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INTERVAL INCLUSIONS FOR DAWSON'S INTEGRAL

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Dawson's integral $f(x) = e^{-x^2} \int_0^x e^{u^2} du$ can be used to calculate the error function for the argument $i \cdot x$; $i = \sqrt{-1}$. In four different intervals $f(x)$ is approximated by different functions $g(x) \approx f(x)$: Padé approximation, Dawson's formula, truncated asymptotic expansion. The corresponding upper bounds $\varepsilon(app)$ of the relative approximation errors are calculated. Because of rounding errors the machine value $\widetilde{g}(x) = g(x)(1 + \varepsilon_g)$ is different from the exact value $g(x)$ and the relative error ε_g is estimated by $|\varepsilon_g| \le \varepsilon(g)$ for each interval. Writing $\widetilde{f}(x) = f(x)(1 + \varepsilon_f)$ the upper bound $\varepsilon(f)$ of the relative error ε_f is given by $|\varepsilon_f| \le \varepsilon(app) + [1 + \varepsilon(app)] \cdot \varepsilon(g) = \varepsilon(f)$. With the machine value $\widetilde{f}(x)$ and $\varepsilon(f)$ an inclusion of the exact function value $f(x)$ can be calculated.

ВКЛЮЧАЮЩИЕ ИНТЕРВАЛЫ ДЛЯ ИНТЕГРАЛА ДОУСОНА

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Интеграл Доусона $f(x) = e^{-x^2} \int_0^x e^{u^2} du$ может быть использован для вычисления функции ошибки для аргумента $i \cdot x$; $i = \sqrt{-1}$. На четырех различных интервалах $f(x)$ аппроксимируется различными функциями $g(x) \approx f(x)$. Используются аппроксимация Паде, формула Доусона, усеченное асимптотическое расширение. Вычисляются соответствующие верхние границы $\varepsilon(app)$ для относительных ошибок аппроксимации. Из-за ошибок округления машинное значение $\widetilde{g}(x) = g(x)(1 + \varepsilon_g)$ отличается от точного значения $g(x)$, и относительная ошибка ε_g оценивается $|\varepsilon_g| \le \varepsilon(g)$ для каждого интервала. Записав $\widetilde{f}(x) = f(x)(1 + \varepsilon_f)$, получаем, что

верхняя граница $\varepsilon(f)$ относительной ошибки ε_f задается выражением $|\varepsilon_f| \le \varepsilon(app) + [1+\varepsilon(app)]\cdot\varepsilon(g) = \varepsilon(f)$. Имея машинное значение $\widetilde{f}(x)$ и $\varepsilon(f)$, можно вычислить включающий интервал для точного значения функции $f(x)$.

1. Introduction

Dawson's integral is defined by: $f(x) = e^{-x^2}\int_0^x e^{u^2}du$, [1,2,3,6]. Because of $\overline{f(-x)} \equiv -f(x)$ we consider only $x \ge 0$. With

$$2\int_0^x e^{u^2}du = -i\sqrt{\pi}\cdot \operatorname{erf}(i\cdot x); \qquad \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}du \qquad (1)$$

it is possible to calculate the error function $\operatorname{erf}(z)$ for $z = i\cdot x$ by means of $f(x)$; $i = \sqrt{-1}$.

The problem is to calculate an inclusion interval $y = [y_1, y_2]$ for a given argument-interval $[x_1, x_2]$ with the following conditions:

(1) $f([x_1, x_2]) \subset y = [y_1, y_2]$;
(2) $y_2 - y_1$ should be as small as possible.

