The Filon – Simpson Code
or :
Numerical Integration of Highly Oscillatory Integrals

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June 1, 2006

Outline:

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2. Filon's integration formula

3. New quadrature rules for a class of oscillatory integrals

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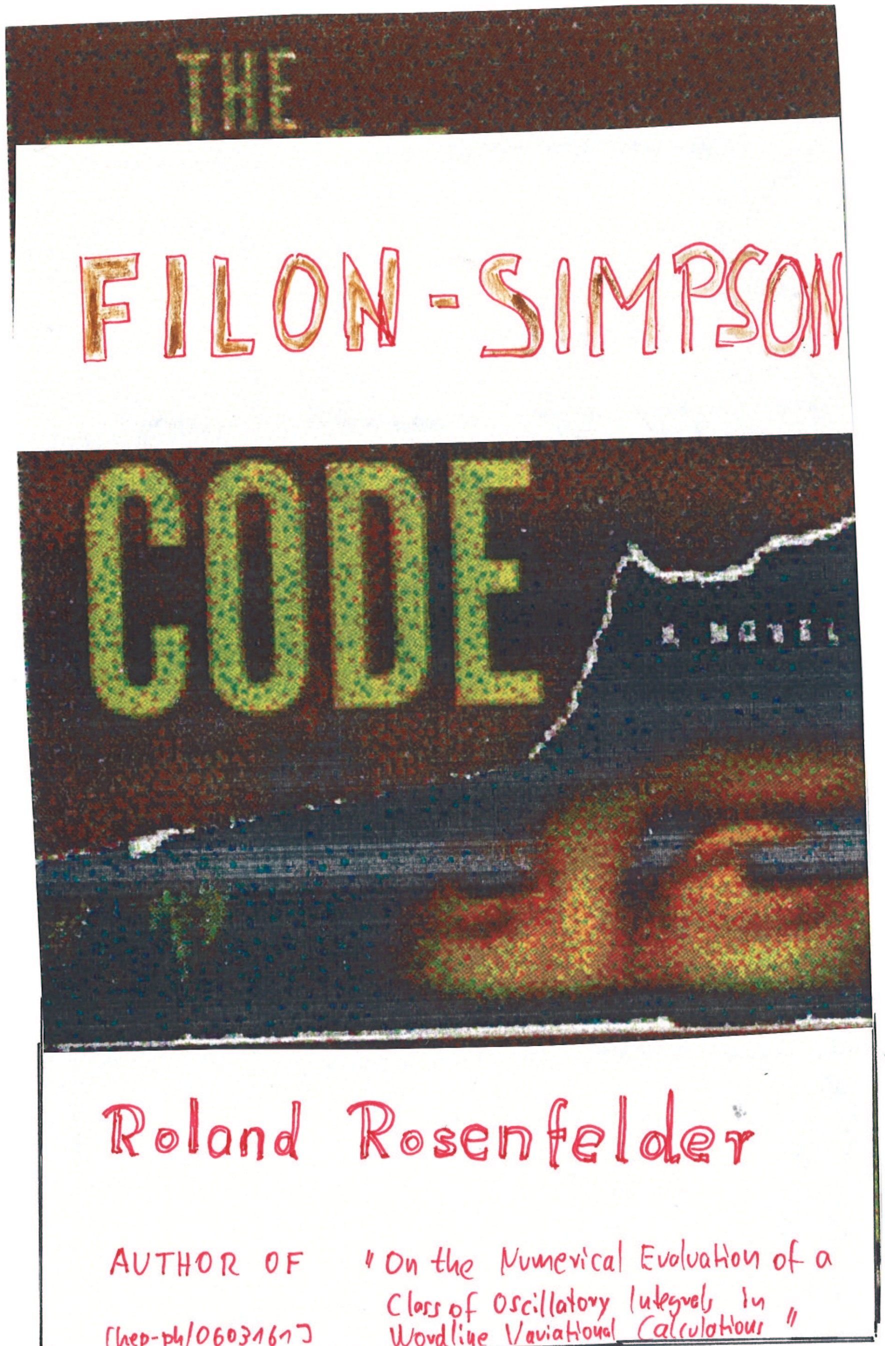
THE
FILON-SIMPSON
CODE
A NOVEL
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AUTHOR OF "On the Numerical Evaluation of a Class of Oscillatory Integrals in Worldline Variational Calculations"
[hep-ph/0603161]

1. Introduction: Simpson, Newton, Gauss, Euler

Numerical Integration:

one-dimensional	**multidimensional**	**functional**
⇓	(*aliter* ...)	(*totaliter aliter* ...)

finite limits

infinite limits

singularities of integrand

oscillatory integrands

⋮

fixed number of integration points

adaptive (automatic) integration

Some integration rules:

