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

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

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

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

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

$$y = \operatorname{inverfc}(x)$$

and methods for computing it. Later, Strecok [2] gave a more detailed treatment' and obtained power series expansions and representations in terms of Chebyshev polynomials.

When x is close to unity, the inverted power series for $\operatorname{erf}(y) = 1 - x$ 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

$$R(x) = \operatorname{inverfc}(1 - x)/[-\ln(2x - x^2)]^{1/2}$$

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 $\operatorname{erfc}(y)$ as a continued fraction [3]:

$$\sqrt{\pi}\, e^{-y^2} \operatorname{erfc}(y) = \cfrac{t}{1 + \cfrac{(t^2/2)}{1 + \cfrac{2(t^2/2)}{1 + \cfrac{3(t^2/2)}{1 + \cdots +}}}} = G(t)$$

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

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$$y^2 = \ln F(x, y)$$

which may be solved iteratively as

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

As a starting value, Philip's approximation

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

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.

x	*Number of terms of power series*	*Number of terms of continued fraction*	*Number of Iterations*
1×10^{-6}	Prohibitive	29	7
1×10^{-4}	Prohibitive	33	8
1×10^{-2}	949	51	11
5×10^{-2}	202	74	14
.1	102	98	16
.2	50	150	21
.3	32	220	27
.4	23	323	52
.5	17	492	179
.6	13	Prohibitive	Prohibitive
.7	10	Prohibitive	Prohibitive
.8	8	Prohibitive	Prohibitive
.9	5	Prohibitive	Prohibitive

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

$$\text{For } x = 10^{-5}, \quad y = 3.123\ 413\ 2743,$$

$$x = 10^{-4}, \quad y = 2.751\ 063\ 9057.$$

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

$$\text{For } x = 10^{-6}, \quad B = 7.186\ 679\ 956 \times 10^{-6},$$

$$x = 10^{-5}, \quad B = 6.540\ 392\ 772 \times 10^{-5},$$

$$x = 10^{-4}, \quad B = 5.828\ 560\ 144 \times 10^{-4},$$

$$x = .05, \quad B = .165\ 307\ 6207.$$

* Calculations made by James C. Caslin on the CDC 6600.

** Philip's "θ" corresponds to "x" in the present paper.

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