To solve this problem we need the upper bound $\varepsilon(f)$ for the absolute value of the relative error $\varepsilon_f(x)$:

$$\varepsilon_f(x) := \frac{f(x) - \widetilde{g}(x)}{f(x)}; \qquad |\varepsilon_f(x)| \le \varepsilon(f) = ?$$

With the approximation function $g(x) \approx f(x)$, which should be easy to evaluate, we have the relative approximation error:

$$\varepsilon_{app}(x) := \frac{f(x) - g(x)}{f(x)}; \qquad |\varepsilon_{app}(x)| \le \varepsilon(app) = ?$$

$\widetilde{g}(x)$ is the machine value of $g(x)$ with the relative error:

$$\varepsilon_g(x) := \frac{g(x) - \widetilde{g}(x)}{g(x)}; \qquad |\varepsilon_g(x)| \le \varepsilon(g) = ?$$

Splitting the errors and using the triangle inequality we get the following expression for $\varepsilon(f)$:

$$\varepsilon(f) := \varepsilon(app) + [1 + \varepsilon(app)]\cdot\varepsilon(g) \qquad (2)$$

The computer result for $f(x)$ is $\widetilde{f}(x) \equiv \widetilde{g}(x)$. To get an inclusion for $f(x) \geq 0$ we have to use the following inequalities:

$$y_1 := \frac{\widetilde{f}(x)}{1+\varepsilon(f)} \leq f(x) \leq \frac{\widetilde{f}(x)}{1-\varepsilon(f)} =: y_2, \tag{3}$$

where the expressions for y_1, y_2 must be evaluated by directed rounding (PASCAL–XSC). So from (2) the main job is to calculate the upper bounds $\varepsilon(app)$, $\varepsilon(g)$.

2. Dawson's approximation formula

With

$$E := 2\sum_{n=1}^{\infty} e^{-\frac{n^2\pi^2}{a^2}} \cdot \cos\frac{2n\pi u}{a}, \quad a \neq 0, \quad \text{we have from [6]:} \tag{4}$$

$$e^{u^2}(1+E) = \frac{a}{\sqrt{\pi}}\left[1 + 2\sum_{n=1}^{\infty} e^{-a^2n^2} \cdot \cosh(2nau)\right]. \tag{5}$$

Integration of (5) from 0 to x with respect to u yields: $f(x) \approx D(a,x,\infty)$, with:

$$D(a,x,\infty) := \frac{a \cdot e^{-x^2}}{\sqrt{\pi}}\left[x + \frac{1}{a}\sum_{n=1}^{\infty}\frac{e^{-a^2n^2}}{n}\sinh(2nax)\right] \quad \text{and:}$$

$$|\varepsilon_{app}| = |E| \leq 2\alpha\left[1 + \alpha^3 + \alpha^8 + \cdots\right]; \qquad \alpha = e^{-\frac{\pi^2}{a^2}} < 1 \tag{6}$$

$$< 2\alpha\left[1 + \alpha^1 + \alpha^2 + \cdots\right] = \frac{2}{e^{\frac{\pi^2}{a^2}} - 1} =: \varepsilon(a) \xrightarrow{a\to 0} 0.$$

Evaluating $D(a,x,\infty)$ with a computer we have to truncate the infinite series in (6) with $n = N$: $D(a,x,\infty) \approx D(a,x,N)$. Using again the geometric series the following upper bound $\varepsilon(a,N,x)$ for the absolute value of the relative approximation error

$$\varepsilon_{a,N}(x) = \frac{D(a,x,\infty) - D(a,x,N)}{D(a,x,N)}$$

is given by [7]:

$$|\varepsilon_{a,N}(x)| < \frac{e^{-a^2(N+1)^2+2(N+1)ax}}{2(N+1)\left[1-e^{-2(N+1)a^2+2ax}\right]\left[ax+\sum_{n=1}^{N}\frac{e^{-a^2n^2}}{n}\sinh(2nax)\right]} \quad (7)$$

$$=: \varepsilon(a,N,x)\,; \qquad N+1 > x/a. \quad (8)$$

$\varepsilon(a,N,x)$ is useless for $x \to 0$; for $x \in [0,c]$ and c not too small $\varepsilon_{a,N}(x)$ is estimated by [7]:

$$|\varepsilon_{a,N}(x)| \leq \frac{e^{-a^2(N+1)^2+2(N+1)ac}}{2ac(N+1)\left[1-e^{-2(N+1)a^2+2ac}\right]} = \delta(a,N,c). \quad (9)$$