Trapezoidal rule ($h = x_1 - x_0 \, , f_i \equiv f\,(x_i)$)

$$\int_{x_0}^{x_1} dx \, f(x) \; = \; \frac{h}{2} \left[f_0 + f_1 \right] - \frac{h^3}{12} f''(\xi) \;\; , \;\; x_0 < \xi < x_1$$

Extended trapezoidal rule ($h = \frac{x_N - x_0}{N} \, , x_0 < \xi < x_N$)

$$\int_{x_0}^{x_N} dx \, f(x) \; = \; h \, \left[\frac{1}{2} f_0 + f_1 + \ldots + f_{N-1} + \frac{1}{2} f_N \right] - \frac{N h^3}{12} f''(\xi)$$

Simpson's rule

$$\int_{x_0}^{x_2} dx \, f(x) \; = \; \frac{h}{3} \left[f_0 + 4 f_1 + f_2 \right] - \frac{h^5}{90} f^{(4)}(\xi)$$

Extended Simpson's rule

$$\int_{x_0}^{x_{2N}} dx\, f(x) = \frac{h}{3}\Big[f_0 + 4\,(f_1 + f_3 + \ldots + f_{2N-1}) + 2\,(f_2 + f_4 + \ldots + f_{2N-2}) + f_{2N}\Big] - \frac{N h^5}{90} f^{(4)}(\xi)$$

Newton-Cotes formulas (examples)

closed type:
$$\int_{x_0}^{x_4} dx\, f(x) = \frac{2h}{45}\Big[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4\Big] - \frac{8h^7}{945} f^{(6)}(\xi)$$

open type:
$$\int_{x_0}^{x_4} dx\, f(x) = \frac{4h}{3}\Big[2f_1 - f_2 + 2f_3\Big] - \frac{28h^5}{90} f^{(4)}(\xi)$$

Gauss-Legendre integration

$$\int_{-1}^{+1} dx\, f(x) \;=\; \sum_{i=1}^{N} w_i\, f(x_i) + R_N$$

with

$$P_N(x_i) \;=\; 0\,, \;\; w_i \;=\; 2\,\frac{[P_N'(x_i)]^2}{1-x_i^2}$$

$$R_N \;=\; \frac{2^{2N+1}(N!)^2}{(2N+1)[(2N)!]^3}\, f^{(2N)}(\xi)\,, \quad -1 < \xi < +1$$

Arbitrary interval: $y = \frac{b+a}{2} + \frac{b-a}{2} x$

Different weight functions $\Longrightarrow$ Gauss-Laguerre, Gauss-Hermite etc.

Euler & tanh sinh-integration

from Borwein et al. : *Experimentation in Mathematics: Computational Paths to Discovery* (2004) p. 309

"Read Euler, read Euler ! He is the master of all of us" (Laplace)

Euler-Maclaurin summation formula

$$\int_a^b dx\, f(x) = h \sum_{i=0}^{N} f(a+ih) - \frac{h}{2}\left[f(a)+f(b)\right] - \sum_{j=1}^{m} \frac{h^{2j} B_{2j}}{(2j)!}\left[f^{(2j-1)}(b) - f^{(2j-1)}(a)\right] + R_m$$

with

$$R_m = -\frac{h^{2m+2}(b-a)B_{2m+2}}{(2m+2)!} f^{(2m+2)}(\xi)$$

When $f(x)$ **and all its derivatives vanish at the endpoints** a and b

then the error of step-function approximation to integral is R_m for **all** m

$\longrightarrow$ error goes to zero more rapidly than any power of h !

Achieved by special transformation $x = g(t)$

$$\int_{-1}^{+1} dx\, f(x) \;=\; \int_{-\infty}^{+\infty} dt\, g'(t)\, f(g(t)) \;=\; h \sum_{j=-\infty}^{+\infty} w_j\, f(x_j) + R$$

$$\text{with} \quad x_j = g(jh) \quad \text{and} \quad w_j = g'(jh)$$

For functions which are analytic in a strip $|\mathrm{Im}\, t| < d$

$$R \;=\; \mathcal{O}\left(e^{-\pi d/h}\right)$$

Recommended transformation:

$$x \;=\; \tanh\left[\,\lambda \sinh t\,\right], \qquad t \in [-\infty, +\infty]\,, \quad \lambda > 0$$

Fast convergence also for $|j| \to \infty$ since

$$w_j \quad \longrightarrow \quad 2\lambda \, \mathrm{exp} \left(-\lambda \, e^{|j| \, h} \right)$$

Examples: ($\lambda = 1$)

h	$\int_0^{\pi/2} dx \, \sin x$	$\int_0^1 dx \, (-\ln x)$	$\int_0^1 dx \, \frac{1}{2\sqrt{x}}$
1.0000	0.997 818 863 766 531	1.006 175 595 0	1.000 562 2
0.5000	0.999 999 556 735 862	0.999 999 700 1	0.999 999 5
0.2500	1.000 000 000 000 006	0.999 999 998 9	0.999 991 5
0.1250	0.999 999 999 999 999	0.999 999 990 6	0.999 978 2

