A Stable Algorithm for Computing the Inverse Error Function in the "Tail-End" Region

By Henry E. Fettis

Abstract. An iterative algorithm, simple enough to be executed on a desk top automatic computer, is given for computing the inverse of the function \( x = \text{erfc}(y) \) for small values of \( x \).

In the present note, a simple method is proposed for computing values of \( y \) for which the function

\[
\text{erfc}(y) = \frac{2}{\pi^{1/2}} \int_y^\infty e^{-\eta^2} \, d\eta
\]

assumes a prescribed value \( x \). This problem occurs in statistics, and also in many problems relating to heat transfer and diffusion. The last mentioned application led Philip [1] to consider the following function

\[
y = \text{inverfc}(x)
\]


When \( x \) is close to unity, the inverted power series for \( \text{erf}(y) = 1 - x \) may be used to advantage. Strecok (loc. cit.) gives the first 200 terms, which may be found from a simple recurrence relation, as well as economized series of Chebyshev polynomials derived from the power series. The series will yield about 20 correct decimal places for \( x > .125 \). For smaller values of \( x \), a new function

\[
R(x) = \frac{1}{\sqrt{\ln(2x - x^2)}} \text{erfc}(1 - x)
\]

is introduced which, in turn, can be expressed, in various intervals of \( x \), by economized series.

In the present note, a simpler method is proposed to handle the region of small \( x \). It is based on the representation of \( \text{erfc}(y) \) as a continued fraction [3]:

\[
\sqrt{\pi} e^{-y^2} \text{erfc}(y) = \frac{t}{1 + \frac{(t^2/2)}{1 + \frac{2(t^2/2)}{1 + \frac{3(t^2/2)}{1 + \cdots}}}} = G(t)
\]

where \( t = 1/y \). Writing \( F(t, x) = G(t)/\pi^{1/2}x \), we obtain the relation
\[ y^2 = \ln F(x, y) \]

which may be solved iteratively as

\[ y_{n+1} = [\ln F(x, y_n)]^{1/2}. \]

As a starting value, Philip's approximation

\[ y \cong [\frac{-\ln \pi^{1/2} x (-\ln x)^{1/2}}{2}]^{1/2} \]

may be used.

The above algorithm works best for small values of \( x \). For larger values, the inverted power series proves to be more economical. One attractive feature of the present algorithm is that it may be used for all values of \( x \) below a certain value, and does not require subdividing this region. Another feature is that it is simple enough to be executed directly on a desk top automatic computer (such as the Hewlett-Packard 9100).

Numerical experiments with the present method indicate that the power series requires more arithmetical operations when \( x < .01 \). The following table lists the comparison in the case where 12 figures of accuracy are required.

<table>
<thead>
<tr>
<th>( x )</th>
<th>Number of terms of power series</th>
<th>Number of terms of continued fraction</th>
<th>Number of Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 ( \times 10^{-6} )</td>
<td>Prohibitive</td>
<td>29</td>
<td>7</td>
</tr>
<tr>
<td>1 ( \times 10^{-4} )</td>
<td>Prohibitive</td>
<td>33</td>
<td>8</td>
</tr>
<tr>
<td>1 ( \times 10^{-2} )</td>
<td>949</td>
<td>51</td>
<td>11</td>
</tr>
<tr>
<td>5 ( \times 10^{-2} )</td>
<td>202</td>
<td>74</td>
<td>14</td>
</tr>
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<td>.1</td>
<td>102</td>
<td>98</td>
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<td>50</td>
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<tr>
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<td>8</td>
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</tr>
<tr>
<td>.9</td>
<td>5</td>
<td>Prohibitive</td>
<td>Prohibitive</td>
</tr>
</tbody>
</table>

Recalculation of Philip's table [1] by the present method* indicates that the following corrections should be made:**

For \( x = 10^{-5} \), \( y = 3.123 \, 413 \, 2743 \),
\[ x = 10^{-4}, \quad y = 2.751 \, 063 \, 9057. \]

The corresponding values of \( B(\theta) = 2/\pi^{1/2} e^{-\theta} \) should be appropriately corrected.

For \( x = 10^{-6} \), \( B = 7.186 \, 679 \, 956 \times 10^{-6} \),
\[ x = 10^{-5}, \quad B = 6.540 \, 392 \, 772 \times 10^{-5}, \]
\[ x = 10^{-4}, \quad B = 5.828 \, 560 \, 144 \times 10^{-4}, \]
\[ x = .05, \quad B = .165 \, 307 \, 6207. \]

* Calculations made by James C. Caslin on the CDC 6600.
** Philip's "\( \theta \)" corresponds to "\( x \)" in the present paper.