We have two approximations: $f(x) \approx D(a,x,\infty) \approx D(a,x,N)$ and again by splitting the errors we find the following expression for the upper bound of the relative error $\varepsilon_{app} = [f(x) - D(a,x,N)]/f(x)$:

$$|\varepsilon_{app}| \leq \varepsilon(a) + [1+\varepsilon(a)]\cdot M = \varepsilon(app,D) \quad (10)$$

$$M := \delta(a,N,c),\ x \in [0,c] \quad \text{and} \quad M := \varepsilon(a,N,x),\ x \geq c > 0.$$

For a large x we need a very large N to keep $\varepsilon(a,N,x)$ small; so we use DAWSON'S formula $D(a,x,N)$ only for $x \in [1.5; 6.3]$.

3. 1.5≤x≤6.3

3.1. Approximation error

$\varepsilon(0.5,24,x)$ is increasing in x, so we have $\varepsilon(0.5,24,x) \leq \varepsilon(0.5,24,6.3) < 2.843\cdot 10^{-18}$ and with $\varepsilon(0.5) < 1.432\cdot 10^{-17}$ we get:

$$|\varepsilon_{app}| < 1.432\cdot 10^{-17} + 1.001\cdot 2.843\cdot 10^{-18} < 1.717\cdot 10^{-17} = \varepsilon(app).$$

3.2. Rounding error

With $e[n] = (e^{-n^2/4})/n$ the function $D(0.5, x, 24)$ can be written as:

$$f(x) \approx D(0.5, x, 24) = \frac{e^{-x^2}}{2\sqrt{\pi}} \left[x + \sum_{n=1}^{24} e[n] \left(e^{nx} - e^{-nx} \right) \right]$$

$$= \frac{e^{-x^2}}{2\sqrt{\pi}} B(x) = g(x)$$

and the main work now is to calculate an upper bound $\varepsilon(B)$ of the relative error with respect to $B(x)$, containing defective machine summands. Doing this we have the following problem: For the machine values $\tilde{u} = u(1+\varepsilon_u)$, $|\varepsilon_u| \le \varepsilon(u)$ and $\tilde{v} = v(1+\varepsilon_v)$, $|\varepsilon_v| \le \varepsilon(v)$ we have to calculate the upper bound $\varepsilon(S)$ for the relative error of the sum: $\widetilde{S} := \tilde{u} \oplus \tilde{v} = S(1+\varepsilon_S)$, $|\varepsilon_S| \le \varepsilon(S)$; $\varepsilon(S)$ is given by:

$$\varepsilon(S) = \varepsilon(+) + [1 + \varepsilon(+)] \cdot \frac{|u| \cdot \varepsilon(u) + |v| \cdot \varepsilon(v)}{|u+v|} \qquad (11)$$

where $\varepsilon(+)$ is the upper bound of the relative error of the floating-point addition $\oplus$. To get an inclusion for $\varepsilon(S)$ we compute the interval extension of expression (11) in PASCAL–XSC. So we can calculate $\varepsilon(B)$ with a recursive program. In the same way we can evaluate the upper bound of the rounding errors in Horner's scheme [5].

To avoid overestimations we have to subdivide our interval into 100 000 interval parts and so we get $\varepsilon(B) = 5.199 \cdot 10^{-17}$. With the error bound $4.14 \cdot 10^{-18}$ of the exponential function we finally have the result $\varepsilon(g) = 5.639 \cdot 10^{-17}$ and (2) yields $\varepsilon(f) = 7.362 \cdot 10^{-17}$.

