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Note

Numerical Analysis and Evaluation of Normalized Repeated Integrals of the Error Function and Related Functions*

INTRODUCTION

Computations in physics and chemistry often require the calculation of functions related to the repeated integrals of the complementary error function [1]

$$i^n \operatorname{erfc} x = \int_x^\infty dt\, i^{n-1} \operatorname{erfc} t$$
$$= 2\pi^{-1/2} \int_x^\infty dt\, e^{-t^2}(t-x)^n/n! \tag{1a}$$

$$i^{-1} \operatorname{erfc} x = 2\pi^{-1/2} e^{-x^2}. \tag{1b}$$

We have encountered them in molecular quantum mechanics involving overlap integrals between an exponential-type atomic orbital ($r^{k-1}e^{-r}$) and a Gaussian-type atomic orbital ($r^{l-1}e^{-\alpha r^2}$), giving rise to [2]

$$S_n = \int_0^\infty r^n e^{-(r+\alpha r^2)}\, dr, \qquad n = k + l. \tag{2a}$$

It can be shown that they are related to the functions of Eq. (1) by

$$S_n = \tfrac{1}{2}\pi^{1/2} n!\, (4x^2)^{(n+1)/2} (i^n \operatorname{erfc} x)\, e^{x^2} \tag{2b}$$

From a numerical point of view, the functions given in Eqs. (1) and (2) are extremely unsatisfactory because they rapidly vary by many orders of magnitude as n and x increase. For this reason a new set of functions, $\operatorname{erfc}_n(x)$, called "Normalized Repeated Error Integrals", is introduced in this note. They are numerically very-well behaved and, on the basis of a brief numerical analysis, a computational method is described by which they can be evaluated without loss of significant figures. A double-precision FORTRAN IV computer program based on this method has been prepared. It evaluates $\operatorname{erfc}_0(x)$ to at least 15 significant figures and $\operatorname{erfc}_n(x)$ for $n \geqslant 1$ to at least 14 significant figures on the IBM 360/65

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NORMALIZATION

The normalized repeated error integrals are defined as

$$\mathrm{erfc}_n(x) = 2^n \Gamma(1 + n/2)(i^n \,\mathrm{erfc}\, x)\, e^{x^2}$$
$$= \left[2/\Gamma\left(\frac{n+1}{2}\right)\right] \int_x^\infty dt(t-x)^n\, e^{-t^2+x^2}, \qquad \text{for} \quad n = 0, 1, \ldots, \tag{3a}$$

$$\mathrm{erfc}_0(x) = e^{x^2}\,\mathrm{erfc}\, x, \tag{3b}$$

$$\mathrm{erfc}_{-1}(x) = 1. \tag{3c}$$

The behavior of these functions for $0 \leqslant n \leqslant 5000$ and $10^{-5} \leqslant x \leqslant 10^4$ is exhibited in Fig. 1.[1] Note that

$$\lim_{n\to\infty} \mathrm{erfc}_n(x) = 0. \tag{3d}$$

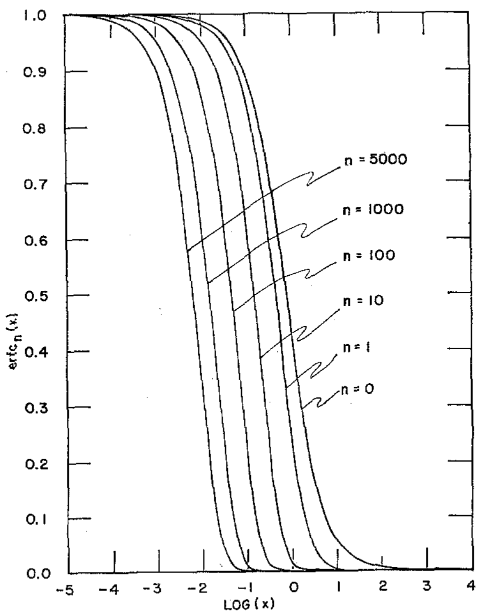

FIG. 1. Behavior of $\mathrm{erfc}_n(x)$.

[1] The logarithms to base 10 and e are denoted by "log" and "ln", respectively.

