Computation of the error functions erf and erfc in arbitrary precision with correct rounding

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IEEE-754 standard for floating-point arithmetic

Floating-point number : $s.m.\beta^e$ or 0, a denormal, $\pm\infty$, NaN.

- s : sign
- m : mantissa $\in [2^{p-1}/2^p, (2^p - 1)/2^p]$, p is the precision
- e : exponent $\in [e_{\min}, e_{\max}]$
- β : basis, usually equal to 2

IEEE-754 standard for floating-point arithmetic :

- fixed formats for single and double precision
- specifies 4 rounding modes
- specifies the arithmetic and algebraic operations $+$, $-$, $\times$, $/$, $\sqrt{\ }$.

Advantages :

- well-specified arithmetic, reproducible results
- error bounds can be established and proofs can be done

Desirable extensions of the IEEE-754 standard

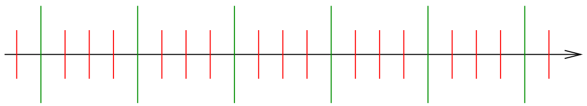
correctly rounded elementary functions :
cf. current revision of the standard

arbitrary precision : (software)
cf. MPFR

correctly rounded special functions :
? ? ?

correctly rounded functions in arbitrary precision :
cf. MPFR for elementary functions
? ? ?

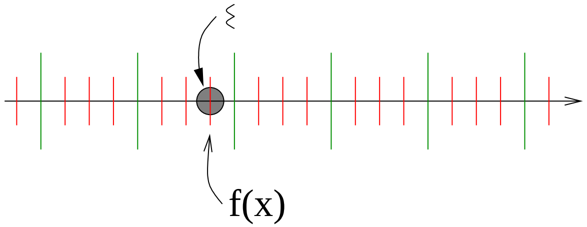
How can one return the correctly rounded evaluation of a function f ?



To return the correctly rounded evaluation of $f(x)$ in precision p :

1- approximate $f(x)$ with larger precision q, error $< \varepsilon$

2- if `can_round` $(f(x), \varepsilon, p)$



then return it

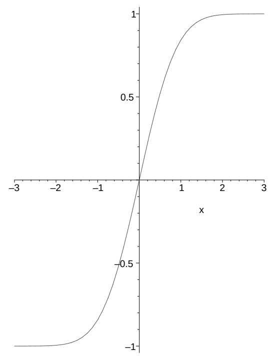
3- otherwise increase q, decrease ε and try again.

Outline of this talk

- the error function erf
- algorithm to return the correctly rounded evaluation of erf(x)
- experimental results
- the complementary error function erfc
- conclusion and hints for improvements
- current work on interval arithmetic and algorithms : MPFI

The error function erf

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$



The error function is very useful in statistics (cf. Gaussian distribution), diffusion equation (special configurations) and other heat transfer problems. . .

Goal : return the correctly rounded value of erf(x) in arbitrary precision.

Possible formulas

$$
\begin{aligned}
\mathsf{erf}(x) &= \tfrac{2}{\sqrt{\pi}} \textstyle\int_0^x e^{-t^2} dt & (1)\\
&= \tfrac{2}{\sqrt{\pi}} \textstyle\sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} & (2)\\
&= \tfrac{2}{\sqrt{\pi}} e^{-x^2} \textstyle\sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3\cdots(2n+1)} & (3)\\
&= \sqrt{2} \textstyle\sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] & (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \, \frac{1}{x+} \, \frac{1/2}{x+} \, \frac{1}{x+} \, \frac{3/2}{x+} \, \frac{2}{x+} \cdots & (5)
\end{aligned}
$$

Possible formulas

$$
\begin{aligned}
\mathrm{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt & (1) \\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} & (2) \\
&= \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3 \cdots (2n+1)} & (3) \\
&= \sqrt{2} \sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] & (4) \\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \, \frac{1}{x+} \, \frac{1/2}{x+} \, \frac{1}{x+} \, \frac{3/2}{x+} \, \frac{2}{x+} \cdots & (5)
\end{aligned}
$$

Discussion of the use of quadrature :

- numerous evaluations of $\exp$: costly (either in computing time or in development time)
- many sources of error : evaluation of $\exp$, quadrature, roundoff

Possible formulas

$$
\begin{aligned}
\mathrm{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt && (1)\\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} && (2)\\
&= \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3\cdots(2n+1)} && (3)\\
&= \sqrt{2} \sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] && (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \frac{1}{x+} \frac{1/2}{x+} \frac{1}{x+} \frac{3/2}{x+} \frac{2}{x+} \cdots && (5)
\end{aligned}
$$

Discussion of the use of alternate power series :

- the remainder is easy to bound
- sum of terms of alternate signs : cancellation