4. 6.3≤x≤13.5

4.1. Approximation function

In this area we use a Padé Approximation:

$$f(x) \approx R(x) = \frac{Z_8(x)}{N_9(x)} \equiv g(x)$$

$$Z_8(x) = a_0 + a_1 x^1 + \cdots + a_8 x^8; \quad N_9(x) = b_0 + b_1 x^1 + \cdots + b_9 x^9.$$

The coefficients a_k, b_k are calculated with the DERIVE-package [4] using the expansion point $x_0 = 8$. For the internal representation of Dawson's integral $f(x)$ in the DERIVE package we use the Taylor series of $f(x)$, where the Taylor coefficients are evaluated by means of a recursion formula, which is easy to derive from the differential equation $f'(x) = -2x \cdot f(x) + 1$.

4.2. Truncation error

To calculate the approximation error we write:

$$f(x) \approx D(a, x, N) \approx R(x) \equiv g(x). \tag{12}$$

Notice, that $g(x) \equiv R(x) = Z_8(x)/N_9(x)$ is the actual approximation function and that we use the first approximation $f(x) \approx D(a, x, N)$ only to be able to evaluate the approximation error. For the first approximation in (12) the upper bound of the approximation error can be calculated by (10) with $a = 0.37$, $N = 90$ and $x = 13.5$ because $\varepsilon(0.37, 90, x)$ is increasing in x:

$$\varepsilon(0.37) + 1.001 \cdot \varepsilon(0.37, 90, 13.5) < 9.801 \cdot 10^{-32} = \varepsilon(app, D).$$

For the second approximation $D(0.37, x, 90) \approx R(x)$ the relative error

$$\varepsilon_{D,R} = \frac{D(0.37, x, 90) - R(x)}{D(0.37, x, 90)}$$

can be evaluated with DERIVE, and the maximum of $|\varepsilon_{D,R}(x)|$ is given by:

$$|\varepsilon_{D,R}(13.5)| < 3.800 \cdot 10^{-17} = \varepsilon(D, R)$$

and for the approximation $f(x) \approx R(x)$ we have analogously to (2):

$$|\varepsilon_{app}| < 9.801 \cdot 10^{-32} + 1.001 \cdot 3.8 \cdot 10^{-17} < 3.804 \cdot 10^{-17} = \varepsilon(app).$$

4.3. Rounding error

With $R(x) = Z_8(x)/N_9(x)$ the machine result $\widetilde{R}(x)$ is given by:

$$\begin{aligned}\widetilde{R}(x) &= [Z_8(x)(1+\varepsilon_Z)] \oslash [N_9(x)(1+\varepsilon_N)] = \\ &= R(x) \cdot \frac{(1+\varepsilon_Z)(1+\varepsilon_{21})}{1+\varepsilon_N} = R(x)(1+\varepsilon_R); \\ |\varepsilon_{21}| &\le \varepsilon(21) = 0.5 \cdot 10^{-21}.\end{aligned}$$

$\varepsilon(21)$ is the upper bound of the relative error for the floating-point division $\oslash$. The upper bounds $\varepsilon(N)$, $\varepsilon(Z)$ of the relative errors ε_N, ε_Z can be calculated with the recursive program [5]:

$$\begin{aligned}\widetilde{Z}_8(x) &= Z_8(x)(1+\varepsilon_Z); \qquad |\varepsilon_Z| \le 9.5648 \cdot 10^{-18} = \varepsilon(Z) \\ \widetilde{N}_9(x) &= N_9(x)(1+\varepsilon_N); \qquad |\varepsilon_N| \le 9.7223 \cdot 10^{-18} = \varepsilon(N) \quad \longrightarrow\end{aligned}$$

$$|\varepsilon_R| \le 1.930 \cdot 10^{-17} = \varepsilon(R) = \varepsilon(g).$$

Now with (2) we finally obtain:

$$|\varepsilon_f| \le \varepsilon(app) + 1.001 \cdot \varepsilon(g) \le 5.736 \cdot 10^{-17} = \varepsilon(f).$$