Figure 1 suggests that it may be useful to write

$$\operatorname{erfc}_n(x) = \operatorname{erfc}_0[xg_n(x)] \quad \text{or} \quad \operatorname{erfc}_n(x) = \operatorname{erfc}_1[xh_n(x)], \tag{4a}$$

where $g_n(x)$ and $h_n(x)$ can be expected to be slowly varying functions. A rough numerical examination yielded the expression

$$\begin{aligned} \log g_n(x) &= g'(\mu) + xg''(\mu), \\ g'(\mu) &= 0.53\mu, \\ g''(\mu) &= \mu(0.59 - 1.49\mu + 0.98\mu^2 - 0.06\mu^3), \\ \mu &= \log(n+1). \end{aligned} \tag{4b}$$

The accuracy of this approximation, as seen from Table I, indicates that this approach can be further refined.

TABLE I

Comparison between $\operatorname{erfc}_n(x)$ and $\operatorname{erfc}_0[xg_n(x)]$.

$\log x$	$\operatorname{erfc}_{10}(x)$	$\operatorname{erfc}_0(xg_{10})$	$\operatorname{erfc}_{100}(x)$	$\operatorname{erfc}_0(xg_{100})$	$\operatorname{erfc}_{1000}(x)$	$\operatorname{erfc}_0(xg_{1000})$
−3	0.995	0.995	0.986	0.986	0.956	0.958
−2.5	0.988	0.988	0.957	0.960	0.866	0.864
−2	0.956	0.961	0.870	0.874	0.640	0.620
−1.5	0.866	0.876	0.640	0.641	0.240	0.192
−1	0.640	0.668	0.244	0.246	0.011	0.010
−0.5	0.240	0.340	0.010	0.021	0.000	0.000
0	0.016	0.044	0.000	0.000	0.000	0.000

Recurrence Relation

The computational method to be described is based on the recurrence relation for the functions (3), viz.,

$$\operatorname{erfc}_n(x) = -x\gamma(n)\operatorname{erfc}_{n-1}(x) + \operatorname{erfc}_{n-2}(x), \qquad n = 2, 3, \ldots, \tag{5a}$$

$$\operatorname{erfc}_1(x) = -x\gamma(1)\operatorname{erfc}_0(x) + 1, \tag{5b}$$

where

$$\gamma(n) = \Gamma\left(\frac{n}{2}\right) \Big/ \Gamma\left(\frac{n+1}{2}\right), \tag{6a}$$

$$\gamma(n) = \frac{(n-2)(n-4)(n-6)}{(n-1)(n-3)(n-5)} \cdots \begin{cases} \cdots \dfrac{3.1}{4.2}\, \pi^{1/2}, & \text{if } n = \text{odd}, \\ \cdots \dfrac{4.2}{5.3}\, 2\pi^{-1/2}, & \text{if } n = \text{even}. \end{cases} \tag{6b}$$

This relation is obtained from the recurrence relation for $i^n \operatorname{erfc} x$ given by Abramowitz [1]. Some approximate values of $\gamma(n)$ are as follows:

n	1	2	3	10	100	1000
$\gamma(n)$	1.772	1.128	0.886	0.459	0.142	0.0447

For very small values of x, the functions

$$\operatorname{erf}_n(x) = 1 - \operatorname{erfc}_n(x) \tag{7}$$

are preferable. They satisfy the relations

$$\operatorname{erf}_n(x) = \operatorname{erf}_{n-2}(x) + x\gamma(n)[1 - \operatorname{erf}_{n-1}(x)], \tag{8a}$$

$$\operatorname{erf}_1(x) = x\gamma(1)[1 - \operatorname{erf}_0(x)], \tag{8b}$$

$$\operatorname{erf}_0(x) = e^{x^2} \operatorname{erf} x + (1 - e^{x^2}), \tag{8c}$$

$$\operatorname{erf}_{-1}(x) = 0. \tag{8d}$$

As one recurs forward, significant figures are lost if n becomes too large. We have been concerned with generating $\operatorname{erfc}_n(x)$ to an accuracy of at least 14 significant figures. In this case, forward recursion is applicable for

$$(n + 1) \leqslant R(x) = 1.3/x^2. \tag{9}$$

The curve $R(x)$ is shown in Fig. 2 where, because of the logarithmic representation, it appears as a straight line. Since, in practice, all functions with $0 \leqslant n \leqslant N$ are needed together, our method and program evaluates and stores all those functions simultaneously. Two cases arise: $N < R(x)$ and $N \geqslant R(x)$. If $N < R(x)$, forward recursion is used. If $N \geqslant R(x)$, backward recursion is used all the way to $n = 0$.

