

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.

TABLE 2
Coefficients for the series expansion of the inverse, formula (8)

n	C_n	n	C_n	n	C_n
1	.88622	69	.00318	86642	08655
2	.23201	70	.00313	89387	67365
3	.12755	71	.00309	06904	57324
4	.08655	72	.00304	38552	24041
5	.06495	73	.00299	83726	39899
6	.05173	74	.00295	41856	52066
7	.04283	75	.00291	12403	51090
8	.03646	76	.00286	94857	58223
9	.03168	77	.00282	88736	29736
10	.02798	78	.00278	93582	76662
11	.02502	79	.00275	08963	95573
12	.02260	80	.00271	34469	30129
13	.02060	81	.00267	69708	99281
14	.01891	82	.00264	14312	96097
15	.01747	83	.00260	67929	51309
16	.01623	84	.00257	30224	23741
17	.01514	85	.00254	00878	95884
18	.01419	86	.00250	79590	76923
19	.01334	87	.00247	66071	12618
20	.01259	88	.00244	60045	01479
21	.01191	89	.00241	61250	16721
22	.01130	90	.00238	69436	33552
23	.01075	91	.00235	84364	61362
24	.01025	92	.00233	05806	80445
25	.00979	93	.00230	33544	82898
26	.00937	94	.00227	67370	17375
27	.00898	95	.00225	07083	37421
28	.00862	96	.00222	52493	53104
29	.00829	97	.00220	03417	85706
30	.00798	98	.00217	59681	25264
31	.00770	99	.00215	21115	90724
32	.00743	100	.00212	87560	92562
					62953
					57568
					04202
					35837
					61335
					84953
					52243
					92453
					83406
					65527
					01777
					89963
					09447
					06481
					69962
					94100
					68714
					53698
					61222
					32984
					30738
					52077
					14999
					71575
					17534
					51350
					21513
					09601
					42631
					83530
					47496
					17663
					59824
					18068
					54319

33	.00718	43865	11268	31244	41163	101	.00210	58861	97659	96675	94849
34	.00694	99911	01064	71485	71204	102	.00208	34870	96301	18461	02249
35	.00672	98950	85341	52981	82763	103	.00206	15445	71134	36921	81473
36	.00652	28451	61450	06176	43492	104	.00204	00449	67963	94615	04750
37	.00632	77293	64343	14323	00182	105	.00201	89751	68249	69068	75947
38	.00614	35577	70384	15591	68944	106	.00199	83225	63197	47031	77333
39	.00596	94462	69734	45629	43731	107	.00197	80750	29335	39871	89774
40	.00580	46028	53834	30176	03007	108	.00195	82209	05477	18178	65060
41	.00564	83159	75551	56001	75138	109	.00193	87489	70981	77808	56061
42	.00549	99446	26203	96350	84038	110	.00191	96484	25225	22697	78422
43	.00535	89098	41686	44547	02891	111	.00190	09088	68206	67349	78892
44	.00522	46874	03687	49060	98435	112	.00188	25202	82216	29019	67351
45	.00509	68015	44706	20556	63718	113	.00186	44730	14498	00798	38444
46	.00497	48194	99739	04039	88281	114	.00184	67577	60844	76142	39462
47	.00485	83467	74958	48553	68178	115	.00182	93655	50068	36592	79292
48	.00474	70230	25884	97662	30607	116	.00181	22877	29290	20822	02917
49	.00464	05184	55559	03192	53643	117	.00179	55159	50002	67757	97464
50	.00453	85306	57907	08485	61814	118	.00177	90421	54854	72098	92192
51	.00444	07818	43527	18353	22720	119	.00176	28585	65118	09528	52763
52	.00434	70163	95021	51030	52998	120	.00174	69576	68793	83614	82027
53	.00425	69987	07182	72882	76970	121	.00173	13322	09321	18773	20596
54	.00417	05112	74126	17157	11220	122	.00171	59751	74853	75644	17219
55	.00408	73529	91109	02163	84896	123	.00170	08797	88069	98468	15080
56	.00400	73376	43498	14205	67945	124	.00168	60394	96487	20067	07082
57	.00393	02925	59306	47814	84431	125	.00167	14479	63250	50261	86294
58	.00385	60574	05048	21755	18009	126	.00165	70990	58369	59241	18616
59	.00378	44831	07473	82581	56007	127	.00164	29868	50378	39710	66003
60	.00371	54308	86126	04792	43302	128	.00162	91055	98393	91654	37246
61	.00364	87713	83679	09283	72093	129	.00161	54497	44552	22200	15137
62	.00358	43838	82744	56894	82347	130	.00160	20139	06800	91282	66518
63	.00352	21555	99297	86878	26452	131	.00158	87928	72028	62354	06210
64	.00346	19810	44137	66023	08552	132	.00157	57815	89513	37042	31735
65	.00340	37614	44872	07088	72919	133	.00156	29751	64672	64082	26346
66	.00334	74042	21855	56472	07579	134	.00155	03688	53099	16666	40669
67	.00329	28225	12303	31717	05625	135	.00153	79580	54867	29153	58463
68	.00323	99347	37504	23107	34137	136	.00152	57383	09095	74357	93174

TABLE 3
Coefficients for telescoped series, formula (12)

C. Hastings [11] essentially approximates the inverse by using rational functions of $(-\ln t^2)^{1/2}$ where $t = 1/(2\pi)^{1/2} \int_x^\infty e^{-z^2/2} dz$. Since these formulas are of limited accuracy, we recommend a slightly different form, which will now be justified.

