

On the Calculation of the Inverse of the Error Function*

By Anthony J. Strecok

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 $\text{erf}(x)$ 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

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

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

2. Formulas for $\text{erf}(y)$. 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

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

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 $C = \cos(2y/5)$.

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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 $y = 0 = x$.

TABLE 1
Coefficients for calculating $\text{erf}(Y)$ from formula (2)

n	A_{1n}	n	A_{2n}
1	.70322	50027	43775
2	.33050	15219	16606
3	.20133	97472	64706
4	.10863	02450	22740
5	.04677	55234	32484
6	.01539	85726	15710
7	.00380	15076	79852
8	.00069	71837	92408
9	.00009	44909	26881
10	.00000	94328	11698
11	.00000	06919	27520
12	.00000	00372	25234
13	.00000	00014	66606
14	.00000	00000	42261
15	.00000	00000	00889
16	.00000	00000	00013
17	.00000	00000	00000
18	.00000	00000	00000
19	.00000	00000	00000

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 $\text{inverf}(1 - x)$ was obtained by Philip [5].

If we now assume that

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

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

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

and

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

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

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

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 $\text{inverf}(x)$ 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	69254	52758	01364	90836
2	.23201	36665	34654	49355	35340
3	.12755	61753	05597	95825	39997
4	.08655	21292	41547	53372	96417
5	.06495	96177	45385	41338	20146
6	.05173	12819	84616	37411	26318
7	.04283	67206	51797	34984	46514
8	.03646	59293	08531	62632	55797
9	.03168	90050	21605	44680	96094
10	.02798	06329	64995	22473	34306
11	.02502	22758	41198	34945	71692
12	.02260	98633	18897	57443	28165
13	.02060	67803	79059	00171	87687
14	.01891	82172	50778	85446	34987
15	.01747	63705	62856	54619	04295
16	.01623	15009	87685	25127	52949
17	.01514	63150	63247	80552	03853
18	.01419	23160	02509	96415	11535
19	.01334	73641	97421	29715	03471
20	.01259	40048	71332	06984	15966
21	.01191	82959	36392	03987	38582
22	.01130	89701	05922	53677	22250
23	.01075	68253	03317	95757	77905
24	.01025	42740	81853	46821	40955
25	.00979	50057	70071	17565	18125
26	.00937	37298	19182	08151	68329
27	.00898	59785	02843	37808	80376
28	.00862	79535	80709	43465	25409
29	.00829	64059	27739	24140	44119
30	.00798	85401	62603	35483	77731
31	.00770	19384	32259	76116	63687
32	.00743	44990	17831	53060	38419

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33	.00718	11268	41163	101	.00210	58861	96675	94849
34	.00694	99911	01064	71204	.00208	34870	96301	18461
35	.00672	98950	85341	52981	.00206	15445	71134	02249
36	.00652	28451	61450	06176	.00204	00449	67963	94615
37	.00632	77293	64343	14323	.00182	104	.00201	04750
38	.00614	35577	70384	15591	.00182	105	.00201	75947
39	.00596	94462	69734	45629	.00182	106	.00199	36921
40	.00580	46028	53834	30176	.03007	107	.00197	81473
41	.00564	83159	75551	56001	.00182	108	.00195	68249
42	.00549	99446	26203	96350	.00182	109	.00193	69068
43	.00535	89098	41686	44547	.00182	110	.00191	77333
44	.00522	46874	03687	49060	.00182	111	.00190	77335
45	.00509	68015	44706	20556	.00182	112	.00188	39871
46	.00497	48194	99739	04039	.00182	113	.00186	89771
47	.00485	83467	74958	48553	.00182	114	.00184	89774
48	.00474	70230	25884	97662	.00182	115	.00182	65068
49	.00464	05184	55559	03192	.00182	116	.00181	68206
50	.00453	85306	57907	08485	.00182	117	.00181	67349
51	.00444	07818	43527	18353	.00182	118	.00179	77892
52	.00434	70163	95021	51030	.00182	119	.00177	77892
53	.00425	69987	07182	72882	.00182	120	.00176	77892
54	.00417	05112	74126	17157	.00182	121	.00175	77892
55	.00408	73529	91109	02163	.00182	122	.00174	77892
56	.00400	73376	43498	14205	.00182	123	.00173	77892
57	.00393	02925	59306	47814	.00182	124	.00173	77892
58	.00385	60574	05048	21755	.00182	125	.00173	77892
59	.00378	44831	07473	82581	.00182	126	.00172	77892
60	.00371	54308	86126	04792	.00182	127	.00171	77892
61	.00364	87713	83679	09283	.00182	128	.00170	77892
62	.00358	43838	82744	56894	.00182	129	.00169	77892
63	.00352	21555	99297	86878	.00182	130	.00168	77892
64	.00346	19810	44137	66023	.00182	131	.00167	77892
65	.00340	37614	44872	07088	.00182	132	.00167	77892
66	.00334	74042	21855	56472	.00182	133	.00166	77892
67	.00329	28225	12303	31717	.00182	134	.00165	77892
68	.00323	99347	37504	23107	.00182	135	.00165	77892
						136	.00152	77892
							.09095	77892
							.74357	77892

