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A Note on the Evaluation of the Complementary Error Function

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Abstract. A modification is proposed to a method of Matta and Reichel for evaluating the complementary error function of a complex variable, so as to improve the numerical stability of the method in certain critical regions.

In the past twenty years, a number of methods have been proposed for evaluating the complementary error function

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2}\,dt \tag{1}$$

of a complex variable $z = x + iy$ by applying the trapezoidal rule or the mid-ordinate rule to the integral representation

$$\operatorname{erfc}(z) = \frac{ze^{-z^2}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}\,dt}{z^2 + t^2} \qquad (x > 0) \tag{2}$$

(see, e.g., Fettis [2], Luke [4], Hunter [3]). More recently, Chiarella and Reichel [1] have suggested a modification which greatly increases the accuracy of the approximation when x is small. Their method has been further extended by Matta and Reichel [5].

The formula of Matta and Reichel [5] may be expressed in the form

$$\operatorname{erfc}(z) = \frac{hze^{-z^2}}{\pi} \sum_{r=-\infty}^{\infty} \frac{e^{-r^2h^2}}{z^2 + r^2h^2} - R(h) - E(h); \tag{3}$$

the summation represents the trapezoidal rule with interval $h > 0$,

$$\begin{aligned} R(h) &= 2/(e^{2\pi z/h} - 1) && \text{if } x < \pi/h, \\ &= 1/(e^{2\pi z/h} - 1) && \text{if } x = \pi/h, \\ &= 0 && \text{if } x > \pi/h, \end{aligned} \tag{4}$$

and the error $E(h)$ is given by the expression

$$E(h) = \frac{2ze^{-z^2-2\pi^2/h^2}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(t+i\pi/h)^2+2\pi it/h}\,dt}{[1 - e^{-2\pi^2/h^2+2\pi it/h}][z^2 + (t + i\pi/h)^2]} \tag{5}$$

(the Cauchy principal value of the integral being taken if $x = \pi/h$). By using the fact that $|z^2 + (t + i\pi/h)^2| \geqq |x^2 - \pi^2/h^2|$, we may derive from (5) the inequality

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(6) $$|E(h)| \leqq \frac{2\,|ze^{-z^2}|\,e^{-\pi^2/h^2}}{\pi^{1/2}(1 - e^{-2\pi^2/h^2})\,|(x^2 - \pi^2/h^2)|} \qquad (x \neq \pi/h).$$

This inequality indicates that, even with relatively large values of h, the approximation obtained by omitting the error term $E(h)$ in (3) has considerable accuracy for nearly all values of z in the right half-plane. In fact, Matta and Reichel [5] show that the accuracy is generally good even when $x = 0$, despite the fact that the representation (2) then breaks down. However, the method obviously fails if $z = nih$ (n an integer), and is numerically unstable if z is close to one of those values.

Matta and Reichel [5] suggest that this difficulty may be overcome by merely altering the value of h—this will, of course, be ineffectual if z is close to zero. The object of this note is to propose an alternative way round the difficulty. Instead of (3), we may use the formula

(7) $$\operatorname{erfc}(z) = \frac{hze^{-z^2}}{\pi} \sum_{r=-\infty}^{\infty} \frac{e^{-(r+1/2)^2h^2}}{z^2 + (r + \frac{1}{2})^2h^2} + R'(h) + E'(h);$$

the summation now represents the mid-ordinate rule, with interval h,

(8) $$\begin{aligned} R'(h) &= 2/(e^{2\pi z/h} + 1) && \text{if } x < \pi/h, \\ &= 1/(e^{2\pi z/h} + 1) && \text{if } x = \pi/h, \\ &= 0 && \text{if } x > \pi/h, \end{aligned}$$

and

(9) $$E'(h) = \frac{2ze^{-z^2-2\pi^2/h^2}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(t+i\pi/h)^2+2\pi it/h}\,dt}{(1 + e^{-2\pi^2/h^2+2\pi it/h})[z^2 + (t + i\pi/h)^2]}.$$

Inequality (6), with $E(h)$ replaced by $E'(h)$, still holds.

Like the original method, this method breaks down for certain values of z, but, fortunately, not the same values as before—in fact, it fails if $z = (n + \frac{1}{2})ih$ (n an integer). This suggests that we adopt the following criterion:

(a) if $\frac{1}{4} \leqq \varphi(y/h) \leqq \frac{3}{4}$, use the formula given by (3);

(b) otherwise, use the formula given by (7).

Here, $\varphi(y/h)$ denotes the fractional part of y/h, i.e., $\varphi(y/h) = y/h - [y/h]$. Note that, in particular, (7) should be used if z is real and small. For example, when $z = 0$, Eq. (7), with $E'(h)$ omitted, gives the value $\operatorname{erfc}(0) = 1$ exactly, whereas the first two terms on the right in (3) both become infinite.

The above criterion is important only if z is close to one of the values $\frac{1}{2}nih$, but it may safely be applied for any value of z in the right half-plane. Finally, if $x < 0$, we have

(10) $$\operatorname{erfc}(z) = 2 - \operatorname{erfc}(-z).$$

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