Possible formulas

$$
\begin{aligned}
\mathrm{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt & (1)\\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} & (2)\\
&= \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3 \cdots (2n+1)} & (3)\\
&= \sqrt{2} \sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] & (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \frac{1}{x+} \frac{1/2}{x+} \frac{1}{x+} \frac{3/2}{x+} \frac{2}{x+} \cdots & (5)
\end{aligned}
$$

Discussion of the use of this power series :

- sum of positive terms : numerical stability
- the remainder is less easy to bound

Possible formulas

$$
\begin{aligned}
\mathsf{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt && (1)\\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} && (2)\\
&= \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3 \cdots (2n+1)} && (3)\\
&= \sqrt{2} \sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] && (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \, \frac{1}{x+} \, \frac{1/2}{x+} \, \frac{1}{x+} \, \frac{3/2}{x+} \, \frac{2}{x+} \cdots && (5)
\end{aligned}
$$

Discussion of the use of Bessel functions of fractional order :

- the problem is now to evaluate the Bessel functions of fractional order

Possible formulas

$$
\begin{aligned}
\mathrm{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt & (1)\\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} & (2)\\
&= \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3\cdots(2n+1)} & (3)\\
&= \sqrt{2} \sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] & (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \, \frac{1}{x+} \, \frac{1/2}{x+} \, \frac{1}{x+} \, \frac{3/2}{x+} \, \frac{2}{x+} \cdots & (5)
\end{aligned}
$$

Discussion of the use of this continued fraction :

- the remainder is less easy to bound
- numerical stability is not ensured

Chosen formula

$$\begin{aligned}
\mathrm{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt && (1)\\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} && (2)\\
&= \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3 \cdots (2n+1)} && (3)\\
&= \sqrt{2} \sum_{n=0}^{+\infty} (-1)^n \left[I_{2n+1/2}(x^2) - I_{2n+3/2}(x^2) \right] && (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \frac{1}{x+} \frac{1/2}{x+} \frac{1}{x+} \frac{3/2}{x+} \frac{2}{x+} \cdots && (5)
\end{aligned}$$

Motivation for the choice of this alternate power series :

- the remainder is easy to bound
- special care to avoid cancellation in the sum of terms of alternate signs

Other useful formulas

$$\mathrm{erf}(-x) = -\mathrm{erf}(x)$$

No argument reduction possible (cf. $\sin(x + 2\pi) = \sin x$ or $\exp(2x) = (\exp x)^2$).

$$\frac{2}{\sqrt{\pi}} \cdot \frac{e^{-x^2}}{x + \sqrt{x^2 + 2}} < \mathrm{erfc}(x) \leq \frac{2}{\sqrt{\pi}} \cdot \frac{e^{-x^2}}{x + \sqrt{x^2 + \frac{4}{\pi}}} \text{ for } x \geq 0.$$

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Algorithm

Input : x, p

Output : correctly rounded value of erf(x) with p bits

1. handle special cases : $x = 0$, $x = \pm\infty$, $x < 0$
2. check whether the last enclosure gives rapidly the answer
3. determine the truncation rank N needed to have an absolute error $\leq \varepsilon$
4. determine the computing precision q to have roundoff error $\leq \varepsilon$
5. evaluate y that approximates erf(x) using the alternate power series ; bound from above the roundoff error $\varepsilon' \leq \varepsilon$, on the fly
6. if $\texttt{can\_round}(y, \varepsilon + \varepsilon', p)$ then
   return y
   else increase N and q and do steps (5) and (6) again

Algorithm : step (2)

Input : x, p

Output : correctly rounded value of erf(x) with p bits

1. handle special cases : $x = 0$, $x = \pm\infty$, $x < 0$
2. check whether the last enclosure gives rapidly the answer
3. determine the truncation rank N needed to have an absolute error $\leq \varepsilon$
4. determine the computing precision q to have roundoff error $\leq \varepsilon$
5. evaluate y that approximates erf(x) using the alternate power series ; bound from above the roundoff error $\varepsilon' \leq \varepsilon$, on the fly
6. if $\texttt{can\_round}(y, \varepsilon + \varepsilon', p)$ then
   return y
   else increase N and q and do steps (5) and (6) again

Algorithm : step (2)

Reminder :

$$\frac{2}{\sqrt{\pi}} \cdot \frac{e^{-x^2}}{x + \sqrt{x^2+2}} < \mathrm{erfc}(x) \leq \frac{2}{\sqrt{\pi}} \cdot \frac{e^{-x^2}}{x + \sqrt{x^2 + \frac{4}{\pi}}} \text{ for } x \geq 0.$$

Step (2) :

compute both sides of this enclosure : y_L, y_R

if `can_round`$(y_L, y_R - y_L, p)$ then return it.

