Error function of complex numbers

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This document describes the current implementation of the error function for use with MATLAB. The error function is briefly introduced and series developments for its evaluation are given. The numerical evaluation of the function for real- and complex-valued numbers is discussed.

1 Introduction

The error function $\operatorname{erf}(z)$ is defined as the integral of the normal distribution from 0 to z scaled such that $\operatorname{erf}(\pm\infty) = \pm 1$.

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\,\mathrm{d}t \tag{1}$$

It is an entire function defined for real- and complex-valued numbers. For real-valued $z = R$, the GNU math library defines the error function `double erf(double z)`. For complex $z = R + \mathrm{i}I$, it can be rewritten as a line integral in the complex plane.

$$\operatorname{erf}(z) = \frac{2z}{\sqrt{\pi}} \int_0^1 e^{-z^2 s^2}\,\mathrm{d}s \tag{2}$$

The error function is odd as a whole as well as by its real and imaginary parts, that is $\operatorname{erf}(-z) = -\operatorname{erf}(z)$ and $\operatorname{erf}(z^*) = \operatorname{erf}(z)^*$ with z^* denoting the complex conjugate. It is zero at the origin, that is $\operatorname{erf}(0) = 0$, which is the only zero on the real axis. For real z, the error function is bound and strictly monotonically increasing, that is $|\operatorname{erf}(R)| \leq 1$ and $\mathrm{d}\operatorname{erf}(R)/\mathrm{d}R > 0$. At $\pm\infty$, it is exactly ± 1 by definition. The error function cannot be written in closed form but the development of the integrand into a Taylor series is simple and reads as

$$e^{-z^2} = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} z^{2n}\,, \qquad \text{which yields} \qquad \operatorname{erf}(z) = \frac{2z}{\sqrt{\pi}} \left(1 + \sum_{n=1}^{\infty} \frac{(-1)^n z^{2n}}{n!(2n+1)} \right). \tag{3}$$

The error function is discussed in detail in standard math textbooks, i.e. Abramowitz and Stegun[1]. Summaries are also found online, see for instance Weisstein[2] or Wikipedia[3].

2 Numerical evaluation

In principal, one can assess the correct value within the numerical precision ε by summing all terms of the Taylor series (3) of at least $\varepsilon|z|^{2n_c}/n_c!(2n_c+1)$ magnitude, where n_c is the index of the largest term. This approach fails for large $|z|$ because the corresponding interval $n \in [n_l, n_u] \ni n_c$ scales with $|z|$. Thanks to the factor $e^{-n^2/4}$, the following series development in Abramowitz and Stegun[1] circumvents this problem as the number of required terms $\Delta n = n_u - n_l + 1$ is independent of z.

$$\operatorname{erf}(z) = \operatorname{erf}(R) + \frac{e^{-R^2}}{\pi}\left\{\frac{1-e^{-2\mathrm{i}RI}}{2R} + 2\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2+4R^2}\left(2R - e^{-2\mathrm{i}RI}(2R\cosh(nI) - \mathrm{i}n\sinh(nI))\right)\right\} \tag{4}$$

$$= \operatorname{erf}(R) + E(z) + F(z) - e^{-2\mathrm{i}RI}(G(z)+H(z)) \tag{5}$$

The evaluation of Eq. (5) with the five partial functions $\operatorname{erf}(R)$, $E(z)$, $F(z)$, $G(z)$ and $H(z)$ can be done with $I \geq 0$. The sign of the imaginary part of the result is then adjusted according to the symmetry rules. Therefore, the first partial function is

$$E(z) = \frac{e^{-R^2}}{\pi}\frac{1-e^{-2\mathrm{i}RI}}{2R} \qquad \text{with the limit} \qquad \lim_{R\to 0} E(z) = \mathrm{i}\frac{I}{\pi}\,. \tag{6}$$

