SCIREA Journal of Mathematics

https://www.scirea.org/journal/Mathematics

August 5, 2019

Volume 4, Issue 4, August 2019

Two New Approximants for the Error Function

D.G. Zaccari[1], C.J. AlturriaLanzardo[2], J.E. Pérez[1,*], J.C. Cesco[3]

[1]Departamento de Física, FCEFQyN, Universidad Nacional de Río Cuarto, Ruta Nac. 36 Km 601, CPX5804BYA, Río Cuarto, Argentina.

[2]Departamento de Matemática, FCEFQyN, Universidad Nacional de Río Cuarto, CONICET, Ruta Nac. 36 Km 601, CP X5804BYA Río Cuarto, Argentina.

[3]Instituto de Matemática Aplicada, Universidad Nacional de San Luis, CONICET; Avda. Ej. de los Andes 950, 1er piso, CP D5700HHW San Luis, Argentina.

*Corresponding author: eperez@exa.unrc.edu.ar

Abstract

In this paper, we present two new approximants for the Error Function. The starting point for obtaining them, is to use two alternative integral representations involving improper integrals. Both integrands include the $\exp(-x^2)$ function. Therefore, by replacing $\exp(x^2)$ by its truncated Taylor's expansion, we obtain a rational approximant for $\exp(-x^2)$ which converges, for each x, to that function. Since these Taylor polynomials have simple roots, the improper integrals can be evaluated with the residues technique of integration in the complex plane, by using an appropriate contour of integration. By just using the roots of the polynomials, we get two new analytical expressions for the Error Function in terms of elementary functions. We show the behaviour of their corresponding errors by giving practical bounds for the absolute and relative errors, respectively.

Keywords: Error function, Complimentary Error function, residues, contour of integration, rational approximant, oscillating integrand, Integral representation, Boys function.

1. Introduction

The Error function [1] page 722

$$erf(x) = \frac{2}{\pi^{0.5}} \int_0^x dz \exp(-z^2) \tag{1}$$

has the following alternative integral representation [2]

$$erf(x) = \frac{2}{\pi} \int_{-\infty}^{+\infty} du\ x\ Sinc(2ux) \exp(-u^2) \tag{2}$$

The Complimentary Error function $erfc(x) = 1 - erf(x)$, also has the following alternative integral representation [2]

$$erfc(x) = \frac{x \exp(-x^2)}{\pi} \int_{-\infty}^{\infty} du \frac{\exp(-u^2)}{u^2 + x^2} \tag{3}$$

With the aim of carrying out their evaluations, we observe that the representations (2) and (3) offer the possibility of replacing the function $\exp(-x^2)$ by a rational approximant [4, 5]; for evaluations in the literature see [3].

Here, we propose the use of the Taylor Polynomial of $\exp(x^2)$ to get the following rational approximating function

$$\exp(-u^2) \cong \left[\sum_{j=0}^{N} \frac{u^{2j}}{j!} \right]^{-1} \equiv A(u,N) \tag{4}$$

for $\exp(-u^2)$. Now, by replacing $\exp(-u^2)$ by $A(u,N)$ in equations (2) and (3), we obtain the following approximants for the Error function and the Complimentary Error function, respectively

$$erfa(x,N) = \frac{2}{\pi} \int_{-\infty}^{+\infty} du\ x\ Sinc(2ux)\ A(u,N) \tag{5}$$

$$erfca(x) = \frac{x \exp(-x^2)}{\pi} \int_{-\infty}^{\infty} du \frac{A(u,N)}{u^2 + x^2} \tag{6}$$

Since for each N, *A(x, N)* has simple poles, which are, in fact, the roots of the corresponding approximating Taylor polynomials of $\exp(x^2)$, the structure of poles of the integrand in equations (5) and (6) is completely known. This fact allows for the *analytical resolution* of these integrations by using well-known integration techniques in the complex plane.