5. $0 \le x \le 1.5$

In this area we again use a Padé Approximation:

$$f(x) \approx R(x) = \frac{x \cdot Z_9(x^2)}{N_{10}(x^2)} \equiv g(x)$$

with the expansion point $x_0 = 0$. The calculation of the polynomial coefficients and the upper bounds $\varepsilon(app)$, $\varepsilon(g)$ can be done analogously to the area $6.3 \le x \le 13.5$. Results:

$$\varepsilon(app) = 2.505 \cdot 10^{-18}; \quad \varepsilon(g) = 9.837 \cdot 10^{-19} \longrightarrow \varepsilon(f) = 3.490 \cdot 10^{-18}.$$

6. 13.5<x<∞

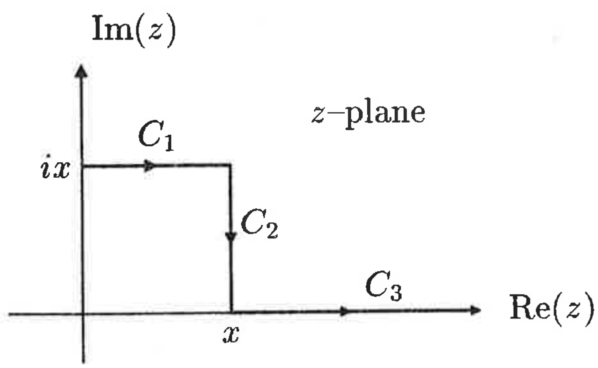
In this area the best approximation function is the truncated asymptotic expansion of $f(x)$. Using the asymptotic of the error function $\mathrm{erf}(x)$ together with an analytic continuation we obtain:

$$f(x) = g_n(x) + r_n(x)\,, \qquad \text{with:} \tag{13}$$

$$g_n(x) = \frac{1}{2x}\left[1 + \frac{1}{(2x^2)^1} + \frac{1\cdot 3}{(2x^2)^2} + \cdots + \frac{1\cdot 3\cdots(2n-1)}{(2x^2)^n}\right], \tag{14}$$

$$r_n(x) = i\cdot e^{-x^2}\left[(-1)^{n+1}\frac{1\cdot 3\cdots(2n+1)}{2^{n+1}}\int_{ix}^{\infty}\frac{e^{-z^2}}{z^{2n+2}}dz - \frac{\sqrt{\pi}}{2}\right]. \tag{15}$$

The path of integration is separated into the parts: C_1, C_2, C_3 :



Upper bounds for the modulus of $I(x) = \int_{ix}^{\infty}\frac{e^{-z^2}}{z^{2n+2}}dz$:

$$C_1: \quad |I(x)| \le \frac{e^{x^2}\cdot\sqrt{\pi}}{2x^{2n+2}}; \qquad C_2: \quad |I(x)| \le \frac{f(x)}{x^{2n+2}};$$

$$C_3: \quad |I(x)| = \frac{\sqrt{\pi}}{2x^{2n+2}}\,[1-\mathrm{erf}(x)] < \frac{\sqrt{\pi}}{2x^{2n+2}}.$$

With this results we find the following estimations [7]:

$$|r_n(x)| < \frac{\sqrt{\pi}}{2}\left[\frac{1\cdot 3\cdots(2n+1)\cdot 1.0002}{2^{n+1}\cdot x^{2n+2}} + e^{-x^2}\right], \quad x \ge 3; \tag{16}$$

$$|r_n(x)| < 1.014\frac{\sqrt{\pi}}{2}\cdot\frac{1\cdot 3\cdots(2n+1)}{2^{n+1}x^{2n+2}}; \qquad x \ge 3n. \tag{17}$$

The first result of (17) is:

$$\lim_{x\to\infty} x^{2n+1}|r_n(x)| = 0\,; \qquad n = 1, 2, \ldots .$$

So for $f(x)$ there really exists an asymptotic expansion! Secondly it is easy to proof that for $x \geq 3n$ the last summand in (14) is an upper bound of the expression in (17), so we get the

