Computation of Exponential Integrals

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Formulas leading to the computation of M member sequences of exponential integrals $E_{N+k}(x)$, $x \geq 0$, $N \geq 1$, $k = 0, 1, \ldots, M - 1$, are presented here and implemented in Fortran subroutine EXPINT. Sequences of exponential integrals can be generated in a numerically stable fashion if recurrence is carried forward or backward away from the integer closest to x. In keeping with this requirement, we select n, the integer closest to x within the constraint $N \leq n \leq N + M - 1$, and use $E_n(x)$ to start the recursion $E_n(x)$ is computed by means of the power series on $0 \leq x \leq 2$ and the confluent hypergeometric function $U(n, n, x)$ on $2 < x < \infty$. $U(n, n, x)$ is, in turn, computed from the backward recursive Miller algorithm for $U(n + k, n, x)$, $k = 0, 1, \ldots$, with a normalizing relation derived from the two-term recursion relation satisfied by $E_n(x)$ and $E_{n+1}(x)$. Truncation error bounds are derived and used in error tests in EXPINT Exponential scaling is also provided as a subroutine option.

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INTRODUCTION

In [5], Gautschi shows that a sequence of exponential integrals $E_{N+k}(x)$, $x \geq 0$, $N \geq 1$, $k = 0, 1, 2, \ldots, M - 1$, can be computed in a stable fashion if recurrence on

$$kE_{k+1}(x) + xE_k(x) = e^{-x} \tag{1}$$

is carried forward or backward away from the integer closest to x, $[x + 0.5]$. In keeping with this stability requirement, Gautschi [2] computes $e^x E_1(x)$ by means of the series for $x \leq 1$ and recurs forward with (1) for $e^x E_n(x)$, $n \geq 1$. For $x > 1$, the (Legendre) continued fraction [1, p. 229] is evaluated for $n = [x + 0.5]$, and the appropriate application of (1) increases or decreases the index to desired values. Even and odd convergents, which bound the limit of the continued fraction to arbitrary accuracy, are computed from series representations [4, p. 29] to guarantee the accuracy of the starting value in (1). A similar implementation is described in [3] for $E_\alpha(x)$, $\alpha > 0$. However, the Algol code developed in [2] appears to be the only one generally available for exponential integrals.

In this paper we present the analytical basis for a Fortran subroutine EXPINT which computes M member sequences $E_{N+k}(x)$ or $e^x E_{N+k}(x)$, $N \geq 1$, $k = 0, 1, \ldots, M - 1$ for real $x \geq 0$. The work in computation of $E_n(x)$ or $e^x E_n(x)$ to start the recursion is comparable to that in [2], but great savings are achieved in the recurrence when N is large and $x \leq 1$ or x is large and $N + M - 1$ is small.

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For $x \le 2$, the power series is implemented. For $x > 2$, the backward recursive Miller algorithm for approximations to $U(n+k, n, x)$, $k = 0, 1, \ldots,$ is used where

$$E_n(x) = e^{-x}x^{n-1}U(n, n, x)$$

and $U(a, b, x)$ is the second confluent hypergeometric function. The analysis to follow is directed toward computation at an index n, the integer closest to x within the constraint $N \le n \le N + M - 1$. Once $E_n(x)$ is computed, (1) is used to generate the remainder of the sequence with indices $N \le k \le N + M - 1$. The nature of the computation allows exponential scaling, which extends the computer argument x over many orders of magnitude, to be introduced conveniently with no overall increase in the amount of computation.

ANALYSIS

Series for $x \le$ XCUT, $n \ge 1$, and XCUT = 1 or 2

For $x \le$ XCUT, the series [1, p. 229]

$$E_n(x) = -\sum_{m=0}^{n-2} \frac{(-x)^m}{(m-n+1)m!} + \frac{(-x)^{n-1}}{(n-1)!}[-\ln x + \psi(n)] - \sum_{m=n}^{\infty} \frac{(-x)^m}{(m-n+1)m!} \tag{2}$$

was implemented where the leading sum does not appear for $n = 1$. Since the terms of each sum are bounded by terms of the exponential series, it can happen that truncation will occur in either the first or the second sum, depending on the size of x and n. We therefore consider the truncation of (2) in two cases and, for convenience, never terminate on the term $m = n - 1$. If we truncate the series at index $m = N$, the remainder is denoted by R_N and we have the following cases.

