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Continued Fraction Evaluation of the Error Function

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Abstract. In this paper, continued fraction expansion of the error function is developed. An efficient and simple computational algorithm based on this expansion is also developed using top-down evaluation procedure. Numerical results of the algorithm are in full agreement at least to fifteen digits accuracy with that of the standard tables.

Introduction

The *error function* erf(z) is the integral of the Gaussian distribution, given by

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

and is an entire function of z with no branch cut discontinuities.

The error function is central to many calculations in statistics, for example the inverse error function is defined as the solution for z in the equation s = erf (z). The inverse error function appears in computing confidence intervals in statistics as well as in some algorithms for generating Gaussian random numbers. On the other hand the error function plays very serious role in many problems of space dynamics. Of these problems are for examples, orbit determination of space objects[1] and space navigation problems[2]. Moreover, the error function is now of common appearance in the determination of cosmic distances[3].

There are several methods available for the evaluation of integral (1), all depending on polynomial evaluations with different degrees of accuracy[4,5].

In fact, continued faction expansions are, generally, far more efficient tools for evaluating the classical functions than the more familiar infinite power series. Their convergence is typically faster and more extensive than the series.

Due to the above importance of erf(z), and on the other hand, due to the efficiency of the continued fraction for evaluating functions are what motivated the present work: to establish computational algorithm for the function erf(z) based on its continued fraction expansion.

erf(z) **In Terms of Confluent Hypergeometric Functions**

- Recalling Equation (1) we have

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

Since

$$e^{-t^2} = \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} t^{2j}$$

then

$$\mathrm{erf(z)} = \frac{2}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \int_0^z t^{2j}\, \mathrm{d}t = \frac{2}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(2j+2)} z^{2j+1}$$

$$= \frac{2z}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!(2j+1)} (-z^2)^j$$

$$= \frac{2z}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)\left(\frac{5}{2}\right)\cdots\left(\frac{2j-1}{2}\right)}{\left(\frac{3}{2}\right)\left(\frac{5}{2}\right)\cdots\left(\frac{2j-1}{2}\right)\left(\frac{2j+1}{2}\right)} (-z^2)^j$$

- That is

$$\mathrm{erf(z)} = \frac{2z}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{\left(\frac{1}{2}\right)_j}{\left(\frac{3}{2}\right)_j \; j!} \left(-z^2\right)^j$$

where

$$(\eta)_j = \eta(\eta+1)(\eta+2)\ldots(\eta+j-1) \quad ; \quad (\eta)_0 = 1.$$

- From the above equation it follows that

$$\text{erf(z)} = \frac{2z}{\sqrt{\pi}} M(\frac{1}{2},\frac{3}{2},-z^2)$$

where $M(\beta, \gamma; z)$ is the *confluent hypergeometric function* defined in terms of the *hypergeometric function* $F(\alpha, \beta, \gamma, z)$ as :

$$M(\beta, \gamma; \mathrm{z}) = \lim_{\alpha\to\infty} F(\alpha, \beta, \gamma, z / \alpha) \tag{2}$$

that is

$$M(\beta,\gamma;z) = \sum_{k=0}^{\infty}\frac{(\beta)_k z^k}{(y)_k \ k!} \ .$$

According to Kummer transformation [*e.g.*, See[5]] which is

$$M(\beta, \gamma; \mathrm{z}) = e^z M(\gamma - \beta, \gamma, -z) \ ,$$

then

$$\text{erf}(z) = \frac{2z}{\sqrt{\pi}} \ e^{-z^2} M(1,\frac{3}{2},-z^2) \tag{3}$$

Continued Fraction Expansion of erf(z):

- The confluent hypergeometric functions satisfy the identities[6]

$$M(\beta+1,\gamma+1;z) - M(\beta,\gamma;z) = \frac{\gamma-\beta}{\gamma(\gamma+1)} zM(\beta+1,\gamma+2;z) \tag{4}$$

$$M(\beta+1,\gamma+2;z) - M(\beta+1,\gamma+1;z) = -\frac{(\beta+1)}{(\gamma+1)(\gamma+2)} zM(\beta+2,\gamma+3;z) \ . \tag{5}$$

- Consider the following sequence of confluent hypergeometric functions defined for n = 0, 1, 2.

$$M_{2n} = M(\beta + n, \gamma + 2n; z) \ , \tag{6}$$

$$M_{2n+1} = M(\beta + n + 1, \gamma + 2n + 1; z) \ , \tag{7}$$

- From identities (4) and (5) we have

$$M_{2n+1} - M_{2n} = \delta_{2n+1} \ zM_{2n+2} \ , \tag{8}$$

$$M_{2n} - M_{2n-1} = \delta_{2n} \ zM_{2n+1} \ , \tag{9}$$

where the odd -and -even labed δ's are determined from

$$\delta_{2n+1} = \frac{\gamma-\beta+n}{(\gamma+2n) \ (\gamma+2n+1)} \ , \tag{10}$$

$$\delta_{2n} = -\frac{\beta + n}{(\gamma + 2n)\ (\gamma + 2n + 1)} \ . \tag{11}$$