We shall assume a relative numerical precision of ε defined as the smallest positive number one can subtract(!) from 1 such that the result inequals 1. Further, we shall assume a numerical dynamic range bound by the smallest positive value $\upsilon > 0$ and the largest positive value $\Upsilon < \infty$. Numbers $|m| < \upsilon$ will underflow and produce ± 0 whereas numbers $|M| > \Upsilon$ will overflow and produce $\pm\infty$. For instance, $E(z)$ underflows for $|R| \gtrsim \sqrt{-\log(\pi\upsilon)}$ but never overflows. The second partial function reads as

$$F(z) \approx R\frac{e^{-R^2}}{\pi}\sum_{n=1}^{\lceil N(\varepsilon)\rceil}\frac{e^{-n^2/4}}{n^2/4+R^2} \tag{7}$$

and underflows for $|R| \gtrsim \sqrt{-\log(\pi\upsilon)-1/4}$. The upper sum index $N(\varepsilon)$ is given by $e^{(1-N^2)/4} \lesssim \varepsilon$, i.e. $N(\varepsilon) \gtrsim \sqrt{1-4\log(\varepsilon)}$, which would also account for the worst case $|R| \gg N$. Because $F(z)$ is real, $N(\varepsilon)$ could be reduced with R such that $R/\pi e^{N^2/4+R^2}(N^2/4+R^2) \lesssim \varepsilon\operatorname{erf}(R)$. As we forced I to be positive, the last partial function

$$H(z) \approx \frac{e^{-R^2}}{2\pi}\sum_{n=1}^{\lceil N(\varepsilon)\rceil}\frac{e^{-nI-n^2/4}}{n^2/4+R^2}(R+\mathrm{i}n/2) \tag{8}$$

can be evaluated with the same constraints as $F(z)$ (without decreasing N). Its evaluation can be skipped if $|I| \gtrsim \sqrt{-\log(\varepsilon)}$ because $\varepsilon|G(z)| \gtrsim |H(z)|$ in this case. Finally, the third partial function reads as

$$\begin{aligned} G(z) &\approx \frac{e^{-R^2}}{2\pi}\sum_{n=\max\{1,\lfloor M(I)-N(\varepsilon)\rfloor\}}^{\lceil M(I)+N(\varepsilon)\rceil}\frac{e^{nI-n^2/4}}{n^2/4+R^2}(R-\mathrm{i}n/2) \\ &= \sum_{n=\max\{1,\lfloor M(I)-N(\varepsilon)\rfloor\}}^{\lceil M(I)+N(\varepsilon)\rceil} e^{nI-n^2/4-R^2-\log(2\pi)-\log(n^2/4+R^2)}(R-\mathrm{i}n/2) \end{aligned} \tag{9}$$

and requires closer attention as the sum term becomes maximal at $n = M(I) > 1$ in general. If we assume again the worst case $|R| \gg N$, the maximum is found at $M(I) \approx 2I$. The numerical precision defines the range of the sum index as before. Because $G(z)$ can overflow as well, the central sum term should obey

$$\log(\upsilon) \lesssim I^2 - R^2 - \frac{1}{2}\log(I^2 + R^2) - \log(2\pi) \lesssim \log(\Upsilon) \,. \tag{10}$$

Violation of the lower bound results in underflow and $G(z) = 0$, whereas violation of the upper limit produces $G(z) = \infty - \mathrm{i}\infty$.

Summary Figure 1 shows the magnitude of the error function in the first quadrant of the complex plane $\mathbb{R}\times\mathrm{i}\mathbb{R}$. For large $|R|$, the partial functions $E(z) \to 0$, $F(z) \to 0$ and $H(z) \to 0$ as well. Furthermore, the partial function $G(z) \to 0$ and hence $\mathrm{erf}(z) \to \mathrm{erf}(R)$ if $|I| \ll |R|$. If the real and imaginary part

