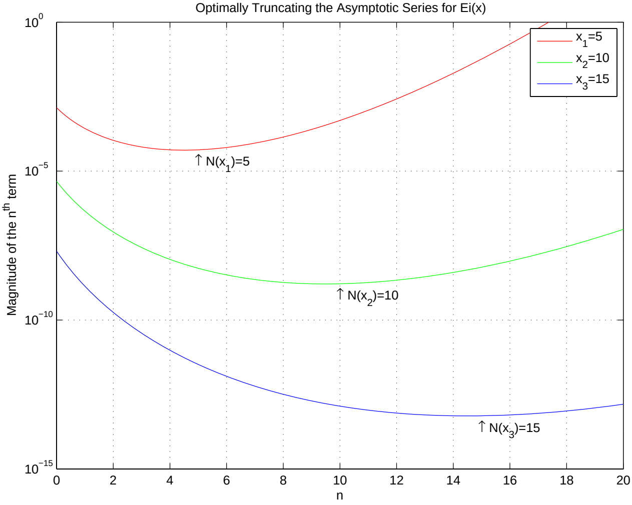
To illustrate the advantages of asymptotic series, we list values of $S_n(x)$ for $n = 0, 1, 2, \ldots$ for $x = 5, 10, 15$.

Table: Partial sums $S_n(x)$ for $x = 5, 10, 15$.

| $n$ | $x = 5$ | $x = 10$ | $x = 15$ |
|---|---|---|---|
| 0 | 1.3475893998(-3) | 4.53999297624(-6) | 2.03934880334(-8) |
| 1 | 1.0780715198(-3) | 4.08599367862(-6) | 1.90339221645(-8) |
| 2 | 1.1858786718(-3) | 4.17679353814(-6) | 1.92151976137(-8) |
| 3 | 1.1211943806(-3) | 4.14955358029(-6) | 1.91789425239(-8) |
| 4 | 1.1729418136(-3) | 4.16044956343(-6) | 1.91886105478(-8) |
| 5 | **1.1211943806(-3)** | 4.15500157186(-6) | 1.91853878732(-8) |
| 6 | 1.1832913001(-3) | 4.15827036680(-6) | 1.91866769430(-8) |
| 7 | 1.0963556128(-3) | 4.15598221034(-6) | 1.91860753771(-8) |
| 8 | 1.2354527126(-3) | 4.15781273551(-6) | 1.91863962123(-8) |
| 9 | 9.8507793300(-4) | 4.15616526286(-6) | 1.91862037112(-8) |
| 10 | 1.4858274922(-3) | **4.15781273551(-6)** | 1.91863320452(-8) |
| 11 | 3.8417846196(-4) | 4.15600051559(-6) | 1.91862379336(-8) |
| 12 | 3.0281361345(-3) | 4.15817517949(-6) | 1.91863132229(-8) |
| 13 | -3.8461538141(-3) | 4.15534811642(-6) | 1.91862479721(-8) |
| 14 | 1.5401858042(-2) | 4.15930600472(-6) | 1.91863088728(-8) |
| 15 | -4.2342177526(-2) | 4.15336917227(-6) | **1.91862479721(-8)** |
| 16 | 1.4243873629(-1) | 4.16286810419(-6) | 1.91863129329(-8) |
| $\mathrm{Ei}(x)$ | 1.1482955912(-3) | 4.15696892968(-6) | 1.91862789214(-8) |

# Asymptotic Series / Divergent Series

Here, we plot the magnitude of the $n^{\text{th}}$ term as a function of $n$.



The series we found for $\mathrm{Ei}(x)$ is called an **asymptotic series**.

The most accurate way to compute $\mathrm{Ei}(x)$ for a given $x$ is to terminate the summation when the first term found to be greater than the previous one is obtained.