2. Filon's integration formula

L. N. G. Filon: "On a quadrature formula for trigonometric integrals", Proc. Royal Soc. Edinburgh **49** (1928), 38 – 47

$$\int_{x_0}^{x_2} dx\, f(x)\, \cos xy \;=\; h \Big\{ \alpha(hy) \Big[-f_0 \sin(x_0 y) + f_2 \sin(x_2 y) \Big] + \beta(hy)\, \frac{1}{2} \Big[f_0 \cos(x_0 y) + f_2 \cos(x_2 y) \Big] + \gamma(hy)\, f_1 \cos(x_1 y) \Big\} + R$$

with

$$\alpha(\Theta) = \frac{1}{\Theta} + \frac{\sin 2\Theta}{2\Theta^2} - \frac{2\sin^2\Theta}{\Theta^3} \quad \xrightarrow{\Theta\to 0} \quad \frac{2\Theta^3}{45} + \ldots$$

$$\beta(\Theta) = 2\left(\frac{1+\cos^2\Theta}{\Theta^2} - \frac{\sin 2\Theta}{\Theta^3} \right) \quad \xrightarrow{\Theta\to 0} \quad \frac{2}{3} + \ldots$$

$$\gamma(\Theta) = 4\left(-\frac{\cos\Theta}{\Theta^2} + \frac{\sin\Theta}{\Theta^3} \right) \quad \xrightarrow{\Theta\to 0} \quad \frac{4}{3} + \ldots$$

i.e. for $y \to 0$: $\Longrightarrow$ Simpson's rule, analogous formula for $\int_{x_0}^{x_2} dx\, f(x)\, \sin xy$

How to derive this formula ?

Write

$$\int_{x_0}^{x_2} dx\, f(x)\, \cos xy \simeq w_0 f_0 + w_1 f_1 + w_2 f_2$$

and require that it is exact for polynomials x^0, x^1, x^2 .

$\Longrightarrow$ system of 3 equations for 3 unknowns

$$\sum_{i=0}^{2} w_i\, x_i^k \;=\; \int_{x_0}^{x_2} dx\, x^k \cos(xy) \;=:\; J_k\,, \quad k = 0, 1, 2, \text{ elementary integrals !}$$

Result:

$$\begin{aligned}
w_0 &= \frac{1}{2h^2}\left[\, x_1\, x_2\, J_0 - (x_1 + x_2)\, J_1 + J_2 \,\right] \\
w_1 &= \frac{1}{2h^2}\left[\, -2x_0\, x_2\, J_0 + 4\, x_1\, J_1 - 2J_2 \,\right] \\
w_2 &= \frac{1}{2h^2}\left[\, x_0\, x_1\, J_0 - (x_0 + x_1)\, J_1 + J_2 \,\right]
\end{aligned}$$

Asymptotic behaviour for $y \to \infty$:

exact:

$$\int_{x_0}^{x_2} dx\, f(x)\, \cos(xy) \quad = \quad f(x)\, \frac{\sin(xy)}{y}\Big|_{x_0}^{x_2} - \frac{1}{y} \int_{x_0}^{x_2} dx\, f'(x)\, \sin(xy)$$

$$\stackrel{y \to \infty}{\longrightarrow} \quad \frac{1}{y} \Big[f_2 \sin(x_2 y) - f_0 \sin(x_0 y) \Big] + \mathcal{O}\left(\frac{\cos}{y^2} \right)$$

Filon:

$$\stackrel{y \to \infty}{\longrightarrow} \; h \Big\{ \underbrace{\alpha(hy)}_{\to 1/(hy)} \Big[-f_0 \sin(x_0 y) + f_2 \sin(x_2 y) \Big] + \ldots \Big\}$$

is correct since the endpoints are included in quadrature formula !

3. New quadrature rules for a class of oscillatory integrals

"In mathematics, I recognize true scientific value only in concrete truths, or to put it more pointedly, only in mathematical (computations)" (Kronecker)

Motivation:

Worldline variational approach to QFT: describe relativistic particles by their worldlines $x_\mu(t)$, $t =$ proper time and not by fields $\Phi(x)$

Quadratic trial action $S_t \sim \int dt \int dt' \, \dot{x}(t) \, A(t-t') \, \dot{x}(t')$
+ Feynman-Jensen variational principle $\langle \exp(-\Delta S) \rangle \geq \exp(-\langle \Delta S \rangle)$

