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Chebyshev Approximation of $(1 + 2x)\exp(x^2)\operatorname{erfc} x$ in $0 \leqslant x < \infty$

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Abstract. We have obtained a single Chebyshev expansion of the function $f(x) = (1 + 2x)\exp(x^2)\operatorname{erfc} x$ in $0 \leqslant x < \infty$, accurate to 22 decimal digits. The presence of the factors $(1 + 2x)\exp(x^2)$ causes $f(x)$ to be of order unity throughout this range, ensuring that the use of $f(x)$ for approximating $\operatorname{erfc} x$ will give uniform relative accuracy for all values of x.

I. Introduction. The functions $\operatorname{erfc} x = (2/\sqrt{\pi})\int_x^\infty \exp(-t^2)\,dt$ and $\exp(x^2)\operatorname{erfc} x$ occur frequently in kinetic theory of gases and related subjects. Calculation of these functions using the identity $\operatorname{erfc} x = 1 - \operatorname{erf} x$, together with available approximations [1] for $\operatorname{erf} x$, usually results in large relative errors for large x because $\operatorname{erf} x \to 1$ as $x \to \infty$. To overcome this difficulty, Clenshaw [2], Luke [3], [4], and Schonfelder [5] have presented Chebyshev approximations in which the range $0 \leqslant x < \infty$ is split into two ranges $0 \leqslant x \leqslant c$ and $c \leqslant x < \infty$, with $\operatorname{erf} x$ being Chebyshev-approximated in $0 \leqslant x \leqslant c$, and $x\exp(x^2)\operatorname{erfc} x$ being Chebyshev-approximated in $c \leqslant x < \infty$. Clenshaw [2] uses $c = 4$, 33 terms for $x \leqslant 4$ and 18 terms for $x > 4$, and obtains an accuracy of twenty decimal places (20D). Corresponding figures for Luke [3], [4] and Schonfelder [5] are $c = 3$, 25 and 22 terms, and 20D; and $c = 2$, 27 and 43 terms, and 30D. These authors use various transformations $t(x)$ to map $c \leqslant x < \infty$ into $-1 \leqslant t < 1$. Use of the identity $\operatorname{erfc}(-x) = 2 - \operatorname{erfc} x$ eliminates the need to approximate $\operatorname{erfc} x$ for negative x.

Schonfelder [5] has also presented a single 43-term Chebyshev expansion of $\exp(x^2)\operatorname{erfc} x$ for the entire interval $0 \leqslant x < \infty$, using a relation of the form $t = (x - k)/(x + k)$ to map this interval into $-1 \leqslant t < 1$. Oldham [6] has presented a simple approximation of $\sqrt{\pi}x\exp(x^2)\operatorname{erfc} x$, having a maximum relative error of one part in 7000 and suitable for hand calculation.

Whenever a function to be Chebyshev-approximated has a zero within its interval of definition or at either end of it, such an approximation is likely to give large relative errors near such a zero because the usual procedures for calculating Chebyshev coefficients minimize maximum *absolute* error. Accordingly, it is advantageous to multiply $\operatorname{erfc} x$ by factors which yield a product of order unity for all x in $(0, \infty)$ and then to Chebyshev-approximate this product function, because one will then obtain good uniformity of relative as well as absolute error. Our chosen function, $f(x) = (1 + 2x)\exp(x^2)\operatorname{erfc} x$, satisfies this criterion. It has limiting values

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of 1 and $2/\sqrt{\pi} \approx 1.13$ at $x = 0$ and $x \to \infty$, respectively. In comparison, Schonfelder's function $\exp(x^2)\text{erfc}\, x$ approaches 0 as $x \to \infty$. Furthermore, our choice contains no irrational coefficients, in contrast with the more obvious choice $(1 + \sqrt{\pi}x)\exp(x^2)\text{erfc}\, x$, which $\to 1$ at $x = 0$ and $x \to \infty$. A graph of $f(x)$ appears in Figure 1.