The ratio of the $(n+1)^{\mathrm{th}}$ to the $n^{\mathrm{th}}$ term in $S_n(x)$ is given by:

$$\left| \frac{(-1)^n \, n! \, x^{-(n+1)} \, e^{-x}}{(-1)^{n-1} \, (n-1)! \, x^{-n} \, e^{-x}} \right| = \frac{n}{x}.$$

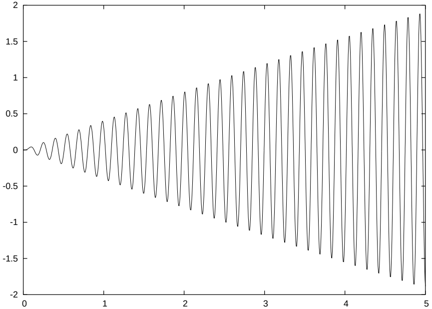
In order to obtain the best approximation for $\mathrm{Ei}(x)$, $n$ must be taken to be the largest integral part of the given $x$.

# Integration by Parts & Transformed Integrals

Let us consider:

$$\int_0^{+\infty} g(x)\, j_\lambda(vx)\,\mathrm{d}x \quad \text{where} \quad g(x) = x^{n_x} \frac{\hat{k}_\nu\left(R\sqrt{a+b\,x^2}\right)}{\left(\sqrt{a+b\,x^2}\right)^m},$$

$$j_n(z) = (-z)^n \left(\frac{\mathrm{d}}{z\mathrm{d}z}\right)^n \left[\frac{\sin(z)}{z}\right], \quad \hat{k}_{n+\frac{1}{2}}(z) = \frac{z^n}{e^z}\sum_{j=0}^{n}\frac{(n+j)!}{j!(n-j)!}\frac{1}{(2z)^j},$$



# Integration by Parts & Transformed Integrals

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

Integration by parts with respect to the operator $\underline{x\,\mathrm{d}x}$:

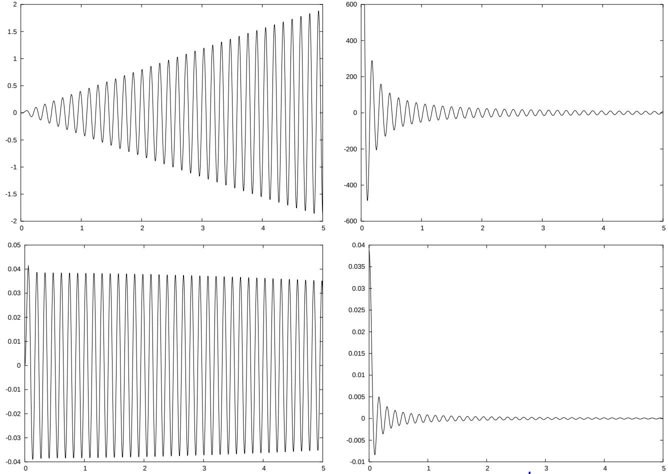
$$\begin{aligned} \int_0^{+\infty} g(x)\, j_\lambda(x)\, \mathrm{d}x \quad &= \quad (-1)^\lambda\, x^{\lambda-1}\, g(x) \left( \frac{\mathrm{d}}{x\mathrm{d}x} \right)^{\lambda-1} \left( \frac{\sin(x)}{x} \right) \Bigg|_0^{+\infty} \\ &+ (-1)^{\lambda-1} \int_0^{+\infty} \left[ \left( \frac{\mathrm{d}}{x\mathrm{d}x} \right) \left( x^{\lambda-1}\, g(x) \right) \right] \left[ \left( \frac{\mathrm{d}}{x\mathrm{d}x} \right)^{\lambda-1} \left( \frac{\sin(x)}{x} \right) \right] x\mathrm{d}x. \end{aligned}$$

Integrating by parts $\lambda$ times:

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

# Integration by Parts & Transformed Integrals

Integrands with $j_\lambda(v\,x)$ $\looparrowright\!\looparrowright$ new integrands with $\sin(v\,x)$:




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

# The Slevinsky-Safouhi formulae (SSF)

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

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

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

If we consider $x^{-3} H(x) = f(x^2)$ and apply the operator $\dfrac{\mathrm{d}}{x\mathrm{d}x}$:

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

For $T(x) = x^2\, f\,(\ln(x))$ : $\quad \left(x \dfrac{\mathrm{d}}{\mathrm{d}x}\right)^k (x^{-2}\, T(x)) = f^{(k)}\,(\ln(x))\,.$

Can we express $\left(\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^k F(x)$ in terms of $\left(\dfrac{\mathrm{d}}{x^m\mathrm{d}x}\right)^i (x^{-n} F(x))$?