Forward Recursion, for $N < R(x)$

In this case, the recurrence relation (5) or (8) is used to generate all the $\operatorname{erfc}_n(x)$. The factors $\gamma(n)$ occurring in it can be calculated from

$$\gamma(n) = \gamma(n-2)[1 - (n-1)^{-1}], \tag{10a}$$

$$\gamma(n)\,\gamma(n+1) = 2/n, \tag{10b}$$

$$\gamma(1) = \pi^{1/2}, \qquad \gamma(2) = 2\pi^{-1/2}. \tag{10c}$$

For the calculation of $\mathrm{erfc}_0(x)$, two ranges of x have to be distinguished. If $x \leqslant 13.3$, the complementary error function (erfc x) can be approximated by a polynomial whose coefficients are obtained from expansions in Chebyshev polynomials [3]. The IBM 360-supplied library subprogram uses this method. This function is then multiplied by e^{x^2} to obtain $\mathrm{erfc}_0(x)$. For $x > 13.3$, e^{x^2} overflows ($>10^{75}$) the computer, and $\mathrm{erfc}_0(x)$ is obtained from the continued fractions given by Abramowitz [1],

$$\pi^{1/2}\,\mathrm{erfc}_0(x) = \frac{1}{x+}\,\frac{1/2}{x+}\,\frac{1}{x+}\,\frac{3/2}{x+}\,\frac{2}{x+}\cdots \qquad \text{for} \quad x > 0. \tag{11}$$

The procedure described by Abramowitz [4] is used in calculating Eq. (11). An exhaustive search for finding the optimal method for evaluating $\mathrm{erfc}_0(x)$ over the entire argument range was not made.

For small values of x the recurrence relations (8) together with $\mathrm{erf}_0(x) = 2\pi^{-1/2}x + 0(x^3)$ yields

$$\mathrm{erf}_n(x) \approx x\{\gamma(n) + \gamma(n-2) + \gamma(n-4) + \cdots + \gamma(1) \text{ or } \gamma(0)\}, \tag{12}$$

where $\gamma(0)$ is defined by $\gamma(0) = \gamma(2)$. From this equation, it is found that

$$\mathrm{erf}_n(x) < 10^{-16.15}, \qquad \text{if} \quad (n+1) < L(x) = 10^{-31.53}\,x^{-1.94}. \tag{13}$$

The line $L(x)$ also appears as a straight line in Fig. 2. Below this line, $\mathrm{erfc}_n(x)$ is indistinguishable from 1 for the computer. Thus, the upward recurrence relation (5) works only for $(n+1) > L(x)$. For $(n+1) < L(x)$ the recurrence relations (8) must be used.

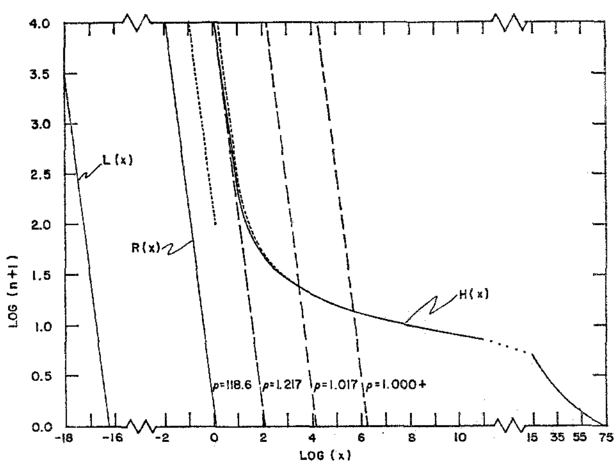

FIG. 2. Regions in the (x, n) plane referring to orders of magnitude and recursive evaluation of $\mathrm{erfc}_n(x)$.

BACKWARD RECURSION, FOR $N \geqslant R(x)$

The choice of starting values required for backward recursion has been carefully discussed by Gautschi [5] for general recursion relations of the type (5). This section is concerned with the implementation of his general results in the present case.