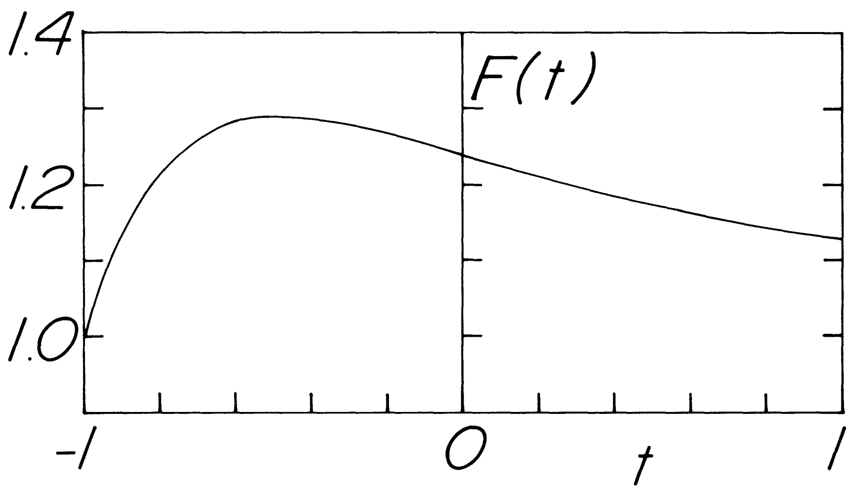

FIGURE 1

Graph of the function $F(t)$ defined by the relation $f(x) = (1 + 2x)\exp(x^2)\text{erfc}\, x$ together with the mapping $t = (x - 3.75)/(x + 3.75)$.

We have used the same transformation as that of Schonfelder [5], i.e. $t = (x - k)/(x + k)$ with $k = 3.75$, to map $0 \leqslant x < \infty$ into $-1 \leqslant t < 1$. Tests of various k values for our $f(x)$ yielded results similar to his, namely that this value gives near-optimum convergence of the resulting Chebyshev series over the precision range of greatest interest, i.e. 8D to 18D. Our calculations were done in IBM quadruple precision, which yields a machine precision of 34D.

II. Calculation of Chebyshev Coefficients. We have used the usual [7] form of an mth-order Chebyshev expansion. Thus, the Chebyshev polynomials $T_j(t)$ are given by

(1) $$T_j(t) = \cos(j \arccos t); \qquad j = 0, 1, 2, \ldots .$$

The above-mentioned $f(x)$ and transformation from x to t define a function $F(t)$ which is expanded as follows:

(2) $$F(t) = \sum_{j=0}^{m} c_j T_j(t),$$

where

(3) $$c_j = \frac{\sum_{k=0}^{m} F(t_k) T_j(t_k)}{\| T_j \|^2},$$

$$t_k = \cos\left(\frac{2k+1}{m+1}\frac{\pi}{2}\right); \qquad k = 0, 1, 2, \ldots, m, \tag{4}$$

$$\|T_0\|^2 = m + 1; \qquad \|T_i\|^2 = \tfrac{1}{2}(m+1) \quad \text{for } i > 0. \tag{5}$$

In order to calculate the required values of $f(x)$, we note that the Taylor expansion

$$\text{erfc}\, x = 1 - \frac{2}{\sqrt{\pi}}\left(t - \frac{t^3}{3} + \frac{t^5}{5 \cdot 2!} - \frac{t^7}{7 \cdot 3!} + \frac{t^9}{9 \cdot 4!} - \cdots\right) \tag{6}$$

can be rearranged [8] into the form

$$\exp(x^2)\text{erfc}\, x = \exp(x^2) - \frac{2x}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{2^n x^{2n}}{1 \cdot 3 \cdot 5 \cdots (2n+1)}, \tag{7}$$

the use of which is less sensitive to roundoff errors.