$\Longrightarrow$ pair of non-linear variational equations for

$$A(E) = 1 + \text{const.} \frac{1}{E^2} \int_0^\infty d\sigma \, \frac{\delta V}{\delta \mu^2(\sigma)} \sin^2 \left(\frac{E\sigma}{2} \right) \qquad \text{"profile function"}$$

$$\mu^2(\sigma) \sim \int_0^\infty dE \, \frac{1}{A(E)} \frac{\sin^2(E\sigma/2)}{E^2} \qquad \text{"pseudotime"}$$

$$V[\mu^2] \sim \langle S_I \rangle$$

is the interaction term averaged over the trial action, specific for the field theory under consideration,

$$\frac{\delta V[\mu^2]}{\delta \mu^2(\sigma)} \xrightarrow{\sigma \to 0} \frac{\text{const.}}{\sigma^{2+r}}$$

the "force" ($r = 0$ for super-renormalizable, $r = 1$ for renormalizable theories)

$$\mu^2(\sigma = t - t') \sim \left\langle \left(x(t) - x(t') \right)^2 \right\rangle \quad \text{mean square displacement}$$

$$\frac{d\mu^2(\sigma)}{d\sigma} \sim \int_0^\infty dE \, \frac{1}{A(E)} \frac{\sin(E\sigma)}{E} \qquad \text{mean "velocity" (also needed for QED)}$$

Large-E, σ limit of $A(E)$ and $\mu^2(\sigma)$ may be obtained analytically

$\Longrightarrow$ restriction to finite integration limits , add the analytically calculated asymptotic contribution to the numerical result

Therefore consider

$$I_1[f](a,b,y) \quad := \quad \int_a^b dx\, f(x)\, \frac{\sin(xy)}{xy}$$

$$I_2[f](a,b,y) \quad := \quad \int_a^b dx\, f(x)\, 4\, \frac{\sin^2(xy/2)}{x^2 y^2}$$

i.e.

$$I_j[f](a,b,y) \; = \; \int_a^b dx\, f(x)\, O_j(xy)\,, \quad O_j(0) \; = \; 1$$

Numerical evaluation of Fourier integrals with infinite upper limits is much more demanding: see NAG routine D01ASF based on strategy in:

Piessens et al.: *QUADPACK, A Subroutine Package for Automatic Integration*, Springer (1983)

requires a delicate extrapolation procedure, not suitable for a numerical solution of the variational equations

"As long as right methods are used, quadrature of highly-oscillatory integrals is very accurate and affordable !" (A. Iserles)

strategy: Choose N points $x_i^{(j)}$ in the interval $[a, b]$, two of them identical with the endpoints and require that the integral over $x^k O_j(xy)$ is exact.

For simplification: $N = 2$, equally spaced points $x_i = a + ih$

$\Longrightarrow$ as in Filon's case

$$w_0^{(j)} = \frac{1}{2h^2}\left[x_1\,x_2\,J_0^{(j)} - (x_1 + x_2)\;J_1^{(j)} + J_2^{(j)}\right]$$
$$w_1^{(j)} = \frac{1}{2h^2}\left[-2x_0\,x_2\,J_0^{(j)} + 4\,x_1\,J_1^{(j)} - 2J_2^{(j)}\right]$$
$$w_2^{(j)} = \frac{1}{2h^2}\left[x_0\,x_1\,J_0^{(j)} - (x_0 + x_1)\;J_1^{(j)} + J_2^{(j)}\right]$$

but now moments involve **special functions**

$$J_k^{(j)} = \frac{1}{y^{k+1}}\left[F_k^{(j)}(by) - F_k^{(j)}(ay)\right]$$
$$\text{with } F_k^{(j)}(z) = \int_0^z dt\, t^k\, O_j(t)$$

We have

$$
\begin{aligned}
F_0^{(1)}(z) &= \mathrm{Si}(\mathrm{z})\,,\ \mathrm{F}_1^{(1)}(\mathrm{z}) = 1-\cos\mathrm{z}\,,\ \mathrm{F}_2^{(1)}(\mathrm{z}) = \sin\mathrm{z} - \mathrm{z}\cos\mathrm{z} \\
F_0^{(2)}(z) &= 2\left[\mathrm{Si}(\mathrm{z}) - \frac{1-\cos z}{z}\right]\,,\ F_1^{(2)}(z) = 2\left[\gamma + \ln z - \mathrm{Ci}(\mathrm{z})\right]\,, \\
F_2^{(2)}(z) &= 2\left[z - \sin z\right]
\end{aligned}
$$

with $\gamma = 0.5772156640\ldots$ (Euler's constant) and

$$
\begin{aligned}
\mathrm{Si}(\mathrm{z}) &:= \int_0^z dt\,\frac{\sin t}{t} && \textbf{Sine integral} \\
\mathrm{Ci}(\mathrm{z}) &:= \gamma + \ln z + \int_0^z dt\,\frac{\cos t - 1}{t} && \textbf{Cosine integral}
\end{aligned}
$$

$y \to 0$: obtain Simpson weights $\Longrightarrow$
new quadrature rules may be called **Filon-Simpson** rules

