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Calculation of the Complementary Error Function of Complex Argument

Error functions of a complex variable arise in several areas of mathematical physics, notably in the dynamic thermoelastic response of solids to rapid heating [1]. In such problems the temperature field satisfies a diffusion equation, while the dynamic response is governed by hyperbolic (wave-type) equations. The resulting forced oscillation is driven by the temperature changes caused by heat addition. For example, the response of a thick spherical shell to internal thermal shock can be expressed in terms of exponentials and error functions of complex arguments [2].

No single, uniformly accurate approximate method exists for calculating the error function complement over the entire complex plane. Series expansions and approximation formulas have limited ranges of validity. The use of existing limited tables of the complex error function or related functions [3] requires bivariate interpolation for both parts of the complex function value. It is desirable to combine computational techniques in a single computer subroutine of general utility. This note describes a FORTRAN function subprogram for calculating the complementary error function of a complex-valued argument at any point in the complex plane.

The error function of complex argument is defined by

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

for an arbitrary integration path in the plane $z = x + iy$. The error function complement is defined by

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty \exp(-\zeta^2)\, d\zeta = 1 - \operatorname{erf}(z) \tag{2}$$

where the integration path is subject to the restriction $\arg(\zeta) \to \theta_0$ with $-\pi/4 < \theta_0 < \pi/4$ as $\operatorname{Re}(\zeta) \to \infty$ along the path [3].

The real and imaginary parts of erf(z) can be expressed as real line integrals in various equivalent forms depending upon the choice of integration path. These forms can be shown to lead to identical results, as they must by virtue of analyticity of erf(z) for finite z. In principle, values of erf(z) can be obtained by numerical evaluation of the defining real integrals. However, the integrands are oscillatory, with frequencies which depend on the real and imaginary parts of z. Thus the numerical integration step size would have to be chosen as a suitable fraction of the period, which in turn depend upon the limit of integration; moreover, evaluation of accuracy would be difficult.

Tabulations of the error function of complex argument are insufficiently dense for most purposes, and it is necessary to develop a rapid computational method for all values of z. Consider the integration path consisting of the line segments $(0, x)$ and $(x, x + iy)$. Then equation (1) can be expressed in the following form:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-\xi^2)\, d\xi + \frac{2i}{\sqrt{\pi}} e^{-x^2} \int_0^y \exp(\eta^2 - 2ix\eta)\, d\eta. \tag{3}$$

To obtain expressions for the real and imaginary parts of erf(z) from the real integrals equivalent to (3), Salzer [4] used the following approximate relation due to Dawson [5]:

$$2\sqrt{\pi}\, \exp(\eta^2) \doteq 1 + 2 \sum_{n=1}^{\infty} \exp(-\mathrm{n}^2/4) \cosh(n\eta). \tag{4}$$

The relative error of this approximation is less than $2 \cdot 10^{-17}$.

In the present work a computational formula was obtained paralleling Salzer's development, retaining the complex representation in (3) and using the exponential equivalent of (4). The first term on the right in equation (3) is the numerically well-known error function of real argument. Using equation (4) in the second term on the right in equation (3), one obtains the following result:

$$\begin{aligned} \operatorname{erf}(z) \doteq{}& \operatorname{erf}(x) + \frac{\exp(-x^2)}{2\pi x}[1 - \exp(-2ixy)] \\ &+ \frac{\exp(-x^2)}{\pi} \sum_{n=1}^{\infty} \frac{\exp(-\mathrm{n}^2/4)}{n^2 + 4x^2} \{4x + i(n + 2ix)\exp[(n - 2ix)y] \\ &- i(n - 2ix)\exp[-(n + 2ix)y]\}. \end{aligned} \tag{5}$$

The relative error in $|\operatorname{erf}(z)|$ using this result is estimated to be about 10^{-16}. The error function complement can be calculated from the right member of equation (2) together with the foregoing result. When $x = 0$ the second term on the right in (5) must be replaced by its limit iy/π.

A computer program was written to calculate the complementary error function of complex argument from equation (5) and the right member of (2), using the complex arithmetic feature available in FORTRAN IV Version 13 programming language. With this feature, complex numbers are regarded as pairs of real numbers corresponding to the real and imaginary parts. Appropriate machine-language subroutines are called to manipulate the real number pairs according to the rules of complex arithmetic.

In the computations, terms of the series in equation (5) are computed successively. The ratio of the square of the length of the incremental complex vector represented by the last computed term, to the squared length of the current sum vector, is compared with the square of a relative length error (ERR) prescribed at 10^{-6}. This accuracy was chosen as reasonably consistent with that of single-precision real arithmetic on the computing equipment used (IBM 7094), in which real constants have precision to 8 decimal digits.

As $z \to \infty$ in $|\arg(z)| < \pi/4$, $\mathrm{erf}(z) \to 1$. Since equation (5) leads to an estimated relative error in $|\mathrm{erf}(z)|$ of 10^{-16}, precision accordingly would be lost in $\mathrm{erfc}(z)$ for large z in this sector of the complex plane. Moreover, the available single-precision subprogram ERF(X) is used to calculate the real complementary error function $\mathrm{erfc}(x)$ which enters into the real part of $\mathrm{erfc}(z)$. For example at $x = 3$, $\mathrm{erfc}(x) = 2 \cdot 10^{-5}$. With 8-digit precision erfc(3) is calculated from $1 - \mathrm{erf}(x)$ with a relative error of $5 \cdot 10^{-4}$.

The complex asymptotic series [3] for $\mathrm{erfc}(z)$ is therefore used in the program for $\mathrm{Re}(z) > 3$ and $|\arg(z)| < \pi/4$:

$$\mathrm{erfc}(z) \sim \frac{\exp(-z^2)}{\sqrt{\pi}\, z} \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{n!(2z)^{2n}}. \tag{6}$$

At $z = 3$ the asymptotic series (real at this point) gives a relative error of about $2 \cdot 10^{-4}$. Precision improves rapidly for larger $\mathrm{Re}(z)$, where the relative error (ERR) in $|\mathrm{erfc}(z)|$ is prescribed at 10^{-6}. Dawson's approximation (4), leading to a relative error of 10^{-16} in (5), nowhere limits the numerical accuracy of the present calculations, and indeed would be adequate for use with equivalent calculations in double-precision real arithmetic.

Coding directly in complex arithmetic is considerably more concise than in equivalent real arithmetic, and simplifies application of numerical convergence tests to terms of the series in (5) and to terms of the asymptotic series (6) as well. For values of $|\mathrm{erfc}(z)|$ as large as 10^6, only 15 terms of the series (5) are required for a relative error of 10^{-6} in the magnitude of the result.

The results of computations using the program were tested against values of the related function $w(z) = \exp(-z^2) \cdot \mathrm{erfc}(-iz)$ tabulated to 6 decimal places [3]. The program was compiled as a closed function subprogram CERFC(Z) to accept an arbitrary complex value of Z and return the desired complex-valued result to the calling program. The source-program listing for this function subprogram is available from the author.

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T. A. Zaker
Engineering Mechanics Division
I.I.T. Research Institute
Chicago, Illinois 60616

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