The asymptotic expansion

$$\exp(x^2)\text{erfc}\, x = \frac{1}{x\sqrt{\pi}}\left(1 - \frac{1}{2x^2} + \frac{1 \cdot 3}{(2x^2)^2} - \frac{1 \cdot 3 \cdot 5}{(2x^2)^3} + \cdots\right) \tag{8}$$

is of limited use when x is large. The continued-fraction expansion

$$\sqrt{\pi}x \exp(x^2)\text{erfc}\, x = \frac{1|}{|1} + \frac{\frac{1}{2x^2}\Big|}{|1} + \frac{\frac{2}{2x^2}\Big|}{|1} + \frac{\frac{3}{2x^2}\Big|}{|1} + \cdots \tag{9}$$

(Perron [9]) yields better precision. Perron [10] gives the following algorithm for use of (9).

We define

$$\begin{aligned} &A_{-1} = 1, \qquad A_0 = b_0, \\ &B_{-1} = 0, \qquad B_0 = 1; \\ &a_i = i/(2x^2), \quad b_i = 1 \quad \text{for } i = 0, 1, 2, 3, \ldots; \\ &b_0 + \frac{a_1|}{|b_1} + \frac{a_2|}{|b_2} + \cdots + \frac{a_n|}{|b_n} = \frac{A_n}{B_n}. \end{aligned} \tag{10}$$

Then A_n and B_n are given recursively by the relations

$$\left.\begin{aligned} A_n &= b_n A_{n-1} + a_n A_{n-2} \\ B_n &= b_n B_{n-1} + a_n B_{n-2} \end{aligned}\right\}, \qquad n = 1, 2, 3, \ldots. \tag{11}$$

At smaller values of x, the convergence of (9) becomes slower. To overcome this, we have used double Aitken δ^2 extrapolation (Burden et al. [11, pp. 56–57]) as follows. If y_j is the approximation obtained by taking j terms of (9), then the sequences of numbers

$$\begin{aligned} y_j' &= y_j - (y_j - y_{j-1})^2/(y_j - 2y_{j-1} + y_{j-2}), \\ y_j'' &= y_j' - (y_j' - y_{j-1}')^2/(y_j' - 2y_{j-1}' + y_{j-2}'), \end{aligned} \tag{12}$$

converge progressively faster to (9). Use of (12) with (9)–(11) improved the fit of the Chebyshev approximation by about five orders of magnitude.

We have used (7) for $x \leqslant 2.83$ and (9)–(12) for $x > 2.83$. This yielded values of $f(x)$ accurate to at least 23D for all x. The resulting Chebyshev coefficients, generated by (3)–(5), are shown in Table 1. Use of these in (2) gives an approximation which reproduces $f(x)$ to at least 22D for all x. Schonfelder [5] generates Chebyshev coefficients using a different method [12], [13] in which an expression equivalent to (2) is substituted into a linear differential equation satisfied by the given function. Together with the boundary conditions satisfied by the same function, this procedure generates an infinite set of simultaneous linear equations for the c_j, a truncated version of which is then solved.

TABLE 1

Y=(1+2X)*EXP(X*X)*ERFC(X)   X=(0,INF)
T=(X-K)/(X+K)   K= 3.75

ORD	C(N)
0	0.11775789345674017540800Q+01
1	-0.45900545806464773310Q-02
2	-0.84249133366517915584Q-01
3	0.59209939998191890498Q-01
4	-0.26658668435305752277Q-01
5	0.9074997670705265094Q-02
6	-0.2413163540417608191Q-02
7	0.4907758365258086 32Q-03
8	-0.69169733025012064Q-04
9	0.4139027986073010Q-05
10	0.77403830661 9849Q-06
11	-0.218864010492344Q-06
12	0.10764999465671Q-07
13	0.4521959811218Q-08
14	-0.775440020883Q-09
15	-0.63180883409Q-10
16	0.28687950109Q-10
17	0.194558685Q-12
18	-0.965469675Q-12
19	0.32525481Q-13
20	0.33478119Q-13
21	-0.1864563Q-14
22	-0.1250795Q-14
23	0.74182Q-16
24	0.50681Q-16
25	-0.2237Q-17
26	-0.2187Q-17
27	0.27Q-19
28	0.97Q-19
29	0.3Q-20
30	-0.4Q-20

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