Let

$$x^2 = (\operatorname{erf} y)^2 = \frac{4}{\pi} \int_0^y e^{-s^2} ds \int_0^y e^{-t^2} dt = \frac{4}{\pi} \int_0^y \int_0^y e^{-(s^2+t^2)} ds dt.$$

The square over which the integration is performed can be decomposed into two regions, ψ_1 and ψ_2 , where ψ_1 is the quarter circle $s^2 + t^2 \leq y^2$, and ψ_2 is the remainder of the square. Converting to polar coordinates, we see that

$$\frac{4}{\pi} \int_{\psi_1} e^{-(s^2+t^2)} ds dt = \frac{4}{\pi} \int_0^{\pi/2} \int_0^y e^{-r^2} r dr d\theta = \int_0^y e^{-r^2} 2r dr = 1 - e^{-y^2}.$$

Since

$$\frac{4}{\pi} \int_{\psi_2} e^{-(s^2+t^2)} ds dt < \frac{4}{\pi} \int_0^{\pi/2} \int_y^{y\sqrt{2}} e^{-r^2} r dr d\theta = e^{-y^2} - e^{-2y^2},$$

this quantity can be neglected relative to $1 - e^{-y^2}$. Thus $x^2 \approx 1 - e^{-y^2}$ and we take $y \approx [-\ln(1 - x^2)]^{1/2}$ or

$$(13) \quad \operatorname{inverf}(x) \approx (-\ln[(1-x)(1+x)])^{1/2}$$

assuming positive x . Because of Eqs. (3) and (4) it is possible to preserve accuracy in $1 - x$.

To simplify notation, $\beta(x)$ will denote $[-\ln(1 - x^2)]^{1/2}$ throughout the remainder of this discussion.

Formula (13) can be improved if we define a new function $R(x)$ such that

$$(14) \quad \operatorname{inverf}(x) = \beta(x) \cdot R(x).$$

For small x , $\beta(x)$ can be expanded in a power series. Because of this, a power series expansion was also generated for $R(x)$ making use of Eq. (8). The resulting series for $R(x)$ was found to be more strongly convergent than the series (8). Unfortunately, more effort is required to evaluate $\beta(x)$ than to compute the extra terms in (8).

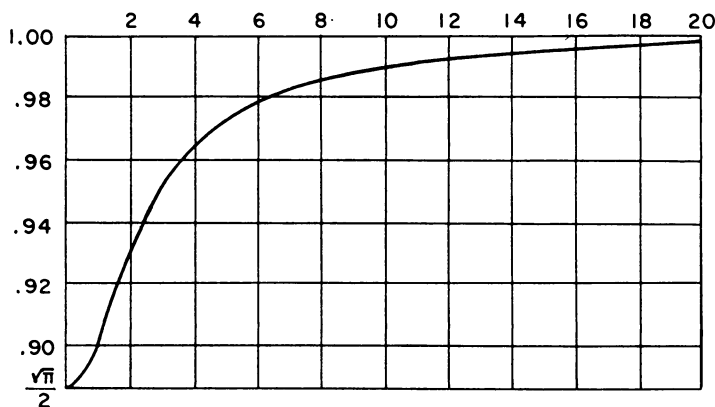


FIGURE 1. $R(X)$ VS. $\operatorname{INVERF}(X)$

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

$$D_1 = -1.54881 \quad 30423 \quad 73261 \quad 65951 \quad 2742,$$

$$D_2 = 2.56549 \quad 01231 \quad 47816 \quad 15192 \quad 8163,$$

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

$$D_3 = -.55945 \quad 76313 \quad 29832 \quad 32254 \quad 36913,$$

$$D_4 = 2.28791 \quad 57162 \quad 63357 \quad 63896 \quad 5891,$$

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

$$D_5 = -9.19999 \quad 23588 \quad 30151 \quad 03127 \quad 8420,$$

$$D_6 = 2.79499 \quad 08201 \quad 24599 \quad 49376 \quad 8426,$$

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 $x = \operatorname{erf}(y)$ is exact. From Taylor's series and Eqs. (5) and (6) we obtain

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

and

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

where

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

and

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

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 $|h_1| = |\operatorname{erf}(y^*) - x| < x \cdot 10^{-23}$. 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 $x \leq \operatorname{erf}(2)$ is known to at least 24 significant decimal places.

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

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

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 $\operatorname{erfc}(y)$ 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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