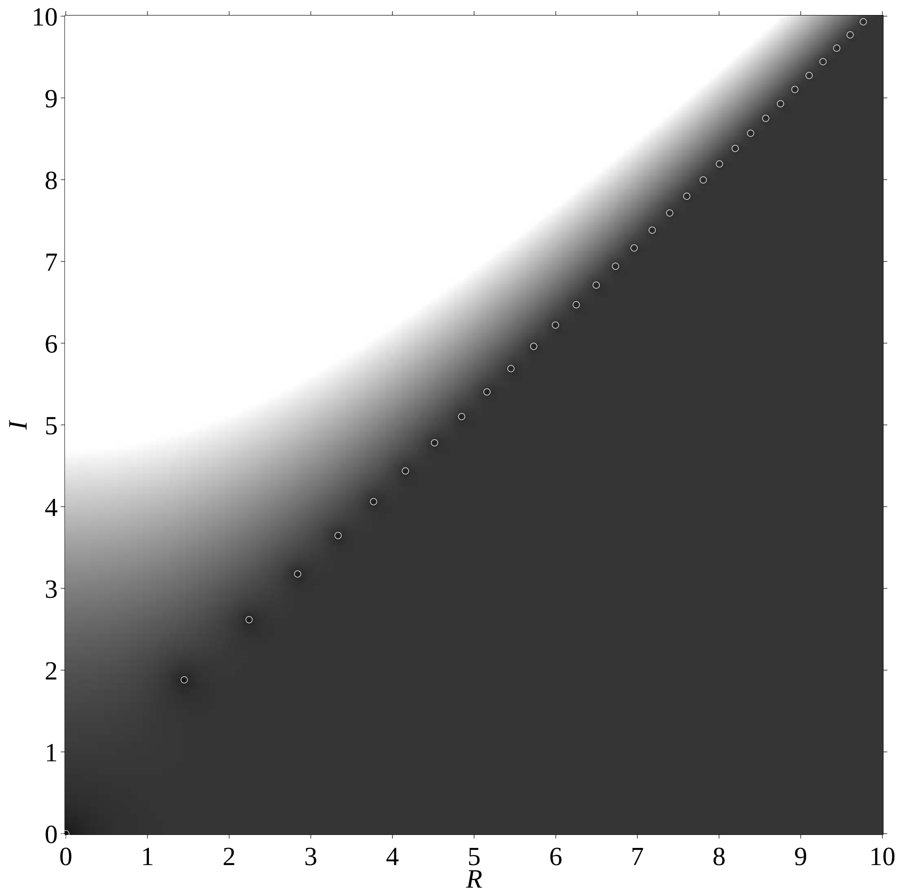

Figure 1: Complex error function $\min\{20, \log|\mathrm{erf}(R + \mathrm{i}I)|\}$. White circles indicate the location of zeros listed in table 1, which are due to phase singularities. The zeros mark the border line above which $\mathrm{erf}(z)$ diverges and below which $\mathrm{erf}(z) \approx \mathrm{erf}(R)$.

$z = R + \mathrm{i}I$	$z = R + \mathrm{i}I$	$z = R + \mathrm{i}I$	$z = R + \mathrm{i}I$
0	4.847970 + 5.101588i	6.960740 + 7.164193i	8.571987 + 8.749670i
1.450616 + 1.880943i	5.158768 + 5.403333i	7.181757 + 7.381187i	8.752713 + 8.927948i
2.244659 + 2.616575i	5.452192 + 5.688837i	7.396234 + 7.591927i	8.929805 + 9.102713i
2.839741 + 3.175628i	5.730854 + 5.960483i	7.604720 + 7.796925i	9.103474 + 9.274167i
3.335461 + 3.646174i	5.996769 + 6.220120i	7.807687 + 7.996629i	9.273911 + 9.442491i
3.769006 + 4.060697i	6.251536 + 6.469216i	8.005553 + 8.191429i	9.441290 + 9.607850i
4.158998 + 4.435571i	6.496444 + 6.708966i	8.198681 + 8.381670i	9.605769 + 9.770396i
4.516319 + 4.780448i	6.732551 + 6.940351i	8.387396 + 8.567659i	9.767493 + 9.930268i

Table 1: The first 32 zeros of $\mathrm{erf}(z)$ in the first quadrant of the complex plane.

are large but of similar magnitude, $G(z)$ stays finite and is the only partial function to be evaluated. However, $G(z)$ and $\mathrm{erf}(z)$ quickly diverge for $|I| > |R|$.