Algorithm : step (3)

Input : x, p
Output : correctly rounded value of erf(x) with p bits

1. handle special cases : $x = 0$, $x = \pm\infty$, $x < 0$
2. check whether the last enclosure gives rapidly the answer
3. determine the truncation rank N needed to have an absolute error $\leq \varepsilon$
4. determine the computing precision q to have roundoff error $\leq \varepsilon$
5. evaluate y that approximates erf(x) using the alternate power series ; bound from above the roundoff error $\varepsilon' \leq \varepsilon$, on the fly
6. if $\texttt{can\_round}(y, \varepsilon + \varepsilon', p)$ then
   return y
   else increase N and q and do steps (5) and (6) again

Algorithm : step (3)

Reminder : power series

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} = \sum_{n=0}^{+\infty} a_n \text{ with } a_n = \frac{2}{\sqrt{\pi}} \frac{(-1)^n x^{2n+1}}{n!(2n+1)}$$

Property : alternate power series $\sum_{n=0}^{+\infty} a_n$ with non-increasing term a_n (for n large enough)
$\Rightarrow$ remainder $|\sum_{n=N}^{+\infty} a_n| = |\,\mathrm{erf}(x) - \sum_{n=0}^{N-1} a_n| \leq |a_N|$.

Step (3) :
$\varepsilon = 2^{-p-8}$: 8 extra bits
evaluate a_n until $a_N \leq \varepsilon$: N is the truncation rank.

Algorithm : step (4)

Input : x, p
Output : correctly rounded value of erf(x) with p bits

1. handle special cases : $x = 0$, $x = \pm\infty$, $x < 0$
2. check whether the last enclosure gives rapidly the answer
3. determine the truncation rank N needed to have an absolute error $\leq \varepsilon$
4. determine the computing precision q to have roundoff error $\leq \varepsilon$
5. evaluate y that approximates erf(x) using the alternate power series ; bound from above the roundoff error $\varepsilon' \leq \varepsilon$, on the fly
6. if $\texttt{can\_round}(y, \varepsilon + \varepsilon', p)$ then
   return y
   else increase N and q and do steps (5) and (6) again

Algorithm : step (4)

Goal : computing precision q such that roundoff error $\leq \varepsilon$.

Technique : cf. Higham, *Accuracy and stability of numerical algorithms*.

Step (4) :

$$q = 1 + \log_2\left(\frac{5^{\frac{N+1}{2}}}{\alpha}\right) \text{ where } \alpha = \min\left(\frac{1}{2}, \frac{\frac{\varepsilon x}{2}}{e^{x^2} - 1 + \frac{\varepsilon x}{2}}\right).$$

Algorithm : step (5)

Input : x, p

Output : correctly rounded value of erf(x) with p bits

1. handle special cases : $x = 0$, $x = \pm\infty$, $x < 0$
2. check whether the last enclosure gives rapidly the answer
3. determine the truncation rank N needed to have an absolute error $\leq \varepsilon$
4. determine the computing precision q to have roundoff error $\leq \varepsilon$
5. evaluate y that approximates erf(x) using the alternate power series ; bound from above the roundoff error $\varepsilon' \leq \varepsilon$, on the fly
6. if $\texttt{can\_round}(y, \varepsilon + \varepsilon', p)$ then
   return y
   else increase N and q and do steps (5) and (6) again

Algorithm : step (5)

Power series :

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)}$$

Problem : cancellation $\Rightarrow$ numerical unstability.

Solution : group the terms by pair (assume N is odd) :

$$\text{erf}(x) = \sum_{n=0}^{N-1} a_n = a_{N-1} + \frac{2x}{\sqrt{\pi}} \sum_{n=0}^{\frac{N-1}{2}} \frac{x^{4n}}{(2n)!} \left(\frac{1}{4n+1} - \frac{x^2}{(2n+1)(4n+3)} \right)$$

Step (5) :

sum using Horner-like scheme.

Algorithm : remaining issues

Increase N and q :
cf. Kreinovich and Rump 2006 : optimal overhead $= 4$ if the computing time is doubled
$N_{i+1} \simeq (2 - \alpha_i)N_i$ with $\alpha_i = 2/(1 + q_i)$,
q_{i+1} depends on N_{i+1}.

Termination :
if there exists a floating-point number x such that erf(x) is a floating-point number, then `can_round` can never answer "yes".
In other words, infinite loop.

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Experimental results : small values of x

x	p	`mpfr_erf`	Maple 6	my_erf
0.25	100	0.21 ms	< 0.10 ms	0.53 ms
0.25	$1\,000$	7.51 ms	20 ms	3.28 ms
0.25	$10\,000$	$1\,020$ ms	580 ms	365 ms

(2003 : on a Pentium II 400MHz, 64MB RAM)

Comments :

for small precisions, our pre-computations (determination of the truncation rank and of the computing precision) is costly ;
this cost is compensated by the gain it provides, for larger precisions.