# The Slevinsky-Safouhi formulae (SSF)

**Theorem** [Slevinsky & Safouhi 2009] The SSF I for any arbitrary $(\alpha, \beta, m, n)$ is given by:

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

The coefficients are given by $[N = (n-\beta-(k-1)(\alpha+1))]$:

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

Moreover, for $m \neq -1$:

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

The SSF II corresponds to the $(\alpha, \beta, m, n) = (0, 0, 1, 0)$.

# Reformulized Integration by Parts

Let $f(x)$ be integrable on $[a, b]$ and have the general form:

$$f(x) = G_0(x)H_0(x)w(x) \quad \text{with} \quad w(x) \neq 0 \ \text{ on } \ (a, b).$$

Let the functionals $G_l(x)$ and $H_l(x)$ be defined by:

$$G_l(x) = (-1)^l \left(\frac{\mathrm{d}}{w(x)\mathrm{d}x}\right)^l G_0(x) \quad \text{and} \quad H_l(x) = \left(\frac{\mathrm{d}}{w(x)\mathrm{d}x}\right)^{-l} H_0(x).$$

If $f(x) \in \mathcal{C}^m[a, b]$ then $\displaystyle\int_a^b f(x)\mathrm{d}x$ has the equivalent representation:

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

# Bessel Integral

The integral that follows appeared in Numerical Recipes:

$$\mathcal{I}_1 = \int_0^b \frac{x}{x^2+1}\, J_0(x)\,\mathrm{d}x = \int_0^\infty w(x)\, G_0(x)\, H_0(x)\,\mathrm{d}x,$$

$$w(x) = x, \quad G_0(x) = \frac{1}{x^2+1} \quad \text{and} \quad H_0(x) = J_0(x).$$

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

Using the generalized $S_n$ and SSF 1, we obtain the equivalent representations:

$$\begin{aligned} \mathcal{I}_1 &= \sum_{l=0}^{n-1} \frac{-2^l\, l!\, x^{l+1}}{(x^2+1)^{l+1}}\, J_{l+1}(x)\Big|_0^\infty + 2^n\, n! \int_a^\infty \frac{x^{n+1}}{(x^2+1)^{n+1}}\, J_n(x)\,\mathrm{d}x \\ &= 2^n\, n! \int_0^\infty \frac{x^{n+1}}{(x^2+1)^{n+1}}\, J_n(x)\,\mathrm{d}x. \end{aligned}$$

# Fresnel Integrals

The integrals are given by:

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

$$w(x) = x, \quad G_0(x) = \frac{1}{x} \quad \text{and} \quad H_0(x) = \sin(v\,x^2).$$

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

Using the generalized $S_n$ and SSF 1, we obtain the equivalent representations for $\mathcal{I}_2(a,v)$:

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

# Airy Functions

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

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

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

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

Using the generalized $S_n$ and SSF 1, we obtain:

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

# The Twisted Tail

The twisted tail proposed in *The SIAM 100-digit challenge*:

$$\mathcal{T} = \int_0^{\infty} \cos(x\,e^x)\,\mathrm{d}x = \int_0^{\infty} w(x)\,G_0(x)\,H_0(x)\,\mathrm{d}x,$$

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

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

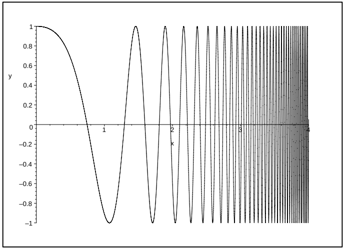
The general form of $G_l(x)$ is:

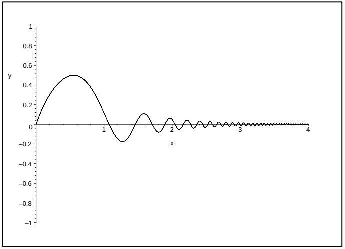
$$G_l(x) = \frac{e^{-(l+1)\,x}}{(1+x)^{2l+1}}\,p_l(x) \qquad \begin{cases} p_0(x) &= 1 \\ p_1(x) &= 2+x \\ p_2(x) &= 9+8x+2x^2 \\ p_3(x) &= 64+79x+36x^2+6x^3 \\ \vdots & \vdots \quad \vdots \end{cases}$$

