

On the Calculation of the Inverse of the Error Function*

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Abstract. Formulas are given for computing the inverse of the error function to at least 18 significant decimal digits for all possible arguments up to $1-10^{-300}$ in magnitude.

A formula which yields $\operatorname{erf}(x)$ to at least 22 decimal places for $|x| \leq 5\pi/2$ is also developed.

1. Introduction. In statistical work, many types of probability integrals or sums are approximated by functions which involve the normal probability integral or its inverse. Examples where the inverse is used in the asymptotic expansions of χ^2 distributions can be found in the first four references which are given at the end of this report. J. R. Philip [5] notes that the solution of a one-dimensional concentration-dependent diffusion equation can be obtained with the aid of the inverse error function, and also suggests some formulas which are useful for computation.

Formulas for the direct computation of the inverse error function have also been discussed by L. Carlitz [6]. Moreover, a computer program which obtains the inverse has recently been designed at the University of Chicago [7].

Throughout the remainder of this paper, we will use the notations

$$x = \operatorname{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-t^2} dt \quad \text{and} \quad y = \operatorname{inverf}(x).$$

Since some formulas for y are obtained from numerical values of $\operatorname{erf}(y)$, it is necessary to consider the calculation of $\operatorname{erf}(y)$ also.

2. Formulas for $\operatorname{erf}(y)$. In the well-known Eq. [8]

$$\sum_{m=-\infty}^{\infty} \exp(-K(m+T)^2) = (\pi/K)^{1/2} \sum_{n=-\infty}^{\infty} \exp(-KT^2 + (KT + in\pi)^2/K),$$

we take $K = 25\pi^2$ and $T \leq \frac{1}{2}$ and obtain

$$e^{-(5\pi T)^2} + \epsilon(T) = \left[1 + 2 \sum_{n=1}^{37} e^{-(n/5)^2} \cos 2n\pi T \right] / (5\sqrt{\pi})$$

where $|\epsilon(T)| < 10^{-25}$. If we take $5\pi T = z$ and integrate with respect to z from 0 to y , we see that

$$(1) \quad \operatorname{erf}(y) \approx \frac{2}{\pi} \left[y/5 + \sum_{n=1}^{37} n^{-1} e^{-(n/5)^2} \sin(2ny/5) \right] \quad \text{for} \quad |y| \leq \frac{5\pi}{2}.$$

In order to circumvent the computation of the 37 values of $\sin(2ny/5)$, we transform (1) essentially into a polynomial in $\alpha = 2C^2 - 1$, where $C = \cos(2y/5)$.

Received September 26, 1966.

* Work performed under the auspices of the U.S. Atomic Energy Commission.

From trigonometric identities, we have

$$\sin (2y(2n - 1)/5) = S \cdot P_{2n-1} \text{ and } \sin (2y(2n/5)) = 2CS \cdot P_{2n}$$

where

$$S = \sin (2y/5), \quad P_{m+1} = [1 + (1 + (-1)^m)(\frac{1}{2} + \alpha)]P_m - P_{m-1} \quad (m \geq 2)$$

with $P_1 = 1 = P_2$. When we substitute the appropriate $S \cdot P_{2n-1}$ and $2CS \cdot P_{2n}$ expressions into (1) and simplify the result, we obtain

$$(2) \quad \operatorname{erf} (y) \approx 2y/(5\pi) + S \sum_{n=1}^{19} (A_{1n} + 2C \cdot A_{2n})\alpha^{n-1}.$$

The coefficients A_{1n} and A_{2n} are given in Table 1. These coefficients, as well as all the others given in this report, were computed on the CDC 3600 computer at Argonne National Laboratory.

Formula (2) was checked by comparing numerical values of $\operatorname{erf} (y)$ with the results of the series expansion

$$\operatorname{erf} (y) \approx \frac{2}{\sqrt{\pi}} y \sum_{n=0}^{25} \frac{(-y^2)^n}{n!(2n + 1)}$$

for $y = 10^{-3}$ (10^{-3}) 10^{-1} . The maximum difference between corresponding values was never found to exceed 10^{-23} in magnitude.

For $y > 2$, we used the continued fraction [9]

$$(3) \quad \int_y^\infty e^{-t^2} dt = \frac{e^{-y^2}}{2y+} \frac{1}{y+} \frac{2}{2y+} \frac{3}{y+} \frac{4}{2y+} \dots$$

to obtain

$$(4) \quad \operatorname{erf} (y) = 1 - \frac{2}{\sqrt{\pi}} \int_y^\infty e^{-t^2} dt.$$

The results of (2) and (4) were compared for $y = 2$ (.01) 7.85, and again no differences between corresponding results were found to exceed 10^{-23} in magnitude.