Case I: $N + 1 \ge n + 1$, $N \ge 2$. In this case,

$$|R_N| = \left| \sum_{N+1}^{\infty} \frac{(-x)^m}{(m-n+1)m!} \right| < \frac{x^{N+1}}{(N+1)!(N-n+2)} < \frac{x^N}{3N!} \tag{3}$$

since the sum is an alternating series and $N - n + 2 \ge 2$.

Case II: $N + 1 \le n - 2$, $N \ge 2$. In this case we have $|m - n + 1| \ge 1$ for all $m \ne n - 1$ and

$$|R_N| \le \sum_{N+1}^{n-2} \frac{x^m}{m!} + \frac{x^{n-1}}{(n-1)!}[-\ln x + \psi(n)] + \sum_{n}^{\infty} \frac{x^m}{m!}.$$

Now, by [1, p. 259],

$$\psi(n) < \ln(n)$$

and

$$0 < -\ln x + \psi(n) < \ln \frac{n}{x}, \qquad 0 < x \le 2, \quad n \ge 3.$$

Note that

$$y = \frac{n-1}{x} - \ln \frac{n}{x} > 0 \qquad \text{for} \quad n \ge 2$$

since y has a single positive minimum at $x = n - 1$, $n \geq 2$. Therefore, since $N \geq 2$ implies $n \geq 5$, we have

$$0 < -\ln x + \psi(n) < \ln \frac{n}{x} < \frac{n-1}{x}$$

and

$$\frac{x^{n-1}}{(n-1)!}[-\ln x + \psi(n)] < \frac{x^{n-2}}{(n-2)!}.$$

Then

$$\begin{aligned}
|R_N| &< \sum_{N+1}^{n-2} \frac{x^m}{m!} + \frac{x^{n-2}}{(n-2)!} + \sum_{n}^{\infty} \frac{x^m}{m!} \\
&< \sum_{N}^{n-3} \frac{x^m}{m!} + \frac{x^{n-2}}{(n-2)!} + \sum_{n-1}^{\infty} \frac{x^m}{m!} \qquad (4) \\
|R_N| &< \frac{x^N}{N!}\left(1 + \frac{x}{N+1} + \frac{x^2}{(N+1)(N+2)} + \cdots\right) \\
|R_N| &< \frac{x^N}{N!}\frac{N+1}{N+1-x} \leq 3\frac{x^N}{N!}, \qquad N+1 \leq n-2, \quad N \geq 2.
\end{aligned}$$

Notice that the term $m = n - 1$ is properly placed between the two sums according to its magnitude and that $(-x)^N/N!$ is computed (recursively) as part of each term. Therefore the truncation error bound $B_N = 3x^N/N!$ or $B_N = x^N/(3N!)$ is easily computed as each term is generated. The actual truncation of the series is made on a relative error test

$$B_N \leq |S_N| \cdot \text{TOL} \tag{5}$$

where $S_N \sim E_n(x)$ is the accumulated sum, and TOL is the relative accuracy desired.

If one wished to terminate the series on an absolute error test with a tolerance TOL $= 10^{-14}$, no more than 23 terms would be necessary. However, the relative error test in (5) is more restrictive and puts an additional requirement on the number of terms. This requirement comes about because $S_N \sim E_n(x)$ as a function of n decreases like

$$\frac{e^{-x}}{x+n} < E_n(x) \leq \frac{e^{-x}}{x+n-1}, \qquad n \geq 2. \tag{6}$$

The minimum index N, which makes (5) true with TOL fixed, causes B_N to decrease with n because $E_n(x)$ (and S_N) decreases slowly with n. Since B_N is monotone decreasing, N must increase slowly with n (see the last line of Table I). In fact, only 36 terms, those which are allowed in EXPINT, are needed to provide for n as high as 10^{12} with TOL $= 10^{-14}$. Table I shows the minimum index N required for (2) when TOL $= 10^{-3}, 10^{-8}, 10^{-14}$.

The function $\psi(n) = \Gamma'(n)/\Gamma(n)$, sometimes called the digamma function, is supplied as a CDC6600-7600 Fortran function DIGAM(N) where only integer arguments are permissible. In the preceding paragraph we noted that 36 terms of the series would accommodate n as high as 10^{12} at a relative error TOL $= 10^{-14}$.

