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

\[ \text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} e^{-t^{2}} \, dt \]

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

\[ \text{erfc}(z) = \frac{2e^{-x^{2}}}{\pi} \int_{-\infty}^{z} e^{-t^{2}} \, dt \quad (x > 0) \]

(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

\[ \text{erfc}(z) = \frac{hz e^{-x^{2}}}{\pi} \sum_{r=0}^{m} \frac{e^{-r^{2}h^{2}}}{z^2 + r^2 h^2} - R(h) - E(h); \]

the summation represents the trapezoidal rule with interval \( h > 0 \),

\[ R(h) = \begin{cases} 2/(e^{2\pi i/h} - 1) & \text{if } x < \pi/h, \\ 1/(e^{2\pi i/h} - 1) & \text{if } x = \pi/h, \\ 0 & \text{if } x > \pi/h, \end{cases} \]

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

\[ E(h) = \frac{2ze^{-x^{2} - 2\pi i/h^{3}}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(t + i\pi/h)(x + 2\pi i/h)^{2}} dt}{1 - e^{2\pi i/h} + 2\pi i/h} |z^2 + (t + i\pi/h)^2| \]

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

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539
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 $z = n\pi h$ ($n$ 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

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

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

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

and

$$E'(h) = \frac{2z e^{-z^2 - 2\pi^2 h^2}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(1 + iy/h)^2 h^2}}{1 + e^{2\pi^2 h^2 + 2\pi i h / h}} dt.$$

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 $\frac{1}{2} \leq \varphi(y/h) \leq \frac{1}{2}$, 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 $\text{erfc}(0) = 1$ 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 $\frac{1}{2}n\pi h$, but it may safely be applied for any value of $z$ in the right half-plane. Finally, if $x < 0$, we have

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