

Recursive Computation of the Repeated Integrals of the Error Function

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1. This paper is concerned with a special technique, originated by J. C. P. Miller [1, p. xviii], of computing a solution f_n of a second-order difference equation

$$(1.1) \quad y_{n+1} + a_n y_n + b_n y_{n-1} = 0 \quad (n = 1, 2, 3, \dots)$$

for $n = 0(1)N$, N large, in cases where (1.1) has a second solution, g_n , which ultimately grows much faster than f_n . Straightforward use of (1.1) is then not adequate, since rounding errors will "activate" the second solution g_n , which in turn will eventually overshadow the desired solution f_n . Miller's device consists of applying (1.1) in backward direction,

$$(1.2) \quad y_{n-1} = -b_n^{-1}(a_n y_n + y_{n+1}) \quad (n = \nu - 1, \nu - 2, \dots, 1; \nu > N),$$

starting with the initial values

$$(1.3) \quad y_{\nu-1} = \alpha, \quad y_\nu = 0,$$

where α is any real number $\neq 0$. If ν is taken sufficiently large the values so obtained turn out to be approximately proportional to f_n in the range $0 \leq n \leq N$. The factor of proportionality may then be determined, e.g., by comparing y_0 with f_0 .

This technique was originally devised [1] for the computation of Bessel functions $I_n(x)$, and has since then been applied to various other Bessel functions [2], [5], [9], to Legendre functions [8], and to the repeated integrals of the error function* [6],

$$(1.4) \quad \begin{aligned} i^n \operatorname{erfc} x &= \frac{2}{\sqrt{\pi}} \int_x^\infty \frac{(t-x)^n}{n!} e^{-t^2} dt \quad (n = 0, 1, 2, \dots), \\ i^{-1} \operatorname{erfc} x &= \frac{2}{\sqrt{\pi}} e^{-x^2}. \end{aligned}$$

An analogous technique for first-order difference equations is described in [4, p. 25].

We shall present in Section 2 a detailed description of Miller's procedure, paying special attention to the error term. In Section 3 we study the procedure as applied to the computation of the functions (1.4) and show that the process converges for any positive x , as $\nu \rightarrow \infty$. In Sections 4-5 estimates will be developed of how large ν must be taken to ensure any prescribed accuracy.

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* In this notation i^n ($n \geq 0$) should be interpreted as the n th power of the integral operator $i = \int_x^\infty$, so that

$$i^0 \operatorname{erfc} x = \operatorname{erfc} x, \quad i^n \operatorname{erfc} x = \int_x^\infty i^{n-1} \operatorname{erfc} t dt \quad (n = 1, 2, \dots).$$

This notation for the repeated integrals of the error function, even though not entirely satisfactory, has become standard.

2. Consider the homogeneous second-order difference equation

$$(2.1) \quad y_{n+1} + a_n y_n + b_n y_{n-1} = 0 \quad (n = 1, 2, 3, \dots)$$

and assume that

$$(2.2) \quad b_n \neq 0 \quad \text{for all } n \geq 1.$$

Let f_n be the (nontrivial) solution of (2.1) to be computed for $n = 0(1)N$. We assume

$$(2.3) \quad f_0 \neq 0.$$

Let there be another solution g_n of (2.1), for which

$$(2.4) \quad g_n \neq 0 \quad \text{for all } n \geq 0,$$

and

$$(2.5) \quad \lim_{n \rightarrow \infty} \left| \frac{f_n}{g_n} \right| = 0.$$

It follows readily that f_n, g_n are linearly independent.

Now let $y_n^{(\nu)}$ ($n = 0, 1, \dots, \nu - 2; \nu > N$) be the result of applying (2.1) in backward direction, starting with

$$(2.6) \quad y_{\nu-1}^{(\nu)} = \alpha, \quad y_{\nu}^{(\nu)} = 0 \quad (\alpha \neq 0).$$

These values, by (2.2), are well defined, and, as will presently be shown, $y_0^{(\nu)} \neq 0$ for ν sufficiently large. Let us then define

$$(2.7) \quad f_n^{(\nu)} = \frac{f_0}{y_0^{(\nu)}} y_n^{(\nu)}.$$

We show that for any fixed n ,

$$(2.8) \quad \lim_{\nu \rightarrow \infty} f_n^{(\nu)} = f_n.$$

Moreover,

$$(2.9) \quad f_n^{(\nu)} = f_n \frac{1 - \frac{f_{\nu}}{g_{\nu}} \frac{g_n}{f_n}}{1 - \frac{f_{\nu}}{g_{\nu}} \frac{g_0}{f_0}}.$$