In the following sections, we give the details of the scheme of approximations proposed, i.e. properties of *A(x,N)*, properties of the relative errors involved together with some graphical examples, the corresponding practical bounds of the relative and absolute errors respectively. We end with some concluding remarks.

2. Properties of the *A(x,N)* function

A(x, N) depends on a polynomial whose terms are all even in the variable "*x*" with positive coefficients. We point out that this polynomial has only conjugated complex roots with multiplicity one. Moreover, given a complex root, its opposite complex number is also a root of the polynomial. This implies that *A(x, N)* has only single poles.

Graphically, the Figure 1 shows the roots in the complex plane for some representative examples.

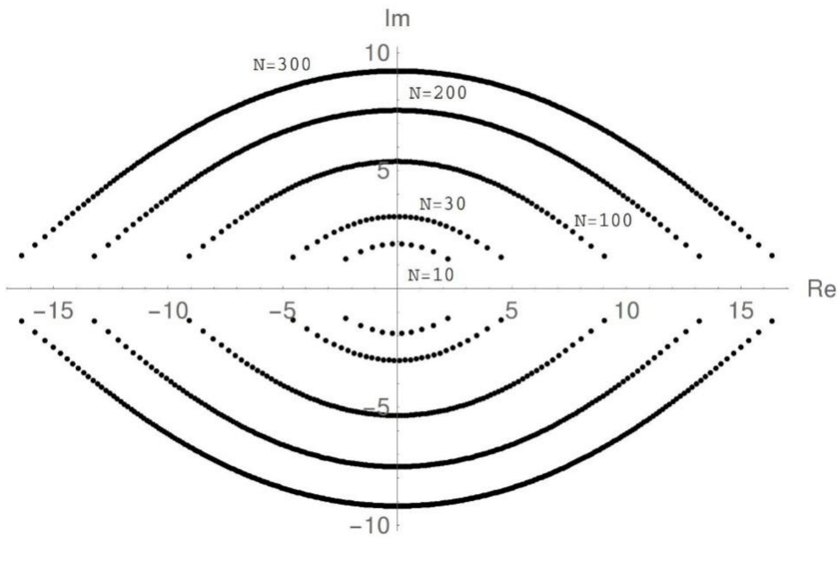

Figure 1

The curves correspond to the roots of the Taylor polynomial of degree 2*N*, for the *A(x, N)* approximant, calculated using the MATHEMATICA software.

We also point out that, for any *u>0*, *A(u, N)* converges to $\exp(-u^2)$ as *N* growth towards infinite, as follows from the next inequalities (see [5])

$$\exp(-u^2) < A(u, N+1) < A(u, N) \tag{7}$$

for *u>0*.

3. Properties of the relative error and, some graphical results.

Let $re(x,N) = \dfrac{\int_0^x du\ A(u,N) - \int_0^x du\ \exp(-u^2)}{\int_0^x du\ \exp(-u^2)}$.

Then, it has the following properties.

Proposition 1: *re(x,N)* is a monotonous non decreasing function of *x*, bounded by

$$\frac{2}{\pi^{0.5}} \int_0^\infty du\ A(u,N) - 1 \tag{8}$$

Proof. The corresponding derivative with respect to x is

$$\frac{\partial er(x,N)}{\partial x} = \frac{\exp(-x^2)\Gamma(N+1,0)}{\int_0^x du\ \exp(-u^2)\ \Gamma(N+1,x^2)} - \frac{\exp(-x^2)\int_0^x du\ \dfrac{\exp(-u^2)\Gamma(N+1,0)}{\Gamma(N+1,u^2)}}{\left[\int_0^x du\ \exp(-u^2)\right]^2} \tag{9}$$

Where

$$\Gamma(x,y) = \int_y^\infty dt\ t^{x-1}\ \exp(-t) \tag{10}$$

$$\frac{\Gamma(N+1,t^2)}{\Gamma(N+1,0)} = \exp(-t^2)\sum_{k=0}^{N} \frac{t^{2k}}{k!} \tag{11}$$