TABLE 2—Continued

n	C_n	n	C_n	n	C_n
137	.00151	37052	88753	46900	41999
138	.00150	18547	95695	96783	41014
139	.00149	01827	55920	30852	62930
140	.00147	86852	15027	68515	76807
141	.00146	73583	33883	02337	79937
142	.00145	61983	84461	74248	37436
143	.00144	52017	45874	34369	65163
144	.00143	43649	00560	02174	34877
145	.00142	36844	30640	99063	54024
146	.00141	31570	14429	67742	55385
147	.00140	27794	23081	37184	52451
148	.00139	25485	17385	32701	97047
149	.00138	24612	44687	68879	62726
150	.00137	25146	35939	99025	61333
151	.00136	27058	02867	28529	24407
152	.00135	30319	35250	31217	42029
153	.00134	34902	98316	37611	89685
154	.00133	40782	30233	92031	55990
155	.00132	47931	39706	01872	81788
156	.00131	56325	03658	27244	78368
157	.00130	65938	65016	82533	90847
158	.00129	76748	30572	43517	89698
159	.00128	88730	68926	74427	36023
160	.00128	01863	08517	08946	00913
161	.00127	16123	35716	37620	96728
162	.00126	31489	93004	71593	55317
163	.00125	47941	77209	69022	46255
164	.00124	65458	37812	26116	08073
165	.00123	84019	75315	49375	00053
166	.00123	03606	39673	39522	26384
167	.00122	24199	28777	30716	42512
168	.00121	45779	86997	40437	200

TABLE 3
Coefficients for telescoped series, formula (12)

n	ξ_n	n	ξ_n
0	.99288	53766	18940
1	.12046	75161	43104
2	.01607	81993	42099
3	.00268	67044	37162
4	.00049	96347	30235
5	.00009	88982	18599
6	.00002	03918	12763
7	.00000	43272	71617
8	.00000	09380	81412
9	.00000	02067	34720
10	.00000	00461	59699
11	.00000	00104	16679
12	.00000	00023	71500
13	.00000	00005	43928
14	.00000	00001	25548
15	.00000	00000	29138
16	.00000	00000	06794
17	.00000	00000	01591
18	.00000	00000	00374
19	.00000	00000	00088

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

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

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).

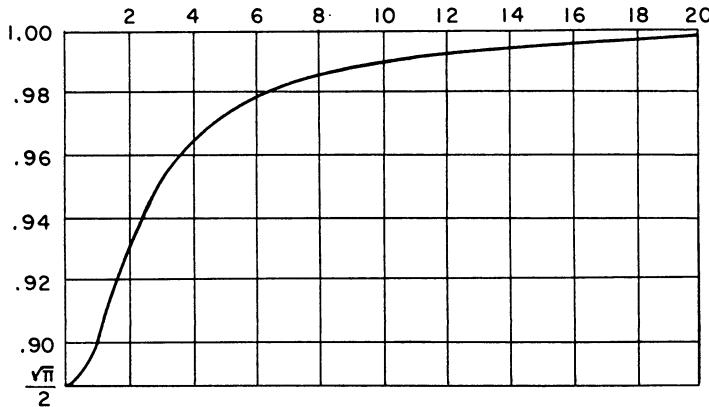


FIGURE 1. $R(X)$ VS. INVERF (X)

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

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

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 $\epsilon_3 < 10^{-19}$.

TABLE 4
Coefficients for calculating $R(x)$ from formula (15)

n	λ_n	n	λ_n	n	λ_n
0	.91215	88034	17553	77330	59200
1	-.01626	62818	67663	69585	46661
2	.00043	35564	72949	44536	50589
3	.00021	44385	70074	45920	65205
4	.00000	26257	51075	76481	30176
5	-.00000	30210	91050	10379	69912
6	-.00000	00124	06061	83675	72157
7	.00000	00624	06609	29999	17380
8	-.00000	00005	40124	79009	57858
9	-.00000	00014	23207	89753	15910
10	.00000	00000	34384	02819	55305
11	.00000	00000	33584	87039	00138
12	-.00000	00000	01458	42885	16512
13	-.00000	00000	00810	58833	21742

TABLE 5
Coefficients for calculating $R(x)$ from formula (16)

n	δ_n	n	δ_n	n	δ_n
0	.95667	97090	20492	52745	26373
1	-.02310	70043	09064	90369	99908
2	-.00437	42360	97508	40773	33218
3	-.00057	65034	22651	18548	09364
4	-.00001	09610	22307	09239	31242
5	.00002	51085	47024	64427	87982
6	.00001	05623	36067	94775	11955
7	.00000	27544	12330	03063	91503
8	.00000	04324	84498	32833	80689
9	-.00000	00205	30336	65520	86916
10	-.00000	00438	91536	66543	16784
11	-.00000	00176	84009	50808	81795
12	-.00000	00039	91289	02804	63420
13	-.00000	00001	86932	41245	59212
14	.00000	00002	72922	73967	46077
15	.00000	00001	32817	21315	65497
16	.00000	00000	31834	24844	82286
17	.00000	00000	01670	06077	51926
18	-.00000	00000	02036	46496	11537

TABLE 6
Coefficients for calculating $R(x)$ from formula (17)

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.

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Argonne National Laboratory
Argonne, Illinois

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