- Devide Equation (8) by M_{2n} and divide Equation (9) by M_{2n+1} and define

$$G_{2n} = \frac{M_{2n+1}}{M_{2n}}, \tag{12}$$

$$G_{2n-1} = \frac{M_{2n}}{M_{2n-1}}, \tag{13}$$

then we get

$$G_{2n} - 1 = \delta_{2n+1}\ zG_{2n+1}\ G_{2n}\ ,$$

$$G_{2n-1} - 1 = \delta_{2n}\ zG_{2n}\ G_{2n-1}\ ,$$

or

$$G_{2n} = \frac{1}{1 - \delta_{2n+1}\ zG_{2n+1}}\ ,$$

$$G_{2n-1} = \frac{1}{1 - \delta_{2n}\ zG_{2n}}\ .$$

- If we put successively $n = 0$, $n = 1$, *etc.,* we derive a continued fraction expansion for $G_0 = M_1 / M_0$.

$$\frac{M(\beta+1,\gamma+1;z)}{M(\beta,\gamma;z)} = \cfrac{1}{1 - \cfrac{\delta_1 z}{1 - \cfrac{\delta_2 z}{1 - \cfrac{\delta_3 z}{\ddots}}}} \tag{14}$$

$$1 - \delta_{2n}\ zG_{2n}$$

and letting n becomes infinite results in an infinite continued fraction.

- Now since $M(0, \gamma,; z) = 1$, then the continued fraction of Eq. (14) represents the function $M(1, \gamma + 1, z)$. Therefore, if we replace γ by $\gamma - 1$, we get

$$M(1,\gamma;z) = \cfrac{1}{1 - \cfrac{\beta_1 z}{1 - \cfrac{\beta_2 z}{1 - \cfrac{\beta_2 z}{1 - \ddots}}}} \tag{15}$$

where

$$\beta_{2n+1} = \frac{\gamma + n - 2}{(\gamma + 2n - 1)(\gamma + 2n)} \quad , \beta_{2n} = \frac{-n}{(\gamma + 2n - 1)(\gamma + 2n - 2)} \tag{16}$$

Finally, from Eq. (15) and (16) we get for the error function the required continued fraction as

$$\mathrm{erf}(z) = \sqrt{\frac{2}{\pi}} e^{-z^2} \cfrac{\hat{z}}{1 - \cfrac{\hat{z}^2}{3 + \cfrac{2\hat{z}^2}{5 - \cfrac{3\hat{z}^2}{7 + \cfrac{4\hat{z}^2}{9 - \ddots}}}}} \quad ; \ \hat{z} = \sqrt{2} z \tag{17}$$

Computational Developments

Top-Down Continued Fraction Evaluation

There are several methods available for the evaluation of continued fraction. Traditionally, the fraction is either computed from the bottom up, or the numerator and denominator of the n*th* convergent were accumulated separately with three term recurrence formulae. The drawback to the first method is, to decide far down the fraction to being in order to ensure convergence. The drawback to the second method is that the numerator and denominator rapidly overflow numerically even though their ratio tends to a well defined limit. Thus, it is clear that an algorithm which works from top down while avoiding numerical difficulties would be ideal from a programming standpoint.

Gautschi[7] proposed a very concise algorithm to evaluate continued fraction from the top down and was recently applied very successfully for the initial value problem[8]. Gautchi's algorithm may be summarized as follows. If the continued fraction is written as:

$$c = \cfrac{n_1}{d_1 + \cfrac{n_2}{d_2 + \cfrac{n_3}{d_3 + \ddots}}} \equiv \frac{n_1}{d_1 +} \frac{n_2}{d_2 +} \frac{n_3}{d_3 +}$$

then initialize the following parameters

$a_1 = 1,$

$b_1 = n_1 / d_1,$

$c_1 = n_1 / d_1$

and iterate (k = 1, 2, ...) according to

$$a_{k+1} = \frac{1}{1 + \left[\frac{n_{k+1}}{d_k d_{k+1}}\right] a_k} ,$$

$$b_{k+1} = [a_{k+1} - 1] b_k ,$$

$$c_{k+1} = c_k + b_{k+1} .$$

In the limit, the c sequence converges to the value of the continued fraction.

Numerical Results

Top-down continued fraction algorithm was applied for the error function erf(z) [Equation (17)] to construct Table 1 erf(z), z = 0(0.1) 2.9 up to fifteen digits accuracy. Within this accuracy, our results agree completely with those given in[5].

In concluding the present paper, an efficient and simple computational algorithm for the error function erf(z), $z \geq 0$ was established using continued fraction expansion. Numerical results of the algorithm are in full agreement at least to fifteen digits accuracy with that of the standard tables.

Table 1. Values of the error function using continued fraction.

z	erf(z)	z	erf(z)	z	erf(z)
0	0	1.0	0.842701	2.	0.995322
0.1	0.112463	1.1	0.880205	2.1	0.997021
0.2	0.222703	1.2	0.910314	2.2	0.998137
0.3	0.328627	1.3	0.934008	2.3	0.998857
0.4	0.428392	1.4	0.952285	2.4	0.999311
0.5	0.5205	1.5	0.966105	2.5	0.999593
0.6	0.603856	1.6	0.976348	2.6	0.999764
0.7	0.677801	1.7	0.98379	2.7	0.999866
0.8	0.742101	1.8	0.989091	2.8	0.999925
0.9	0.796908	1.9	0.99279	2.9	0.999959

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تقييم دالة الخطأ بطريقة الكسر المستمر

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المستخلص. تم فى هذا البحث تمثيل دالة الخطأ بطريقة الكسر المستمر، وتم أيضًا تشييد طريقة حسابية فعالة وبسيطة لهذا التمثيل باستخدام طريقة القمة والهبوط للتقييم .

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