Divide $[a, b]$ in N intervals and apply FS-rules in each interval
$\Longrightarrow$ **Extended** **Filon-Simpson** quadrature rules

Asymptotic behaviour for $y \to \infty$:

Exact:

$$I_1[f](a=0,b,y) \quad \stackrel{y\to\infty}{\longrightarrow} \quad \frac{\pi f(0)}{2y} + \frac{1}{y^2}\left[f'(0) - f(b)\frac{\cos yb}{b}\right] + \mathcal{O}\left(\frac{\sin by}{y^3}\right)$$

$$I_2[f](a=0,b,y) \quad \stackrel{y\to\infty}{\longrightarrow} \quad \frac{\pi f(0)}{y} + \frac{2}{y^2}\left[\, f'(0)\, \ln y + C(b)\,\right] + \mathcal{O}\left(\frac{\sin by}{y^3}\right)$$

with

$$C(b) \;=\; (\,\gamma + \ln b\,)\; f'(0) - \frac{f(0)}{b} + \int_0^b dx\, \frac{f(x) - f(0) - x f'(0)}{x^2}$$

Filon-Simpson rules:

give the exact **asymptotic** and the correct (for $h \to 0$) **sub-asymptotic** behaviour – including the logarithmic terms !

4. Results

Test functions

$$f_l \; = \; x^l e^{-x} \;\; , \quad l = 0, 1$$

upper limit of integration $= 20$
asymptotic contribution obtained analytically and added

Need fast & reliable routine for Sine & Cosine integral

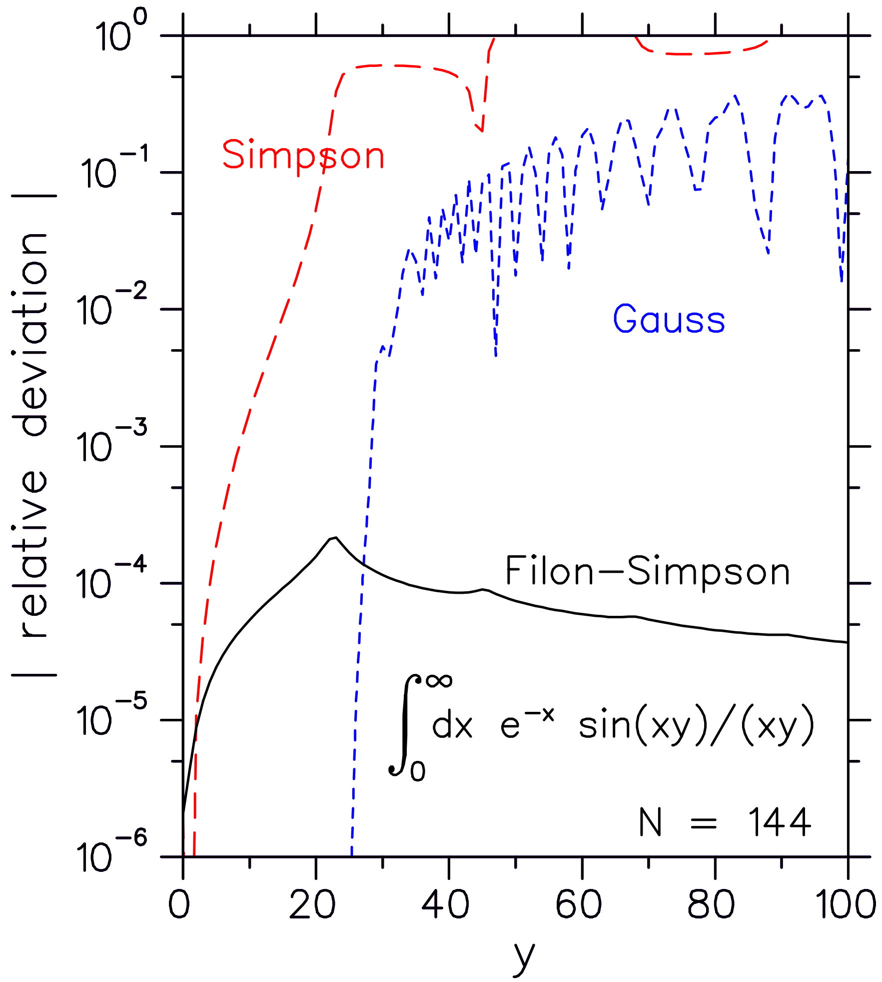
Use expansion in **Chebyshev polynomials** $T_n(x) = \cos(n \arccos(x))\, , \;\; |x| < 1$,
e.g. for $x \le 8$

$$\begin{aligned} \mathrm{Si}(x) &= \sum_{n=0} b_n \, T_{2n+1} \left(\frac{x}{8} \right) \\ \mathrm{Ci}(x) &= \gamma + \ln x - \sum_{n=0} a_n \, T_{2n} \left(\frac{x}{8} \right) \end{aligned}$$