The algorithm as applied to $\operatorname{erfc}_n(x)$ is as follows. First, a set of functions $P_n = K \operatorname{erfc}_n(x)$ is found, where K is independent of n but not of x. If N is the maximum value of n desired, and p the number of significant digits desired, the two starting functions required for the backward recursion are chosen as

$$P_\nu = 0, \qquad P_{\nu-1} = \text{an arbitrary constant,} \tag{14}$$

where the index ν must satisfy

$$\nu \geqslant N[1 + (p \ln 10 + \ln 2)/2(2N)^{1/2}x]^2.$$

In our case $p = 15$ and, thus, we choose

$$\nu = N\rho, \tag{15}$$

where

$$\rho = \rho(N, x) = (1 + 12.4566/xN^{1/2})^2 \tag{16}$$

The values of P_n for $n < \nu - 1$ are then generated using the backward recursion relation,

$$P_{n-2} = x\gamma(n)\, P_{n-1} + P_n \tag{17}$$

until P_0 is obtained. This P_0 is compared with $\operatorname{erfc}_0(x)$, and K^{-1} is found as

$$K^{-1} = \operatorname{erfc}_0(x)/P_0\,. \tag{18}$$

The desired functions are then obtained from

$$\operatorname{erfc}_n(x) = K^{-1}P_n\,, \qquad 1 \leqslant n \leqslant N. \tag{19}$$

The function $\operatorname{erfc}_0(x)$ and the factors $\gamma(n)$ are calculated as before. From Fig. 1, it is evident that the values of P_n will increase during backward recursion. For this reason, the constant in Eq. (14) is chosen as 10^{-75}.

The factor ρ in Eq. (15) is always > 1. It is of some interest to know its dependence upon N and x. It is apparent that the lines $\rho =$ constant will also be straight lines in Fig. 2. Some of them are shown, with the appropriate ρ value indicated, as dashed lines. The largest ρ value, namely $\rho = 118.6$, occurs for the line $R(x)$, which denotes the lower limit of the downward recursion region. The values of ν, corresponding to points on *this* line according to Eq. (15), are indicated by a dotted straight line in Fig. 2.

If, for a given x and N, ν is chosen smaller than the value of Eq. (15), then the accuracy obtained deteriorates more and more below 15 significant figures, as ν is decreased below the value of Eq. (15). On the other hand, no further improvement in accuracy within the first 15 figures occurs, if one chooses ν larger than the value of Eq. (15).

Upper Limit for Backward Recursion

For sufficiently large values of x and N, the functions $\operatorname{erfc}_n(x)$ will underflow a given computer. For large values of x, the limiting behavior is

$$\operatorname{erfc}_n(x) \approx \Gamma(1 + n/2)/\pi^{1/2}x^{n+1}. \tag{20}$$

The curve where $\operatorname{erfc}_n(x) = 10^{-75}$ is indicated by $H(x)$ in Fig. 2. Hence, $\operatorname{erfc}_n x = 0$ for $n > H(x)$ on our computer. In particular, one has $\operatorname{erfc}_0(x) = 0$ for $x = 10^{74.75}$; hence this is the largest x value for which any $\operatorname{erfc}_n(x)$ is nonzero. For $n \geqslant 1$, the curve $H(x)$ is given by

$$(\log H + 2\log x - 4.16)(\log H + 0.1\log x - 1.66) = 0.33, \quad \text{if } 0 < \log x \leqslant 1.70, \tag{21a}$$

$$(\log H + 2\log x - 4.16) = 7.02(\log H - 0.04\log x - 2.05), \quad \text{if } 1.70 < \log x < 37. \tag{21b}$$

It has the straight line $\log(n + 1) = 4.16 - 2\log x$ as an asymptote. The latter corresponds to a ρ value of 1.217.

It can be seen that no overflow or underflow problems occur in the use of Eqs. (18) and (19) if the initial value of ν in Eq. (14) is chosen to be $<H(x)$ and $P_{\nu-1} = 10^{-75}$ as mentioned before. Hence, $\operatorname{erfc}_n(x)$ is set equal zero for all n values $\geqslant H(x)$ and Eq. (15) is replaced by

$$\nu = \min\{N\rho, H(x)\}. \tag{22}$$

The difference between ν and N, as given by Eq. (15), is negligible for N lying on the line $H(x)$. This can be seen from the dotted curve which gives the ν value corresponding to N values on $H(x)$.

The functions $i^n \operatorname{erfc} x$ and $S_n(x)$, mentioned in the introduction, yield considerably more limited computational schemes, because the orders of magnitude of these functions change much more drastically with n and x.

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