Evaluating Error Function on Complex Numbers

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This document outlines an algorithm for computing the error function $\mathrm{erf}(z)$ where z is a complex number. We assume that we can already evaluate $\mathrm{erf}(x)$ for any real number x. The algorithm comes from the note "Error function of complex numbers" by Marcel Leutenegger [2], and it is based on the series expansion given in Abramowitz and Stegun [1]. This document is a rewrite of [2], and I wrote it because I think Leutenegger did a very bad job explaining things.

1 Introduction

- The *error function* is given by:

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

Note that it is a definite integral of the Gaussian distribution wit mean 0 and standard deviation 1. The integral is scaled so that $\mathrm{erf}(+\infty) = 1$.

- For all $z \in \mathbb{C}$, we have that
  - $\mathrm{erf}(-z) = -\mathrm{erf}(z)$, and
  - $\mathrm{erf}(z^*) = \mathrm{erf}(z)^*$ where z^* is the complex conjugate of z.

- The Taylor series expansion of the error function can be derived from the Taylor series of e^{-z^2}:

$$e^{-z^2} = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} z^{2n}.$$

This yields:

$$\mathrm{erf}(z) = \frac{2z}{\sqrt{\pi}} \bigg(1 + \sum_{n=1}^{\infty} \frac{(-1)^n z^{2n}}{n!(2n+1)} \bigg). \tag{1}$$

2 Numerical Evaluation

- One can evaluate $\mathrm{erf}(z)$ upto precision ε by first finding an integer n_c where

$$\frac{|z|^{2n_c}}{n_c!(2n_c+1)} \le \varepsilon.$$

and then add up the first n_c terms of (1). However, n_c depends on the magnitude of z, and this is not good for big $|z|$.

- Abramowitz and Stegun gives a series expansion whose accuracy does not depend on $|z|$:

$$\begin{aligned}\operatorname{erf}(x+iy) = \operatorname{erf}(x) &+ \frac{e^{-x^2}(1-e^{-2ixy})}{2\pi x} \\ &+ \frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2/4+x^2}[2x - e^{-2ixy}(2x\cosh(ny) - in\sinh(ny))] + \epsilon(x,y) \qquad (2)\end{aligned}$$

  where $|\epsilon(x,y)| \approx 10^{-16}|\operatorname{erf}(x+iy)|$.

- Leutenegger proposes breaking (2) — without the $\epsilon(x,y)$ term — into 5 constituent functions:

$$\operatorname{erf}(x+iy) \approx \operatorname{erf}(x) + E(x,y) + F(x,y) - e^{-2ixy}(G(x,y) + H(x,y))$$

  where

$$\begin{aligned}E(x,y) &= \frac{e^{x^2}(1-e^{-2ixy})}{2\pi x} \\ F(x,y) &= \frac{xe^{-x^2}}{\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2/4+x^2}.\end{aligned}$$

  The last two functions come from the derivation:

$$\begin{aligned}&\frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2/4+x^2}[-e^{-2ixy}(2x\cosh(ny) - in\sinh(ny))] \\ &= -e^{-2ixy}\left(\frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2/4+x^2}\left(2x\frac{e^{ny}+e^{-ny}}{2} - in\frac{e^{ny}-e^{-ny}}{2}\right)\right) \\ &= -e^{-2ixy}\left(\frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2/4+x^2}\left(e^{ny}(x-in/2) + e^{-ny}(x+in/2)\right)\right) \\ &= -e^{-2ixy}\left(\frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{ny-n^2/4}}{n^2/4+x^2}(x-in/2) + \frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{-ny-n^2/4}}{n^2/4+x^2}(x+in/2)\right).\end{aligned}$$

  So, we set

$$\begin{aligned}G(x,y) &= \frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{ny-n^2/4}}{n^2/4+x^2}(x-in/2), \text{ and} \\ H(x,y) &= \frac{e^{-x^2}}{2\pi}\sum_{n=1}^{\infty}\frac{e^{-ny-n^2/4}}{n^2/4+x^2}(x+in/2).\end{aligned}$$

- We now seek to evaluate $E(x,y)$, $F(x,y)$, $G(x,y)$, and $H(x,y)$ as accurately as possible relative to a floating point number representation. We make the following assumption about it:
  - Let ε be the *unit in the last place* (ulp) of the system.
  - Let ξ be a positive number such that, if $|x| < \xi$, then x underflows to 0.
  - Let Ξ be a positive number such that, if $|x| > \Xi$, then x overflows to $\pm\infty$
- $E(x,y)$ will underflow if $|x| \geq \sqrt{-\ln(\pi\xi)}$, so there's no need to evaluate it in this case.
- For $F(x,y)$, Leutenegger proposes the following criteria:
  - Skip the evaluation if $|x| \geq \sqrt{-\ln(\pi\xi) - 1/4}$ because the term will underflow.

- Otherwise, evaluate the sum up to $n \approx \sqrt{1 - 4\ln\varepsilon}$.

- Let us define the number of terms we need to evaluate the sum as $N(\varepsilon) = \sqrt{1 - 4\ln\varepsilon}$.
- For $G(x, y)$ and $H(x, y)$, we now assume that $y > 0$ as we can use the rule $\mathrm{erf}(z^*) = \mathrm{erf}(z)^*$ otherwise.
- Given that $y > 0$, here are the criteria for evaluating $H(x, y)$:
  - Skip the evaluation if $|y| \geq \sqrt{-\ln\varepsilon}$ because $\varepsilon|G(x, y)| \geq |H(x, y)|$.
  - Otherwise, evaluate the sum up to $n \approx N(\varepsilon)$.
- Finally, here are the criteria for evaluting $G(x, y)$ given that $y > 0$:
  - Evaluate the sum only if

$$\ln\xi \leq y^2 - x^2 - \frac{1}{2}\ln(y^2 + x^2) - \ln(2\pi) \leq \ln\Xi.$$

    IF the lower equality is violated, then $G(x, y)$ underflows and we can skip the evaluation.
    If the upper inequality is violated, then $G(x, y)$ will overflow, and we can set the whole function equal to $\infty - i\infty$
  - Otherwise, evaluate the sum from $n = \max\{1, \lfloor 2y - N(\varepsilon)\rfloor\}$ to $n = \lceil 2y + N(\varepsilon)\rceil$.
- If the evaluation is done with the IEEE `double`, we have thta $\varepsilon = 2^{-53}$, $\xi = 2^{-1022}$, and $\Xi = (1-\varepsilon)2^{1024}$. We also have that:
  - $N(\varepsilon) \leq 12.2$.
  - As a result, no more than 13 terms are sufficient to evaluate $F(x, y)$ and $H(x, y)$.
  - Also, no more than 27 terms are sufficient to evaluate $G(x, y)$ if $|y| < |x|$.
  - If $|y| < |x|$, the constituent functions underflow to zero if $|x| > 26.6$.
  - We have that, if $|y| > |x|$ and

$$|y| > \sqrt{\ln\Xi + \log(2\pi) + x^2 + \frac{1}{2}\log(2x^2)} \approx \sqrt{712 + x^2 + \ln x},$$

    then there's a good chance that $G(x, y)$ overflows.

References

[1] Milton Abramowitz and Irene A. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables.* Dover, New York, ninth dover printing, tenth gpo printing edition, 1964.

[2] Marcel Leutenegger. Error function of complex numbers. `http://www.mathworks.com/matlabcentral/fileexchange/18312`, 2008.