We claim that $re(x,N)$ is a monotone non-decreasing function of x. To prove this, we will show that, for each N, $\dfrac{\partial\ er(x,N)}{\partial x}$ is a non-negative function. In fact, this claim is equivalent to prove that the following

$$Q(x,N)=\frac{\dfrac{\exp(-x^2)\Gamma(N+1,0)}{\int_0^x du\ \exp(-u^2)\ \Gamma(N+1,x^2)}}{\dfrac{\exp(-x^2)\int_0^x du\ \dfrac{\exp(-u^2)\Gamma(N+1,0)}{\Gamma(N+1,u^2)}}{\left[\int_0^x du\ \exp(-u^2)\right]^2}}=$$

$$=\frac{\dfrac{\Gamma(N+1,0)}{\Gamma(N+1,x^2)}}{\dfrac{\int_0^x du\ \dfrac{\exp(-u^2)\Gamma(N+1,0)}{\Gamma(N+1,u^2)}}{\int_0^x du\ \exp(-u^2)}}=$$

$$=\frac{h(x,N)}{\langle h(x,N)\rangle} \tag{12}$$

where

$$h(x,N)=\frac{\Gamma(N+1,0)}{\Gamma(N+1,x^2)} \tag{13}$$

is, for each x, greater or equal to one. But this follows easily by noting that, for each x, the denominator $\langle h(x,N)\rangle$ in (12) is always an average of $h(.,N)$, with respect to the nonnegative weight function $\dfrac{\exp(-u^2)}{\int\limits_0^x du \exp(-u^2)}$ on the interval $[0,x]$, and due the fact that that $h(.,N)$ is a non-decreasing function on that interval.

Consequently, and because *re(x,N)* is a continuous function of *x*, its limit value at infinite provides an upper bound for it, namely,

$$er(x,N)<\frac{\int_0^\infty du\ A(u,N)}{\int_0^\infty du\ \exp(-u^2)}-1$$

$$=\frac{2}{\pi^{0.5}}\int_0^\infty du\ A(u,N)-1\,.\ \blacksquare \tag{14}$$

Some results concerning to the relative errors of the approximants for $erf(x)$ are appreciated in the Figures 2, 3 and 4, as the parameter N is increased.

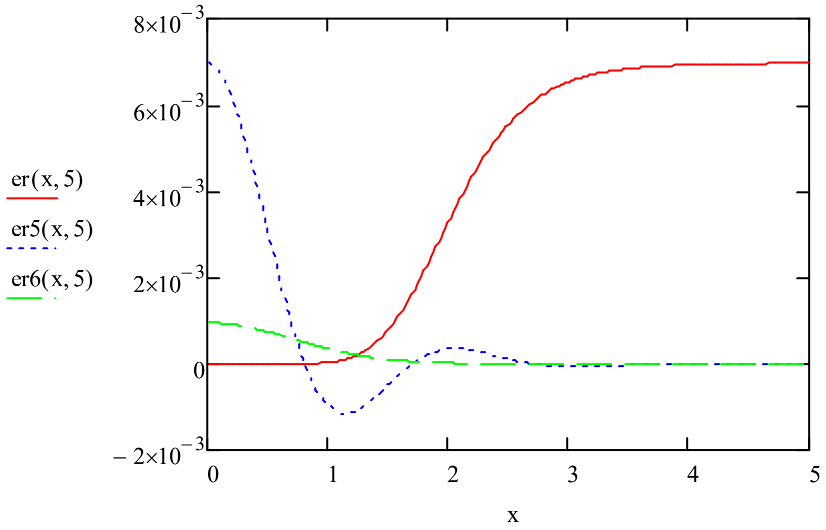

Figure 2.