Table I. Truncation Index N for Series with Relative Errors $B_N \leq 10^{-3}, 10^{-8}, 10^{-14}$

	n						
x	1	2	4	8	16	64	1024
0.2	4	3	4	5	5	5	6
	7	7	7	8	8	9	9
	11	11	11	11	12	12	13
0.4	4	4	5	8	6	7	8
	9	9	9	9	10	10	11
	13	13	13	13	16	14	15
0.6	5	5	6	8	7	8	9
	10	10	10	10	11	12	13
	14	15	15	15	16	16	17
0.8	6	6	7	8	8	9	10
	11	11	11	12	13	13	14
	16	16	16	16	17	18	19
1.0	5	7	7	8	9	10	11
	12	12	12	13	16	14	15
	17	17	18	18	18	19	20
1.2	7	8	8	8	10	11	12
	12	13	13	14	16	15	16
	18	19	19	19	19	21	21
1.4	7	9	9	9	11	11	13
	13	14	14	16	16	16	18
	19	20	20	20	20	22	23
1.6	9	9	10	10	12	12	14
	15	15	15	16	16	17	19
	21	21	21	21	22	23	24
1.8	10	10	11	11	12	13	14
	16	16	16	17	17	18	20
	22	22	22	22	23	24	25
2.0	11	11	11	12	13	14	15
	17	17	17	17	18	19	20
	23	23	23	23	24	25	26

Because the convergence of (2) is rapid, the $n - 1$ term, where $\psi(n)$ is needed, is reached only when n is relatively small, and truncation always occurs on the first sum when n is greater than 36. Consequently, one need only supply a table of $\psi(n)$ at integer arguments as high as 36 to cover most single-precision requirements. However, since EXPINT is almost portable, the implementation described below for DIGAM will allow an easy conversion to machines having longer word lengths or higher precision and requiring correspondingly smaller relative errors.

DIGAM returns a value $\psi(n)$ from a table look-up if $n \leq 100$. This single-precision table was generated in CDC6600 double-precision arithmetic from the relations [1, p. 258]

$$\psi(1) = -\gamma = -0.5772156649015328606065 12\ldots \tag{7}$$

$$\psi(n+1) = \psi(n) + \frac{1}{n}, \qquad n \geq 1$$

where γ is the Euler constant. For $n > 100$, the asymptotic expansion

$$\psi(n) \sim \ln n - \frac{1}{2n} - \sum_{k=1}^{3} \frac{B_{2k}}{2kn^{2k}}$$

is evaluated where [1, p. 810]

$$B_2 = \frac{1}{6}, \qquad B_4 = \frac{-1}{30}, \qquad B_6 = \frac{1}{42}, \qquad B_8 = \frac{-1}{30}$$

are Bernoulli numbers and the error is bounded by the next term of the sum. At $n = 100$, the relative error is 0.91×10^{-19}. If $n > 10^8$, the relative error, expressed by the first term of the sum, is less than 0.45×10^{-18}, and only the two leading terms are used for $\psi(n)$.

BACKWARD RECURSIVE ALGORITHM FOR $x >$ XCUT

In [10] Temme uses the three-term recursion relation

$$k_{n+1}(z) - b_n k_n(z) + a_n k_{n-1}(z) = 0, \qquad n = 1, 2, \ldots, \tag{8}$$

$$a_n = \frac{(n - \frac{1}{2})^2 - \nu^2}{n^2 + n}, \qquad b_n = \frac{2(n + z)}{n + 1}$$

for

$$k_n(z) = (-1)^n (\nu, n) U(\nu + \tfrac{1}{2} + n, 2\nu + 1, 2z), \qquad n = 0, 1, \ldots,$$

$$(\nu, n) = (-1)^n \cos \pi\nu \frac{\Gamma(\frac{1}{2} + \nu + n)\Gamma(\frac{1}{2} - \nu + n)}{\pi n!}$$

to compute the $K_\nu(z)$ Bessel function, $z > 0$,

$$K_\nu(z) = \sqrt{\pi}\,(2z)^\nu e^{-z} U(\nu + \tfrac{1}{2}, 2\nu + 1, 2z), \qquad -\tfrac{1}{2} < \nu < \tfrac{1}{2}.$$