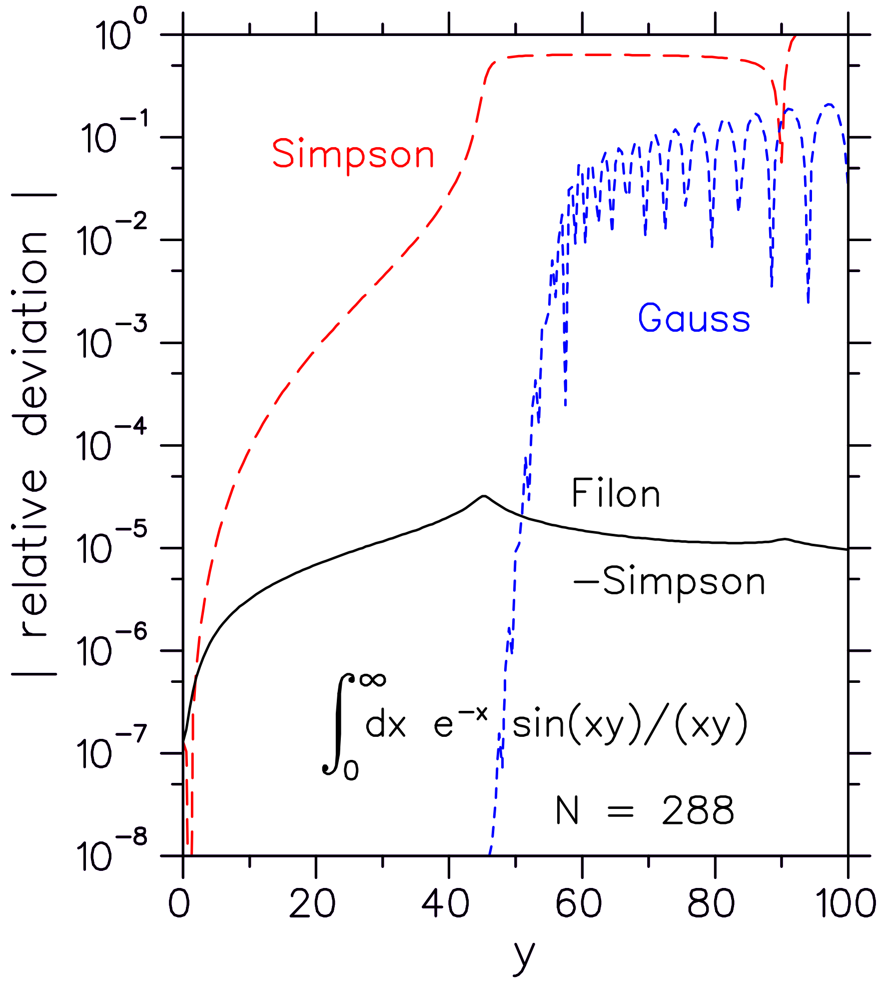
and similar expansions for $x \ge 8$

Y. L. Luke: *The Special Functions and Their Approximations*, vol. II, Academic Press (1969), p. 325

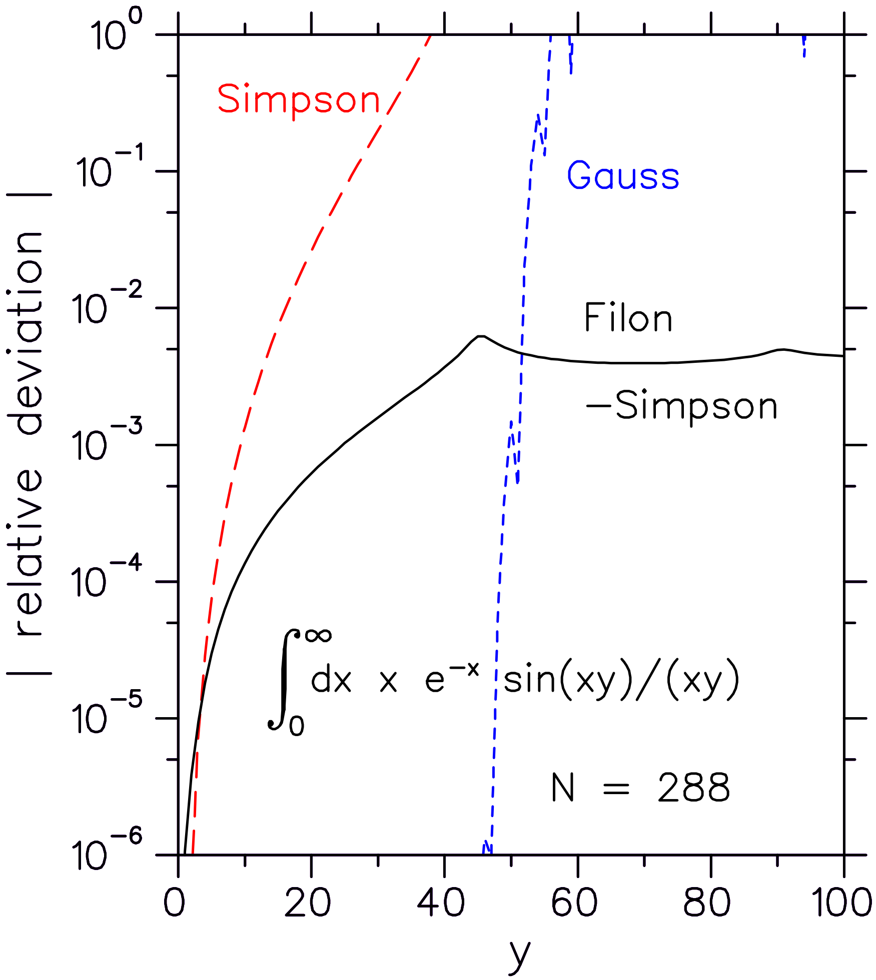
n	b_n
0	1.95222 09759 53071 08224
1	-0.68840 42321 25715 44408
2	0.45518 55132 25584 84126
3	-0.18045 71236 83877 85342
4	0.04104 22133 75859 23964
5	-0.00595 86169 55588 85229
6	0.00060 01427 41414 43021