It is sufficient to prove (2.9), since (2.8) then follows from (2.5). Let $y_n^{(\nu)}$ be extended to all $n > \nu$ by means of (2.1). Then for every fixed ν the sequence $\{y_n^{(\nu)}\} (n = 0, 1, 2, \dots)$ is a solution of (2.1), and therefore representable in the form

$$y_n^{(\nu)} = A^{(\nu)} f_n + B^{(\nu)} g_n \quad (n \geq 0).$$

By (2.6),

$$(2.10) \quad \begin{aligned} A^{(\nu)} f_{\nu-1} + B^{(\nu)} g_{\nu-1} &= \alpha, \\ A^{(\nu)} f_{\nu} + B^{(\nu)} g_{\nu} &= 0. \end{aligned}$$

Certainly, $A^{(\nu)} \neq 0$, since otherwise, by (2.4), $A^{(\nu)} = B^{(\nu)} = 0$, which contradicts the first equation in (2.10). From the second equation, $B^{(\nu)}/A^{(\nu)} = -f_\nu/g_\nu$. Therefore

$$y_n^{(\nu)} = A^{(\nu)} \left(f_n + \frac{B^{(\nu)}}{A^{(\nu)}} g_n \right) = A^{(\nu)} \left(f_n - \frac{f_\nu}{g_\nu} g_n \right).$$

If ν is sufficiently large it follows because of (2.3) and (2.5) that $y_0^{(\nu)} \neq 0$. By (2.7),

$$f_n^{(\nu)} = \frac{f_0 A^{(\nu)} \left(f_n - \frac{f_\nu}{g_\nu} g_n \right)}{A^{(\nu)} \left(f_0 - \frac{f_\nu}{g_\nu} g_0 \right)} = f_n \frac{1 - \frac{f_\nu}{g_\nu} \frac{g_n}{f_n}}{1 - \frac{f_\nu}{g_\nu} \frac{g_0}{f_0}},$$

which proves (2.9).

It is convenient to define

$$(2.11) \quad \rho_n = \frac{f_n g_0}{g_n f_0} \quad (n = 0, 1, 2, \dots),$$

so that $\rho_n \rightarrow 0$ as $n \rightarrow \infty$, and

$$f_n^{(\nu)} = f_n \frac{1 - (\rho_\nu/\rho_n)}{1 - \rho_\nu}.$$

The relative error of $f_n^{(\nu)}$ is given by

$$(2.12) \quad \frac{f_n^{(\nu)} - f_n}{f_n} = \frac{\rho_\nu}{1 - \rho_\nu} \left(1 - \frac{1}{\rho_n} \right).$$

The approximations $f_n^{(\nu)}$ obviously do not depend on α , so that α can be chosen at will. If a high-speed computer is employed it is advisable to choose a small value for α to guard against "overflow" in the values of $y_n^{(\nu)}$.

3. Now let

$$(3.1) \quad f_n = i^{n-1} \operatorname{erfc} x, \quad \times 70 \quad (n = 0, 1, 2, \dots).$$

Then f_n is a solution of

$$(3.2) \quad y_{n+1} + \frac{x}{n} y_n - \frac{1}{2n} y_{n-1} = 0 \quad (n = 1, 2, 3, \dots)$$

as is readily verified by writing

$$i^n \operatorname{erfc} x = \frac{2}{\sqrt{\pi}} \left(\frac{1}{n} \int_x^\infty \frac{(t-x)^{n-1}}{(n-1)!} t e^{-t^2} dt - \frac{x}{n} \int_x^\infty \frac{(t-x)^{n-1}}{(n-1)!} e^{-t^2} dt \right)$$

and evaluating the first integral by parts. A second solution of (3.2) is given by

$$(3.3) \quad g_n = (-1)^n i^{n-1} \operatorname{erfc}(-x) \quad (n = 0, 1, 2, \dots).$$

It is clear that the assumptions (2.2)–(2.4) are satisfied in this case. We shall now verify (2.5), i.e.

$$(3.4) \quad \lim_{n \rightarrow \infty} \frac{i^n \operatorname{erfc} x}{i^n \operatorname{erfc}(-x)} = 0 \quad (x > 0).$$

This then will prove the convergence of the procedure in Section 2, as applied to (3.2).

We recall that the repeated integrals of the error function are related to the parabolic cylinder functions $D_\nu(x)$ by [7, p. 76]

$$i^n \operatorname{erfc} x = \frac{e^{-\frac{1}{2}x^2}}{2^{(n-1)/2}\sqrt{\pi}} D_{-n-1}(x\sqrt{2}).$$

It is furthermore known [3, p. 123] that

$$D_{-n-1}(z) = \frac{\sqrt{\pi}e^{-\sqrt{n}z}}{2^{(n+1)/2}\Gamma\left(\frac{n}{2} + 1\right)} \left[1 + O\left(\frac{1}{\sqrt{n}}\right) \right] \quad (n \rightarrow \infty, z \text{ bounded}).$$

Therefore we obtain immediately for any fixed x , real or complex,

$$(3.5) \quad i^n \operatorname{erfc} x = \frac{e^{-\frac{1}{2}x^2}}{2^n \Gamma\left(\frac{n}{2} + 1\right)} e^{-\sqrt{2}nx} \left[1 + O\left(\frac{1}{\sqrt{n}}\right) \right] \quad (n \rightarrow \infty).$$

Hence,

$$\frac{i^n \operatorname{erfc} x}{i^n \operatorname{erfc} (-x)} \sim e^{-2\sqrt{2}nx} \quad (n \rightarrow \infty),$$

which proves (3.4).