Temme shows, on the basis of the work in [8] and [9], that $k_n(z)$ is a minimal solution of (8), making backward recursion appropriate for numerical stability. The Miller algorithm is employed to compute quantities $\tilde{k}_n^N(z)$ starting with

$$\tilde{k}_{N+1}^N = 0, \qquad \tilde{k}_N^N = 1.$$

This yields convergent ratios $\tilde{k}_{n+1}^N(z)/\tilde{k}_n^N(z)$ and fixes an approximate solution of (8), $k_n^N(z)$, to within a multiplicative constant. This constant is determined by truncating the normalizing relation

$$\sum_{k=0}^{\infty} k_n(z) = (2z)^{-\nu-(1/2)} \tag{9}$$

and replacing k_n by k_n^N. Temme also analyzes the error $|k_n - k_n^N|$ given by Olver [6, p. 116; 7] when the infinite system (8) is truncated to an $N \times N$ system, assuming the normalizing constant $k_0(z)$ is known. Olver's equations are

$$E_N = \sum_{k=N}^{\infty} \frac{e_k}{p_k p_{k+1}}, \qquad |k_n(z) - k_n^N(z)| = E_N p_n, \qquad n \geq 1 \tag{10}$$

where $p_k \geq 0$, $k = 0, 1, \ldots$, is a computed solution of (8) obtained from $p_0 = 0, p_1 = 1$ by forward recursion. The fact that $b_n \geq 1 + a_n$ guarantees that the sequence $\{p_k\}$ is monotone increasing. The $\{e_n\}$ sequence is obtained from

$$e_0 = k_0(z), \qquad e_n = a_n e_{n-1}, \qquad n = 1, 2, \ldots,$$

and is given explicitly by

$$e_n = \frac{k_0(z)(-1)^n(\nu, n)}{(n+1)!}.$$

Temme further analyzes E_N in (10) to get a simple bound in terms of N and p_N,

$$E_N \leq \frac{k_0 \cos \pi\nu N^{-3/2} p_N^{-2}}{2\pi\sqrt{2z}}.$$

There is an additional error term which comes from the truncation of series (9), and this appears to be the dominant factor in determining N in [10]. In the analysis that follows, the normalizing relation terminates and there is no truncation error from this source.

To compute exponential integrals, we propose to use the analysis outlined above on a reparameterization of (8) so that $U(a, a, x)$ in

$$E_a(x) = e^{-x} x^{a-1} U(a, a, x) \tag{11}$$

can be computed. Thus

$$n = m + \frac{a}{2}, \qquad \nu = \frac{a}{2} - \frac{1}{2}, \qquad z = \frac{x}{2}, \qquad a \text{ even}, \qquad m = 0, 1, 2, \ldots$$

carries (8) over to a new recurrence

$$y_{m+1}(x) - b_m y_m(x) + a_m y_{m-1}(x) = 0, \qquad m = 1, 2, \ldots, \tag{12}$$

$$a_m = \frac{m(a + m - 1)}{(a/2 + m)(a/2 + m + 1)}, \qquad b_m = \frac{(a + 2m + x)}{(a/2 + m + 1)},$$

with an explicit solution, except for normalizing constants independent of m, given by

$$y_m = \frac{(1)_m (a)_m}{(1 + a/2)_m} U(m + a, a, x). \tag{13}$$

In (13) $m = 0$ gives $y_0 = U(a, a, x)$ for (11). Now we notice that this sequence can be normalized by means of the two-term recursion relation (1) in the form

$$aE_{a+1}(x) + xE_a(x) = e^{-x} \tag{14}$$

if $E_{a+1}(x)$ can be expressed in terms of y_m, $m = 0, 1, 2, \ldots$. This we do by means of the contiguous relation

$$zU(b, c + 1, z) = (c - b)U(b, c, z) + U(b - 1, c, z)$$

with $b = a + 1$, $c = a$, and $z = x$ for $U(a + 1, a + 1, x)$ in (11). Thus

$$xU(a + 1, a + 1, x) = U(a, a, x) - U(a + 1, a, x), \tag{15}$$

and the normalizing relation (14), in terms of y_0 and y_1 from (11), (13), and (15), becomes

$$(x + a)y_0 - (1 + a/2)y_1 = x^{1-a}. \tag{16}$$

This relation specifies the $\{y_m\}$ sequence uniquely, and

$$E_a(x) = e^{-x}x^{a-1}y_0, \qquad E_{a+1}(x) = e^{-x}x^{a-1}\left[y_0 - \frac{(1 + a/2)y_1}{a}\right]. \tag{17}$$

While this approach appears to be new, it can actually be related to the continued fraction for $E_a(x)$ [1, p. 229]. This comes about by writing the continued fraction for $r_0 = y_1/y_0$,

$$r_0 = \frac{a_1}{b_1-}\frac{a_2}{b_2-}\frac{a_3}{b_3-}\cdots,$$

doing an equivalence transformation (multiplying a_m, b_m, and a_{m+1} by $p_m = a/2 + m + 1$, $m = 1, 2, \ldots$) and using (16) and (17) with $y_1 = r_0 y_0$ to express $E_a(x)$ in terms of r_0. The result is the even contraction of the Legendre continued fraction for $E_a(x)$ [2].