Example If the evaluation is done with the standard IEEE `double` precision, $\varepsilon = 2^{-53}$, $\upsilon = 2^{-1022}$ and $\Upsilon = (1-\varepsilon)2^{1024}$, respectively. Therefore, $N(\varepsilon) \gtrsim 12.2$, which means that summing 13 terms is sufficient to get $F(z)$ and $H(z)$ and no more than 27 terms are required for $G(z)$. The partial functions $E(z)$, $F(z)$ and $H(z)$ all underflow to 0 for $|R| \gtrsim 26.6$. Furthermore, $F(z)$ only requires evaluation up to $n \lesssim N(\varepsilon)\sqrt{1 - R^2/5.82^2}$. The upper bound of $|I|$ before $G(z)$ overflows is reached for $|I| \gtrsim |R|$, that is

$$|I| \lesssim \sqrt{\log(\Upsilon) + \log(2\pi) + R^2 + \frac{1}{2}\log(2R^2)} \approx \sqrt{712 + R^2 + \log(R)}\,. \tag{11}$$

3 Implementation

The error function of a real number is currently implemented piecewise by polynomes with ten non-zero coefficients. For $|R| < 0.3$, the polynome is given directly by the Taylor series (3) with the sum evaluated up to the 9^{th} term. For $0.3 \le |R| < 6$, a total of 57 polynomes of 9^{th} order approximate $\mathrm{erf}(R)$ within intervals of length $\Delta R = 0.1$ to the desired `double` precision. For $|R| \ge 6$, this implementation returns ± 1 as $1 - \mathrm{erf}(|R|) < \varepsilon$.

For complex numbers z, each partial function is only evaluated if it contributes to the result. For instance, none of them is evaluated if $I = 0$ (as all would yield zero) and their real parts do not require evaluation if $R = 0$. Table 2 lists the evaluation conditions for the individual partial functions, where E_r denotes the real part of $E(z)$.

4 MATLAB functions

This software package contains two MATLAB functions `e=erf(r)` and `e=erfz(z)` as MEX-files for Windows. `erf` overloads the default MATLAB error function of real-valued numbers r, but this implementation is about 5–6× faster. `erfz` enhances `erf` to evaluate the error function of complex numbers z too. If called with real numbers r, it is identical to `erf` and equally fast. Users can replace `erf` by `erfz`

Partial function	Evaluated if $I \neq 0$ and
$E(z)$	$R \neq 0$
$E_r(z)$	$\lvert R\rvert < 6.0$
$F(z)$	$0 < \lvert R\rvert < 5.8$
$G_r(z)$	$R \neq 0$
$H(z)$	$\lvert I\rvert < 6.1$ and $\lvert R\rvert < 107$
$H_r(z)$	$R \neq 0$

Table 2: Conditions for the evaluation of the partial functions if $I \neq 0$.

directly if they do not request `erf` to print an error when called with complex numbers. For compatibility with operating systems other than Windows on x86 processors, `erfz` is egally implemented as a normal MATLAB M-file. The M-file relies upon the default `erf` by MATLAB for calculation of $\mathrm{erf}(R)$.

References

[1] M. Abramowitz, I. A. Stegun (ed.), ”Error Function and Fresnel Integrals,” in *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, chapt. 7, 297–309, 9^{th} ed., New York: Dover (1972).

[2] E. W. Weisstein, ”Erf,” from MathWorld–A Wolfram Web Resource, http://mathworld.wolfram.com/Erf.html (Jan 23, 2006).

[3] Wikipedia, ”Error function,” http://en.wikipedia.org/wiki/Error_function (Dec 24, 2007).