# Reformulized Integration by Parts

Applying the first order transformation:

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




$\mathcal{T}$ has the equivalent representations:

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

$$+ \int_0^{\infty} \frac{p_n(x)\, e^{-nx}}{(1+x)^{2n}} \cos\left(x\, e^{x} - \frac{n\pi}{2}\right) \mathrm{d}x.$$

# Numerical Results

$\mathcal{T}$ has an asymptotic expansion given by:

$$\int_0^\infty \cos(x\, e^x)\, \mathrm{d}x \sim \sum_{l=0}^{\infty} -p_l(0)\, \cos\left((l+1)\frac{\pi}{2}\right).$$

Table: Computing the twisted tail $\mathcal{T}$ using the asymptotic expansion. Calculation performed using Maple.

| $l$ | $\mathcal{T}$ |
|---|---|
| 130 | .323 367 431 677 |
| 180 | .323 367 431 677 778 |
| 220 | .323 367 431 677 778 761 |
| 270 | .323 367 431 677 778 761 399 |
| 320 | .323 367 431 677 778 761 399 370 |
| 370 | .323 367 431 677 778 761 399 370 087 |
| 430 | .323 367 431 677 778 761 399 370 087 952 |

# The Staircase Algorithm

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

- For $a < x_0 < b$, initialize the first approximation $S_0$:

$$S_0 = \int_a^{x_0} G_0(x)\, H_0(x)\, w(x)\,\mathrm{d}x,$$

Then, we consider $\int_{x_0}^b G_0(x)\, H_0(x)\, w(x)\,\mathrm{d}x$:

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

- For $a < x_0 < x_1 < b$, we define the second approximation by:

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

Then, we consider $\int_{x_1}^{b} G_1(x)\, H_1(x)\, w(x)\, \mathrm{d}x$:

$$\int_{x_1}^{b} G_1(x)\, H_1(x)\, w(x)\, \mathrm{d}x = G_1(x)\, H_2(x)\Big|_{x_1}^{b} + \int_{x_1}^{b} G_2(x)\, H_2(x)\, w(x)\, \mathrm{d}x.$$

- For $x_1 < x_2 < b$, we define the third approximation $S_2$ by:

$$S_2 \;=\; S_1 + G_1(x)\, H_2(x)\Big|_{x_1}^{b} + \int_{x_1}^{x_2} G_2(x)\, H_2(x)\, w(x)\, \mathrm{d}x.$$

- For the sequence $\{x_l\}_{l=1}^{n}$ satisfying $x_{l-1} < x_l < b$, 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 $\int_a^b f(x)\, \mathrm{d}x$ form the sequence $\{S_l\}_{l=0}^{n}$.