Now we wish to analyze Olver's expression (10) for the error in the Miller algorithm when applied to (12). Since we are only interested in order-of-magnitude estimates, we use $\lesssim$ and $\sim$ in the sense of approximate inequality in many of the subsequent estimates, realizing that a multiplicative constant may have to be inserted in our final result to make any bound rigorous. Since

$$e_0 = y_0, \qquad e_m = a_m e_{m-1}, \qquad m = 1, 2, \ldots,$$

we have explicitly

$$\begin{aligned} e_m &= \frac{(1)_m(a)_m}{(a/2 + 1)_m(a/2 + 2)_m} y_0 \\ &= \frac{\Gamma(m + 1)\Gamma(a + m)}{\Gamma(a/2 + m + 1)\Gamma(a/2 + m + 2)} \cdot \frac{\Gamma(a/2 + 1)\Gamma(a/2 + 2)}{\Gamma(a)} y_0. \end{aligned} \tag{18}$$

The relations

$$\Gamma(z) = \frac{2^{z-1}}{\sqrt{\pi}}\Gamma\left(\frac{z}{2}\right)\Gamma\left(\frac{z+1}{2}\right), \qquad \frac{\Gamma(z + a)}{\Gamma(z + b)} \sim z^{a-b} \qquad \text{for} \quad z \to \infty$$

produce an estimate for the ratio

$$\frac{\Gamma(a/2 + 1)\Gamma(a/2 + 2)}{\Gamma(a)} = \frac{\sqrt{\pi}(a/2)(a/2 + 1)\Gamma(a/2 + 1)}{2^{a-1}\Gamma((a + 1)/2)} \sim \frac{(a/2)^{3/2}(a/2 + 1)\sqrt{\pi}}{2^{a-1}}.$$

Since a and m can be large independently of one another in (18), asymptotic estimates for ratios of gamma functions in the first term of (18) are not appropriate. In this case, we use the Stirling approximation for $\Gamma(z)$, $z > 0$, and arrive at

$$e_m \sim \frac{2y_0(a/2)^{3/2}(a/2 + 1)\sqrt{\pi}}{(m + a/2)(m + 1 + a/2)} W(m) \tag{19}$$

where

$$W(m) = \left(\frac{m+a}{2m+a}\right)^a \left[\frac{m(m+a)}{(m+a/2)^2}\right]^m \sqrt{\frac{m}{m+a}} < 1$$

is monotone decreasing for $a > 2$. This can be seen by logarithmic differentiation of W with the relations

$$\frac{W'}{W} = \ln\left[\frac{m(m+a)}{(m+a/2)^2}\right] + \frac{a/2}{m(m+a)}, \qquad \frac{m(m+a)}{(m+a/2)^2} < 1$$

$$\ln\left[\frac{m(m+a)}{(m+a/2)^2}\right] = \ln\left[1 - \frac{a^2/4}{(m+a/2)^2}\right] \le \frac{-a^2/4}{(m+a/2)^2},$$

and

$$\frac{W'}{W} \le \frac{-a^2/4}{(m+a/2)^2} + \frac{a/2}{m(m+a)} = \frac{a}{2}\frac{[(1-a/2)m^2 + a(1-a/2)m + a^2/4]}{m(m+a)(m+a/2)^2}.$$

While $W(m)$ for $a = 2$ is monotone increasing, $W(m)$ only varies from 0.2436 to 0.2500 for $m \ge 1$. It is convenient here to invoke our rule of approximate inequality for order-of-magnitude estimates and use $W(m+k) \le W(m)$ for $a \ge 2$.