Theorem. *For $x \geq 3n$ the absolute value of the remainder term is less than or equal to the last used summand of the asymptotic.*

6.1. Approximation error

With (16) an estimation of the relative approximation error is given by:

$$|\varepsilon_{app}(x)| < \frac{\sqrt{\pi}}{2\cdot f(x)}\left[\frac{1\cdot 3\cdot \;\cdots\; \cdot(2n+1)\cdot 1.0002}{2^{n+1}\cdot x^{2n+2}} + e^{-x^2}\right], \qquad x \geq 3.$$

Now for $x \geq 13.5$ we have to calculate a lower bound for $f(x) \geq ?$ And this is quite easy with our last theorem! Writing $n = 4$ we have the result:

$$|r_4(x)| \leq \frac{1}{2x}\cdot\frac{1\cdot 3\cdot 5\cdot 7}{(2x^2)^4}, \quad \text{if } x \geq 12.$$

So the sum of the positive last summand of $g_4(x)$ and $r_4(x)$ cannot be negative, and with this result we have:

$$f(x) \geq \frac{1}{2x}\left[1 + \frac{1}{(2x^2)^1} + \frac{1\cdot 3}{(2x^2)^2} + \frac{1\cdot 3\cdot 5}{(2x^2)^3}\right] > \frac{1}{2x}; \quad x \geq 12 \quad \longrightarrow$$

$$\begin{aligned} |\varepsilon_{app}(x)| &< \sqrt{\pi}\left[\frac{1\cdot 3\cdot \;\cdots\; \cdot(2n+1)\cdot 1.0002}{2^{n+1}\cdot(x)^{2n+1}} + x\cdot e^{-x^2}\right] \\ &\equiv K(n,x), \;\; x \geq 13.5. \end{aligned} \tag{18}$$

The two summands in (18) are decreasing in $x \geq 13.5$ and with $n = 10$ we obtain:

$$\begin{aligned} |\varepsilon_{app}(x)| &< K(10, 13.5) \\ &< 2.181\cdot 10^{-17} = \varepsilon(app), \quad x \geq 13.5, \quad n = 10. \end{aligned}$$

6.2. Rounding error

With (14) and $n = 10$ the approximationfunction can be written as:

$$g(x) = \frac{1}{2x}\left[1 + \zeta + 3\cdot\zeta^2 + 3\cdot 5\cdot\zeta^3 + \cdots + 3\cdot 5\cdot \cdots \cdot 19\cdot\zeta^{10}\right];$$

$$= \frac{1}{2x}\cdot P_{10}(\zeta);\quad \zeta = \frac{1}{2x^2};$$

$$\widetilde{g}(x) := [1 \oslash (2 \odot x)] \odot \widetilde{P}_{10}(\tilde{\zeta});$$

$$\widetilde{\zeta} := 0.5 \odot [(1 \oslash x) \odot (1 \oslash x)] = \zeta(1 + \varepsilon_\zeta).$$

With $\varepsilon(\zeta) = 2.001 \cdot 10^{-20}$ (BCD data format with 21 mantissa-digits) together with the recursive program for Horner's–scheme we find:

$$\widetilde{P}_{10}(\tilde{\zeta}) = P_{10}(\zeta)(1 + \varepsilon_P);\quad \varepsilon(P) = 3.474 \cdot 10^{-17}.$$

Simple applications of the error calculus yield: $\varepsilon(g) = 3.476 \cdot 10^{-17}$;

$$|\varepsilon_f| \le \varepsilon(app) + 1.001 \cdot \varepsilon(g) < 5.661 \cdot 10^{-17}.$$

The maximum of the $\varepsilon(f)$-values in the four considered areas is the error bound in the whole area $x \ge 0$:

$$\varepsilon(f) = 7.362 \cdot 10^{-17}.$$

With this value an interval-function for $f(x)$ will be realized in the BCD data format of PASCAL-XSC.

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