Experimental results : intermediate values of x

x	p	`mpfr_erf`	Maple 6	my_erf
π	100	0.73 ms	$<$ 0.10 ms	1.33 ms
π	1 000	19.3 ms	60 ms	8.7 ms
π	10 000	2 040 ms	7 320 ms	560 ms
π	100 000	340.7 s	1692 s	149.6 s

(times in seconds, Pentium II 400MHz, 64MB RAM)

Comments : ibidem
for small precisions, our pre-computations (determination of the truncation rank and of the computing precision) is costly ;
this cost is compensated by the gain it provides, for larger precisions.

Experimental results : large values of x

x	p	`mpfr_erf`	Maple 6	my_erf
100	$1\,000$	0.0022 ms	< 0.10 ms	0.22 ms
100	$10\,000$	0.0065 ms	< 0.10 ms	0.22 ms
100	$14\,446$	$191\,200$ ms	0.20 ms	0.22 ms
100	15000	$196\,100$ ms	0.40 ms	$75\,600$ ms

(2003 : on a Pentium II 400MHz, 64MB RAM)

Comments :

erf(x) is very close to 1 ;

here, Maple computes erfc(x) and then erf$(x) = 1-$ erfc(x).

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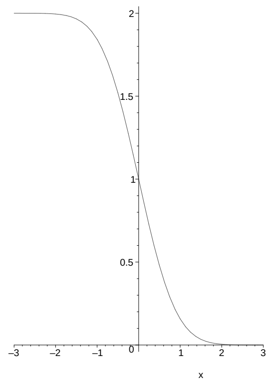
The complementary error function erfc



$$\text{erfc}(x) = 1 - \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^{+\infty} e^{-t^2} dt$$

Why not use erf for large x ?
because this would require to compute a large number of bits of erf(x) to cancel them

$$1 - \text{erf}(x) = 1.000 \cdots - 0.111 \cdots 10 b_1 b_2 \cdots b_p = 0.000 \cdots 01 \cdots$$

Possible formulas

$$
\begin{aligned}
\text{erfc}(x) &= \frac{2}{\sqrt{\pi}} \int_x^{+\infty} e^{-t^2} dt & (1)\\
&= 1 - \frac{2}{\sqrt{\pi}} \sum_{n=0}^{+\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)} & (2)\\
&= 1 - \frac{2}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{+\infty} \frac{2^n x^{2n+1}}{1.3 \cdots (2n+1)} & (3)\\
&= \frac{e^{-x^2}}{x\sqrt{\pi}} \left(1 + \sum_{n=1}^{+\infty} (-1)^n \frac{1.3 \cdots (2n-1)}{(2x^2)^n}\right) & (4)\\
&= \frac{e^{-x^2}}{\sqrt{\pi}} \frac{1}{x+} \frac{1/2}{x+} \frac{2/2}{x+} \frac{3/2}{x+} \cdots & (5)
\end{aligned}
$$

Chosen formula : the continued fraction (5).

Algorithm

Input : x, p

Output : correctly rounded value of erfc(x) with p bits

1. handle special cases : $x = 0$, $x = \pm\infty$, $x < 0$
2. determine the truncation rank N needed to have an absolute error $\leq \varepsilon$
3. determine the computing precision q to have roundoff error $\leq \varepsilon$
4. evaluate y that approximates erfc(x) using the continued fraction ; (two methods : compute the fraction or compute separately the numerator and the denominator)
5. if $\texttt{can\_round}(y, 2\varepsilon, p)$ then
   return y
   else increase N and q and do steps (5) and (6) again

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Conclusion and future work

Realization :

efficient implementation of correctly rounded error functions erf and erfc.
Termination ? Table's Maker Dilemma.

Future work :

- small precisions : avoid costly determination of the truncation rank
- choose between erf and erfc depending on the value of x, to avoid cancellation
- when `can_round` fails, change the heuristic to increase N to reach an optimal overhead factor of 4
- exceptions (under/overflow) not totally taken care of yet

Current work on interval arithmetic and algorithms : MPFI

MPFI (Multiple Precision Floating-point Interval arithmetic library) :

- development of this C library, based on MPFR.
- design of MPFI vs standardization of intervals in C++ (proposal)

Algorithms :

- automatic adaptation of the computing precision
- Newton method for univariate problems
- linear recurrences
- global optimization for univariate problems (approximations of an elementary function by a polynomial)
- future work : linear algebra, multivar. Newton, multivar. global opt.

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