The relative errors for *erf(x)*: *er(x,N)* corresponds to equation (8), *er5(x,N)* corresponds to equations (2) and (5) and, *er6(x,N)* corresponds to equation (3) and (6).

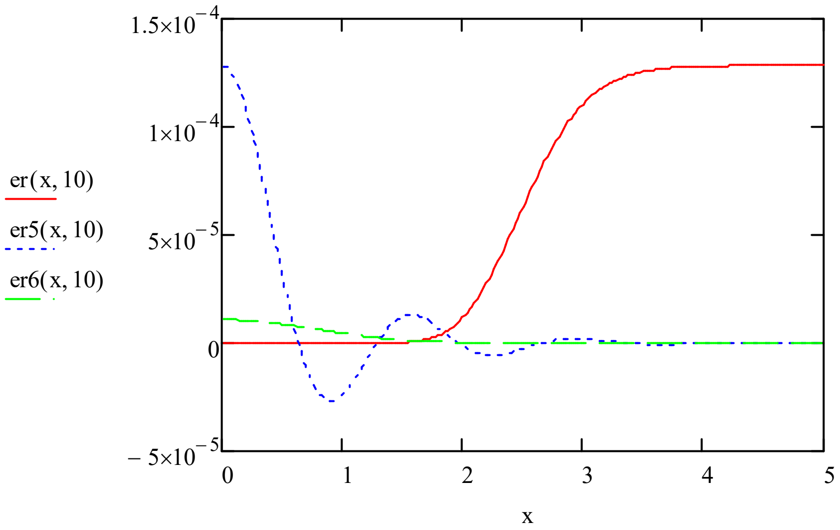

Figure 3.

The relative errors for *erf(x)*: *er(x,N)* corresponds to equation (8), *er5(x,N)* corresponds to equations (2) and (5) and, *er6(x,N)* corresponds to equation (3) and (6).

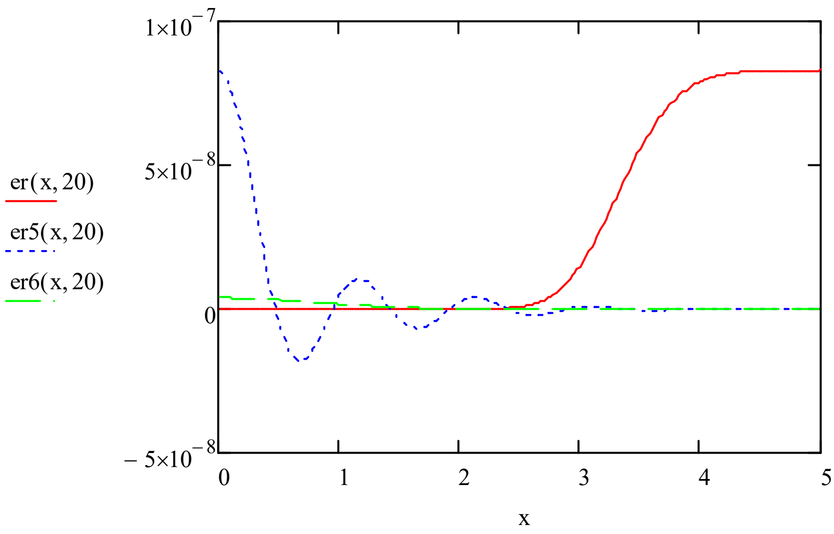

Figure 4.

The relative errors for *erf(x)*: *er(x,N)* corresponds to equation (8), *er5(x,N)* corresponds to equations (2) and (5) and, *er6(x,N)* corresponds to equation (3) and (6).

From Figures 2, 3 and 4, we observe the following property: $er(\infty, N) = er5(0, N)$ i.e. $6.97\ 10^{-3}, 1.28\ 10^{-4}$ *and* $8.30\ 10^{-8}$ corresponding to *N=5,10 and 20,*respectively. According to equation (14), we get a practical bound theoretically sounded.