3. The Calculation of $\operatorname{inverf}(x)$ for Small x . If primes indicate differentiation with respect to x , then from $x = \operatorname{erf} (y)$, we have $1 = (2/\sqrt{\pi})e^{-y^2}y'$, or

$$(5) \quad y' = \frac{\sqrt{\pi}}{2} e^{y^2}.$$

Then

$$(6) \quad y'' = 2yy'y'.$$

Carlitz [6] has developed a series expansion from a differential equation similar to (6). However, we will proceed in a different manner.

Equation (6) can be written as $y''(y')^{-2} = 2y$ and integrated to produce $-1/y' = 2 \int y dx + C$. From (5), it is evident that $y' = \sqrt{\pi}/2$ when $y = 0 = x$.

Consequently,

$$(7) \quad -1/y'(x) = 2 \int_0^x y(t)dt - 2/\sqrt{\pi} .$$

Equation (7) can be used for analogue machine computation, since all values at $x = 0$ are known.

It may also be noted that if Eqs. (5) and (7) are combined, then

$$\int_0^x y(t)dt = (1 - e^{-y^2(x)})/\sqrt{\pi} .$$

A similar result which involves $\operatorname{inverf}(1 - x)$ was obtained by Philip [5].

If we now assume that

$$(8) \quad \operatorname{inverf}(x) = \sum_{n=1}^{\infty} C_n x^{2n-1}$$

for small x , then from (7)

$$(9) \quad 1 + \left(\sum_{m=1}^{\infty} (2m - 1) C_m x^{2m-2} \right) \left(\sum_{n=1}^{\infty} n^{-1} C_n x^{2n} - 2/\sqrt{\pi} \right) = 0 .$$

The C_n values can be determined by multiplying the series of (9) and equating the coefficient of each power of x^2 to zero.

The first 200 values of C_n were computed and are given in Table 2. No attempt was made to determine the accuracy of these coefficients directly. Instead, Eq. (8) was used in the calculation of

$$(10) \quad \epsilon_1 = |x^{-1} \operatorname{erf}(\operatorname{inverf}(x)) - 1|$$

and

$$(11) \quad \epsilon_2 = |y^{-1} \operatorname{inverf}(\operatorname{erf}(y)) - 1|$$

for $x = .001$ (.001) .875. In this range, the test calculations have not found any ϵ_1 or ϵ_2 as large as 10^{-22} .

Since the operations which produced Eq. (8) are also valid for complex values $x = z$, it should be possible to obtain good results from (8) whenever the inverse is unique. In this way, it should be feasible to obtain the inverse of Dawson's integral $\int_0^y e^{t^2} dt$ or other special functions for small arguments.

The first 200 terms of (8) were telescoped [10] by W. J. Cody, Jr. of Argonne for the range $|x| \leq .8$. The result, equivalent in accuracy to (8), is expressed in the form

$$(12) \quad \operatorname{inverf}(x) = x \left\{ \xi_0 + \sum_{n=1}^{38} \xi_n T_n \left(\frac{x^2}{.32} - 1 \right) \right\} ,$$

where $T_n(\lambda)$ is the Chebyshev polynomial of degree n in λ and the ξ_n are the coefficients in Table 3.

4. Asymptotic Forms. Philip [5] suggests using a continued logarithm to obtain $\operatorname{inverf}(x)$ for large values of x . However, this asymptotic expansion appears to be accurate only for values of x which are very close to unity.

In Fig. 1 is a plot of $R(x)$ versus y . As the graph illustrates, $R(x)$ increases monotonically from $\sqrt{\pi}/2$ to 1 as y increases from 0 to ∞ , showing that the relative error due to formula (13) is never larger than $2/\sqrt{\pi} - 1$.

The formulas for $R(x)$ which are given below were obtained by applying Chebyshev interpolation [12] to $\text{inverf}(x)/\beta(x)$.

For $.8 \leq x \leq .9975$,

$$(15) \quad R(x) \approx \sum_{n=0}^{26} \lambda_n T_n(D_1 \beta(x) + D_2),$$

where

$$\begin{aligned} D_1 &= -1.54881 \quad 30423 \quad 73261 \quad 65951 \quad 2742, \\ D_2 &= \quad 2.56549 \quad 01231 \quad 47816 \quad 15192 \quad 8163, \end{aligned}$$

and the coefficients λ_n are given in Table 4.

For $25 \cdot 10^{-4} \geq 1 - x \geq 5 \cdot 10^{-16}$,

$$(16) \quad R(x) \approx \sum_{n=0}^{37} \delta_n T_n(D_3 \beta(x) + D_4),$$

where

$$\begin{aligned} D_3 &= -.55945 \quad 76313 \quad 29832 \quad 32254 \quad 36913, \\ D_4 &= \quad 2.28791 \quad 57162 \quad 63357 \quad 63896 \quad 5891, \end{aligned}$$

and the coefficients δ_n are given in Table 5.