7	-0.00004 44708 32910 74925
8	0.00000 25300 78230 75133
9	-0.00000 01141 30759 30294
10	0.00000 00041 85783 94210
11	-0.00000 00001 27347 05516
12	0.00000 00000 03267 36126
13	-0.00000 00000 00071 67679
14	0.00000 00000 00001 36020
15	-0.00000 00000 00000 02255
16	0.00000 00000 00000 00033



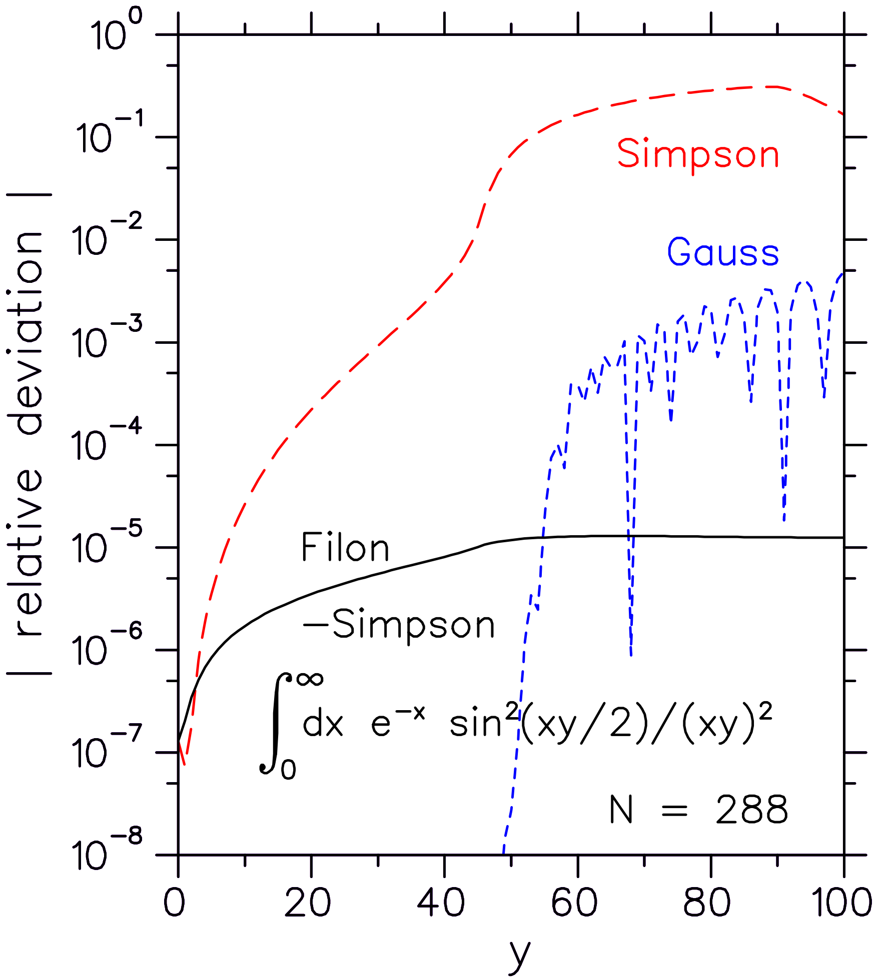
| relative deviation |
y
Simpson
Gauss
Filon–Simpson
$\int_0^\infty dx\ e^{-x}\ \sin(xy)/(xy)$
N = 144