Also, we have that *er6(0,N)* = $9.52\ 10^{-4}, 1.08\ 10^{-5}$ *and* $3.8\ 10^{-9}$ corresponding to *N = 5, 10 and 20,* respectively; defining a better bound for this case.

4. Another upper bound for the error associated to *erf(x)*

The alternative expression (2) for the Error function allows us to perform another error study. Let us call by *a.e.(x,N)* the absolute error $\frac{2}{\pi}\int_{-\infty}^{\infty} du x Sinc(2ux) A(u,N) - erf(x)$. Then. we have the following result.

Proposition 2: For each *x,*

$$a.e(x,N) \leq \frac{1}{\pi}\left[\int_{-\infty}^{+\infty} du \frac{A(u,N) - \exp(-u^2)}{|u|}\right] \tag{15}$$

Proof. Since

$$a.e.(x,N) \leq \frac{2}{\pi}\int_{-\infty}^{+\infty} du\, |x|\, |Sinc(2ux)| \left[A(u,N) - \exp(-u^2)\right]$$

$$\leq \frac{1}{\pi}\int_{-\infty}^{+\infty} du \quad \frac{|Sin(2ux)|}{|u|}\left[A(u,N)-\exp(-u^2)\right]$$

$$\leq \frac{1}{\pi}\int_{-\infty}^{+\infty} du \quad \frac{\left[A(u,N)-\exp(-u^2)\right]}{|u|}$$

because $|Sin(w)| \leq 1$ for any value of the argument and, the integrand in equation (15) is a well behaved function of *u* around *u=0.*■

The equation (15) shows a bound of the absolute error, which is a decreasing function of *N*.

5. An upper bound of the absolute error of *erfca(x,N)*

Now, let us call by *a.e.c(x,N)* the absolute error

$$a.e.c.(x,N) = erfca(x,N) - erfc(x)$$

Then, we have the following bound.

Proposition 3: For each x,

$$a.e.c.(x,N) < \frac{2\; Max(x\,\exp(-x^2))}{\pi}\int_0^{\infty} du\; \frac{\left[A(u,N)-\exp(-u^2)\right]}{u^2} \qquad (16)$$

Proof.

From (3) and (6), and taking into account (7) again, we get that $a.e.c.(x,N) \leq \frac{Max(|x|\,\exp(-x^2))}{\pi}\int_{-\infty}^{\infty} du\; \frac{\left[A(u,N)-\exp(-u^2)\right]}{u^2+x^2}$

$\leq \frac{Max(|x|\,\exp(-x^2))}{\pi}\int_{-\infty}^{\infty} du\; \frac{\left[A(u,N)-\exp(-u^2)\right]}{u^2}$. But since the integrand in the right member of the later inequality is an even function in *u*, it follows that

$$a.e.c.(x,N) \leq 2\frac{Max(|x|\,\exp(-x^2))}{\pi}\int_0^{\infty} du\; \frac{\left[A(u,N)-\exp(-u^2)\right]}{u^2}.■$$

The equation (16) shows a bound of the absolute error, which is a decreasing function of *N*.

6. An analytical expression for *erfa(x,N)*

Using the contour shown in Figure 5 to the integral in equation (5), we get the following expression for approximating the error function

$$erfa(x,N) = \frac{2}{\pi}\int_{-\infty}^{+\infty} du\ x\ Sinc(2ux)\ A(x,N) =$$

$$= \frac{2x}{\pi}\operatorname{Im}\left\{2\pi i \sum_{u_0} \operatorname{Re} s\left[\frac{e^{i2xu}\ A(u,N)}{2u}, u_0\right] + \pi i \operatorname{Re} s\left[\frac{e^{i2xu}\ A(u,N)}{2u}, u=0\right]\right\}. \qquad (17)$$

Here u_0 denotes the simple poles that the integrand has in the upper half of the complex plane.