For $5 \cdot 10^{-16} \geq 1 - x \geq 10^{-300}$,

$$(17) \quad R(x) \approx \sum_{n=0}^{25} \mu_n T_n(D_5 / (\beta(x))^{1/2} + D_6),$$

where

$$\begin{aligned} D_5 &= -9.19999 \quad 23588 \quad 30151 \quad 03127 \quad 8420, \\ D_6 &= \quad 2.79499 \quad 08201 \quad 24599 \quad 49376 \quad 8426, \end{aligned}$$

and the coefficients μ_n are given in Table 6.

Considering the limitations of our formulas, function subroutines, and roundoff errors, these results are not as accurate as the length of the numbers given in Tables 4, 5, and 6 would seem to imply. Twenty-five decimals are given because it is not known which digits are significant.

Test cases which obtained ϵ_2 in (11) from equations (14) through (17) showed that $\epsilon_2 < 10^{-22}$.

A more severe test case using equations (3), (4), (14), (15), (16), and (17) which obtained

$$\epsilon_3 = |\lambda^{-1}[1 - \text{erf}(\text{inverf}(1 - \lambda))] - 1|$$

showed a larger error, with $\epsilon_3 < 10^{-19}$.

5. Comments on Errors. Since the result produced by the formulas of the preceding section includes an error, Dr. D. Woodward of Argonne contributed some of the ideas discussed below.

Let $y^* = y + \epsilon$ assuming $x = \text{erf}(y)$ is exact. From Taylor's series and Eqs. (5) and (6) we obtain

$$(18) \quad \text{inverf}(\text{erf}(y^*)) = \text{inverf}(\text{erf}(y)) + \sqrt{\pi e^{y^2} h_1} / 2 + \pi(y + \theta_1 \epsilon) / 4 (e^{2(y + \theta_1 \epsilon)^2} h_1^2)$$

and

$$(19) \quad \begin{aligned} & \text{inverfc}(\text{erfc}(y^*)) \\ & = \text{inverfc}(\text{erfc}(y)) + \sqrt{\pi e^{y^2} h_2} / 2 + \pi(y + \theta_2 \epsilon) / 4 (e^{2(y + \theta_2 \epsilon)^2} h_2^2) \end{aligned}$$

where

$$h_1 = \text{erf}(y^*) - \text{erf}(y), \quad 0 < \theta_1 < 1,$$

and

$$h_2 = \text{erfc}(y^*) - \text{erfc}(y), \quad 0 < \theta_2 < 1.$$

If $\eta_m = \sqrt{\pi e^{y^2} h_m} / 2$, ($m = 1, 2$), then Eqs. (18) and (19) can be written as

$$(20) \quad \epsilon = y^* - y = \eta_m + (y + \theta_m \epsilon) \exp \{2\theta_m \epsilon (2y + \theta_m \epsilon)\} \eta_m^2.$$

Equation (20) shows that the error in y is approximately equal in magnitude to η_m when η_m is sufficiently small. For $y \leq 2$, the computer program interpolated for y^* subject to the condition that $|h_1| = |\text{erf}(y^*) - x| < x \cdot 10^{-23}$. Thus $|\eta_1| < \sqrt{\pi e^{y^2} / 2} \cdot x \cdot 10^{-23} < 10^{-21}$. This shows that it is possible to obtain y from x to at least 21 decimal places on the 3600 computer whenever $x \leq \text{erf}(2)$ is known to at least 24 significant decimal places.

For $y > 2$, y^* was obtained with the restriction that

$$|h_2| = |\text{erfc}(y^*) - 1 + x| < (1 - x) 10^{-22}.$$

Then

$$|\eta_2| < \frac{\sqrt{\pi}}{2} e^{y^2} \left(\frac{2}{\sqrt{\pi}} \int_y^\infty e^{-t^2} dt 10^{-22} \right) < 10^{-22}.$$

Since y is never larger than 27 for the range under consideration, formula (20) implies that we can obtain y to at least 21 decimal places for $y > 2$ whenever $\text{erfc}(y)$ is known to at least 22 significant figures.

Since y^* is assumed to be larger than .5, the relative error in y cannot be larger than 2ϵ .

6. Conclusion. Extensive testing with thousands of arguments of 24-decimal significance in the range $0 < |x| \leq 1 - 10^{-300}$ and $0 < |y| \leq 26.2$ showed that we should expect at least 18-decimal significance in the results of all formulas which were developed in this report.

7. Acknowledgments. In addition to those mentioned previously, the author would like to express deep gratitude to Drs. A. Jaffey, R. F. King, and H. C.

Thacher, Jr., of Argonne for many valuable suggestions which were incorporated into this report.

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