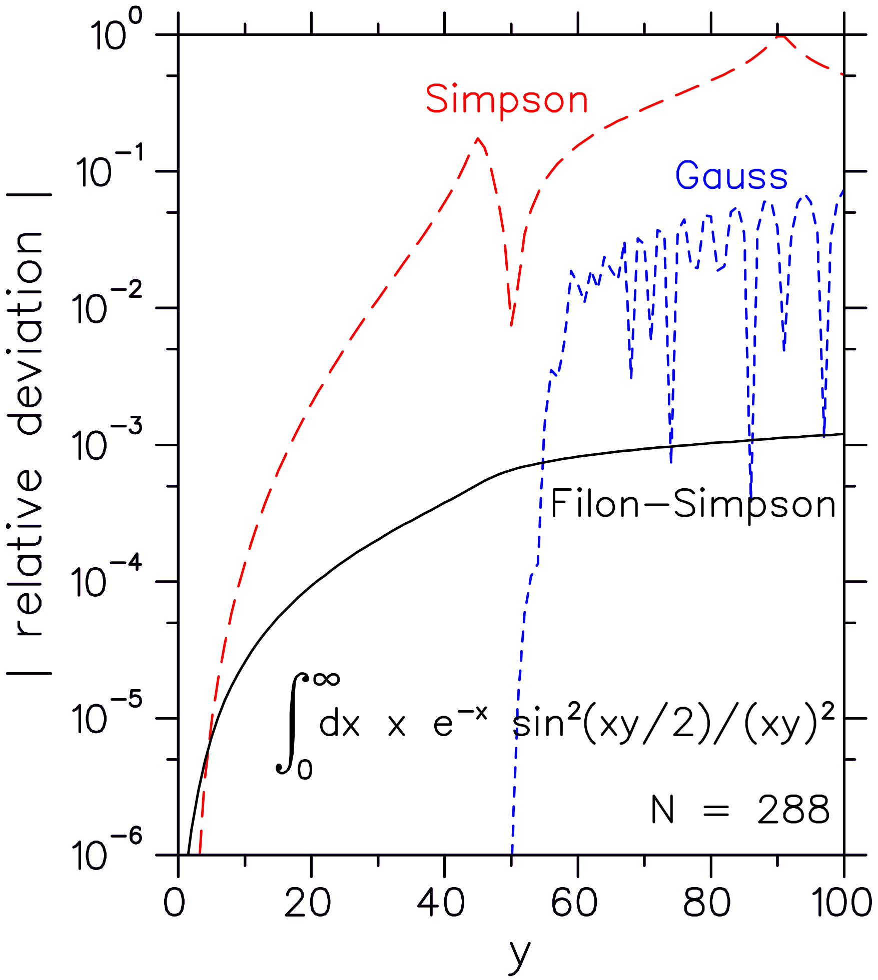


| relative deviation |
y
Simpson
Gauss
Filon
−Simpson
$\int_0^\infty dx\ e^{-x} \sin(xy)/(xy)$
N = 288



| relative deviation |
Simpson
Gauss
Filon
−Simpson
$\int_0^\infty dx\ x\ e^{-x}\ \sin(xy)/(xy)$
N = 288
y
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
0
20
40
60
80
100


| relative deviation |
y
Simpson
Gauss
Filon
−Simpson
$\int_0^\infty dx\ e^{-x}\ \sin^2(xy/2)/(xy)^2$
N = 288
10^0
10^−1
10^−2
10^−3
10^−4
10^−5
10^−6
10^−7
10^−8
0
20
40
60
80
100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10^0
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10^{-6}
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20
40
60
80
100

5. Summary

- Oscillatory integrals can be calculated precisely & reliably for **all** values of the frequency by Filon-type rules **if** the endpoints are included

- Filon-Simpson rules have been derived for particular weight functions $O_j(xy)$ which have removable ("hebbare") singularities

$$\int_{x_0}^{x_N} dx\, f(x)\, O_j(xy) \simeq \sum_{i=0}^{N} w_i^{(j)}(x_0, h; y)\, f(x_i)\ , \quad h \equiv \frac{x_N - x_0}{N}$$

$$O_j = j^2 \frac{\sin^j(xy/j)}{(xy)^j}\ , \quad j = 1, 2$$

- Exact for $y \to \infty$!

- Increase accuracy by applying **extended** Filon-Simpson rules with N (even) integration points

- Weights $w_i^{(j)}(x_0, h; y)$ are given in terms of elementary functions + Sine & Cosine integrals and have to be calculated for each value of the frequency parameter y (bad ?)

- However, fast & accurate routines for these special functions are available $\Longrightarrow$ CPU time nearly neglible (e.g. 3 sec on 600 MHz Alpha for $N = 288$ and 200 y-values) (good !)

- The Filon-Simpson Code is available to the public – both to

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