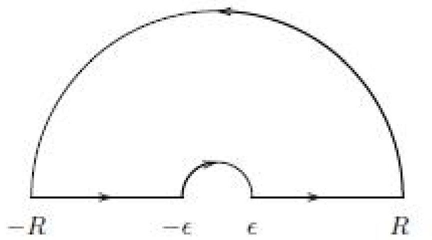

Figure 5.

This contour encloses all the simple poles that the integrand has in the upper half of the complex plane, see Figure 1, and incorporates the simple pole at *z = 0* as usual, when $\varepsilon \to 0$ *and* $R \to \infty$, respectively. See reference [4].

7. Concluding remarks

The decreasing trend of the relative errors *er5(x,N)* and *er6(x,N)* shown in Figures (2), (3) and (4), together with the existence of bounds, as *N* grows, are important properties of the approximants proposed in this work. In all cases, the bound given in equation (14) acts as a kind of reference value. However, the e*r6(x,N)* seems to be superior to e*r5(x,N)* because it has a better behaviour near *x=0* and it does not oscillate.

Relative errors of about 10^{-7} and better are already obtained with *N* = *20, as it is shown* at the end of section 4.

Notably, the approximants given by equations (5) and (6) give the proper behaviour for large values of *x.*

A direct perspective of the present work is the possibility of getting an analytical representation for the Boys function $F_m(x)$ [6], which is useful in Molecular Physics. A particular application [7, 8] involves only the simplest one, i.e. $F_0(x) = \dfrac{\pi^{0.5}\, erf(x^{0.5})}{2\, x^{0.5}}$.

Acknowledgments

Are appreciated grants from SeCyT Universidad Nacional de Río Cuarto and IMASL Universidad Nacional de San Luis–CONICET.

References

[1] Boas M.L., *Mathematical Methods in the Physical Sciences,*3rd ed. John Whiley & Sons, Inc. USA (2006).

[2] Edward W. Ng, Murray Geller, *A Table of Integrals of the Error Functions,* JOURNAL OF RESEARCH of the National Bureau of Standards - B. Mathematical Sciences, Vol. 73B, No. 1, January-March 1969

[3] M. Mori, *A Method for Evaluation of the Error Function of Real and complex Variable with High Relative Accuracy*, Pub. RIMS, Kioto Univ., Vol. 19, 1081-1094 (1983).

[4] J.C. Cesco, J.E. Pérez, C.C. Denner, G.O. Giubergia, A.E. Rosso, *Rational Approximants to evaluate four-center repulsion integrals for 1s hydrogen Slater type functions*, Applied numerical mathematics, vol 55, Issue 2, 173-190 (2005).

[5] S. Särkkä, R. Piché, *On the convergence and accuracy of state-space approximations of squared exponential covariance functions,* 2014 IEEE INTERNATIONAL WORKSHOP ON MACHINE LEARNING FOR SIGNAL PROCESSING, Sept. 21-24, 2014, REIMS, FRANCE.

[6] S.F. Boys, *Electronic wave functions,* Proc. R. Soc. (1950) A200, 542.

[7] J.E. Pérez, O.E. Taurian, J.C. Cesco, A.E. Rosso, C.C. Denner,C.J. Alturria Lanzardo, F.S. Ortiz and A. Bouferguene, *A Basis Set Composed of Only 1s Slater Orbitals and 1s Gaussian Orbitals to Perform Molecular Calculations, SCF-LCAO Approach,* Advances in Quantum Chemistry, Vol 67, Elsevier, 2013, p. 55-64.

[8] J.E. Pérez, J.C. Cesco, C.J. Alturria Lanzardo, D.G. Zaccari, F.S. Ortiz, A.T. Soltermann, P. E. Hoggan, *Considering a mixed atomic basis set composed of only 1s*

STO and 1s GTO in molecular calculations, Chemistry Research Journal, 2019, 4(1):60-66.