# Bessel Integral

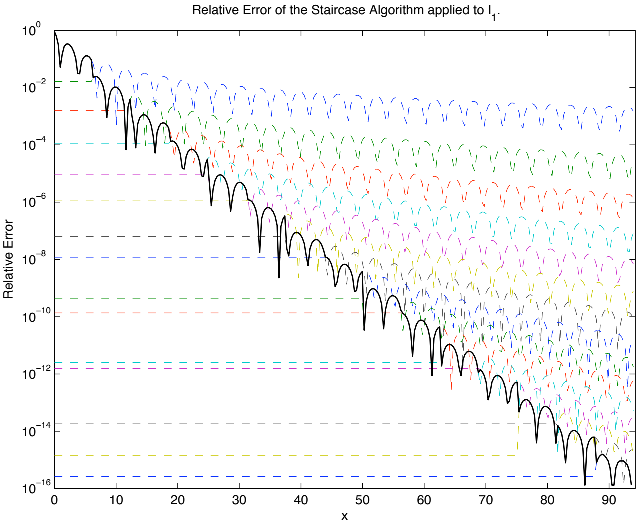



Figure: $x_l = 2\pi(l + 1)$

# Fresnel Integrals

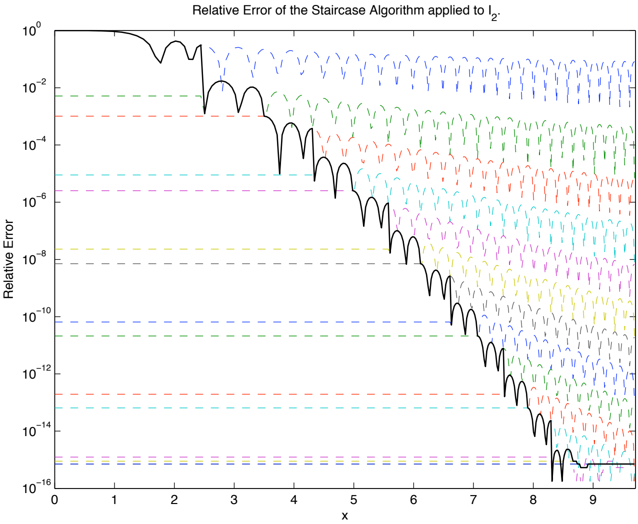



Figure: $x_l = \sqrt{2\pi(l+1)/v}$

# Airy Functions

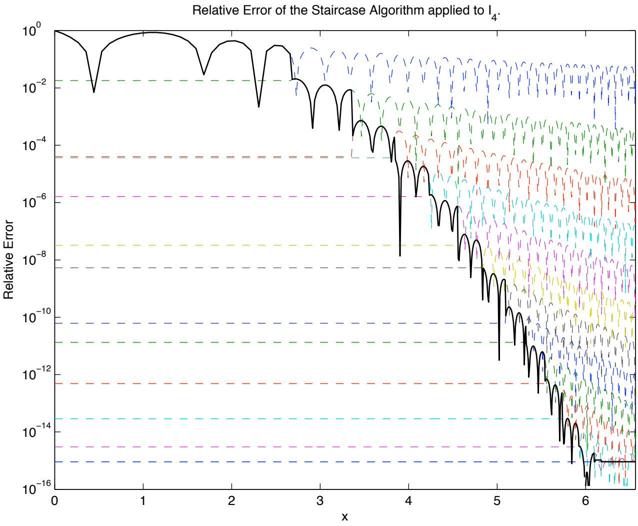



Figure: $x_l = \sqrt[3]{6\pi(l+1)}$

# Twisted Tail

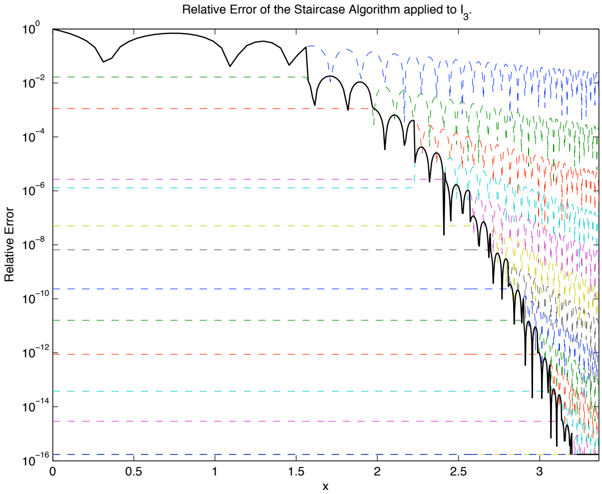



Figure: $\{x_l\}_{l=0}^{n} = \left\{ \ln(2\pi(l+2)) - \ln(\ln(2\pi(l+2))) + \frac{\ln(\ln(2\pi(l+2)))}{\ln(2\pi(l+2))} \right\}_{l=0}^{n}$

# Conclusion

- The Slevinsky-Safouhi formulae for differentiation present an important tool in numerical integration.
- Reformulized integration by parts can be very useful in numerical integration and can be applied to a larger class of integrals.
- Asymptotic expansions, more favourable from a computational point of view.
- Transformed integrals have better convergence / asymptotic properties.
- The staircase algorithm is robust and allow for accurate numerical evaluation

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**Thank you all for listening!**