4. With f_n, g_n defined by (3.1) and (3.3) we have for the quantities ρ_n in (2.11)

$$(4.1) \quad \rho_n = (-1)^n \frac{i^{n-1} \operatorname{erfc} x}{i^{n-1} \operatorname{erfc} (-x)} \quad (n = 0, 1, 2, \dots).$$

It is shown in this section that for any fixed $x > 0$ the sequence $\{|\rho_n|\}$ is monotonically decreasing, i.e.,

$$(4.2) \quad \left| \frac{\rho_{n+1}}{\rho_n} \right| = \frac{i^n \operatorname{erfc} x}{i^{n-1} \operatorname{erfc} x} \cdot \frac{i^{n-1} \operatorname{erfc} (-x)}{i^n \operatorname{erfc} (-x)} < 1 \quad (n \geq 0).$$

Inequality (4.2) is obvious if $n = 0$ and, by (1.4), equivalent to

$$\int_x^\infty (t-x)^{n-1} e^{-t^2} dt \int_{-x}^\infty (s+x)^n e^{-s^2} ds - \int_x^\infty (t-x)^n e^{-t^2} dt \int_{-x}^\infty (s+x)^{n-1} e^{-s^2} ds > 0$$

if $n > 0$. By introducing new variables of integration, $t = u + x, s = v - x$, and writing the left-hand side as a double integral, one obtains

$$(4.3) \quad \iint_Q u^{n-1} v^{n-1} (v-u) e^{-(u+x)^2 - (v-x)^2} du dv > 0,$$

where Q denotes the first quadrant $u \geq 0, v \geq 0$. Let Q_1, Q_2 denote the regions

$$Q_1: \quad 0 < u < v, \quad Q_2: \quad 0 < v < u.$$

Interchanging variables of integration gives

$$\iint_{Q_2} u^{n-1} v^{n-1} (v-u) e^{-(u+x)^2 - (v-x)^2} du dv = - \iint_{Q_1} u^{n-1} v^{n-1} (v-u) e^{-(v+x)^2 - (u-x)^2} du dv.$$

Therefore (4.3) is equivalent to

$$\iint_{Q_1} u^{n-1} v^{n-1} (v-u) [e^{-(u+x)^2 - (v-x)^2} - e^{-(v+x)^2 - (u-x)^2}] du dv > 0.$$

Now, $u^{n-1} v^{n-1} (v-u) > 0$ in Q_1 , and the same is true for the expression in brackets, since

$$-(u+x)^2 - (v-x)^2 > -(v+x)^2 - (u-x)^2 \quad \text{for } u < v.$$

This proves (4.3), and thus (4.2).

5. We are now in a position to estimate ν such that for any given integer p ,

$$|(f_n^{(\nu)} - f_n)/f_n| \leq 10^{-p} \quad \text{for } n = 0, 1, \dots, N+1.$$

Here, $f_n^{(\nu)}$ denotes the approximations to $f_n = i^{n-1} \operatorname{erfc} x$ obtained by the procedure of Section 2.

Since, by (2.12),

$$|(f_n^{(\nu)} - f_n)/f_n| \leq |\rho_\nu| (1 + |\rho_n|^{-1}) + O(\rho_\nu^2),$$

and since $|\rho_n|^{-1}$ increases with n , by (4.2), it is sufficient to choose ν such that

$$(5.1) \quad |\rho_\nu| (1 + |\rho_{N+1}|^{-1}) \leq 10^{-p}.$$

From (3.5) and (4.1) we have

$$(5.2) \quad |\rho_{n+1}| = e^{-2\sqrt{2}nx} \left[1 + O\left(\frac{1}{\sqrt{n}}\right) \right].$$

Assuming N large enough to neglect the O -term in (5.2) for $n \geq N$, the requirement (5.1) may be simplified to

$$e^{-2\sqrt{2}\nu x} \leq \frac{10^{-p}}{1 + e^{2\sqrt{2}Nx}},$$

or even to

$$(5.3) \quad e^{-2\sqrt{2}\nu x} \leq \frac{10^{-p}}{2e^{2\sqrt{2}Nx}},$$

having made the right-hand bound smaller. Inequality (5.3) yields

$$\nu \geq \left(\frac{2\sqrt{2}Nx + p \ln 10 + \ln 2}{2\sqrt{2}x} \right)^2,$$

which gives us the desired estimate of ν .

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