Now $x \ge 0$ and $a \ge 2$ imply that $b_m \ge 1 + a_m$ for all m, and this guarantees [7] that $p_{m+1} \ge p_m$. Consequently [10] becomes

$$|y_m - y_m^M| = p_m E_M, \qquad E_M \le \sum_M^\infty \frac{e_m}{p_m^2}, \qquad m = 1, 2, \ldots. \tag{20}$$

However, Temme [10] notes that (12) has minimal and dominant solutions, with asymptotic estimates [8, p. 80], given by

$$\begin{aligned} d_m(x) &= \frac{\Gamma(m+1)\Gamma(m+a)}{\Gamma(m+1+a/2)} U(m+a, a, x) \\ &\sim \frac{\Gamma(m+1)}{\Gamma(m+1+a/2)} C_1(x) n^{(a-1)/2} K_{a-1}(2\sqrt{xn}), \\ D_m(x) &= \frac{\Gamma(m+a)}{\Gamma(m+1+a/2)} {}_1F_1(m+a, a, x) \\ &\sim \frac{\Gamma(m+a)}{\Gamma(m+1+a/2)} C_2(x) n^{(1-a)/2} I_{a-1}(2\sqrt{xn}), \qquad n = m + \frac{a}{2} \end{aligned} \tag{21}$$

where $y_m(x) = \beta d_m(x)$ is also minimal and K_{a-1} and I_{a-1} are modified Bessel functions. Any other solution of (12), namely, p_m, is a linear combination of d_m and D_m. This makes p_m dominant, and asymptotically

$$p_m \sim \alpha C_2(x)(m+a/2)^{-1/2} I_{a-1}(2\sqrt{x(m+a/2)}). \tag{22}$$

Now we insert p_m and e_m into (20) and replace the sum by a bounding integral to obtain

$$E_M \le \frac{2y_0(a/2)^{3/2}(a/2+1)\sqrt{\pi}}{\alpha^2 C_2^2(x)} W(M) \int_M^\infty \frac{dm}{(m+a/2) I_{a-1}^2(2\sqrt{x(m+a/2)})}.$$

This latter integral, with a change of variable $v^2 = 4x(m + a/2)$, becomes

$$2\int_{v_M}^{\infty} \frac{dv}{vI_{a-1}^2(v)} = 2\frac{K_{a-1}(v_M)}{I_{a-1}(v_M)}, \qquad v_M = 2\sqrt{x\left(M + \frac{a}{2}\right)},$$

which is the Wronksian of the Bessel functions $K_\nu(z)$ and $I_\nu(z)$ written in integral form

$$\frac{K_\nu(z)}{I_\nu(z)} = \int_z^{\infty} \frac{dv}{vI_\nu^2(v)}.$$

Now we approximate K_ν and I_ν with first-term *uniform* asymptotic expressions [1, p. 378]

$$K_\nu(z) \sim \sqrt{\frac{\pi t}{2\nu}}\, e^{-\nu\xi}, \qquad I_\nu(z) \sim \sqrt{\frac{t}{2\pi\nu}}\, e^{\nu\xi},$$
$$t = \frac{1}{\sqrt{1 + (z/\nu)^2}}, \qquad \xi = \frac{1}{t} - \frac{1}{2}\ln\left(\frac{1+t}{1-t}\right) \tag{23}$$

to obtain an order-of-magnitude estimate of the ratio

$$\frac{K_\nu(z)}{I_\nu(z)} \sim \pi e^{-2\nu\xi} \sim \frac{t}{2\nu I_\nu^2(z)}$$

or, with (22),

$$\frac{K_{a-1}(2\sqrt{x(M + a/2)})}{I_{a-1}(2\sqrt{x\,(M + a/2)})} \sim \frac{\alpha^2 C_2^2(x)}{2p_M^2(M + a/2)\sqrt{(a-1)^2 + 4x(M + a/2)}}.$$

Thus with (19) we can write

$$E_M \le y_0 B_M$$
$$B_M = \frac{e_M}{P_M^2} \cdot \frac{M + a/2 + 1}{\sqrt{(a-1)^2 + 4x(M + a/2)}}. \tag{24}$$

If one uses the Bessel function expansions for large argument (large M) in place of the uniform expansions, the additive term $(a - 1)^2$ under the square root does not appear and the bound is much too large when a is large. In an error test, this forces M to be too large and results in much higher accuracies and more computation than desired.

In order to compute the relative error in y_0^M, we apply (20) and (24) for $m = 1$,

$$|y_1 - y_1^M| \le y_0 B_M.$$

Note that $y_1 = r_0 y_0$ and $y_1^M = \tilde{r}_0^M y_0$ are both normalized on y_0 where

$$r_0 = \frac{y_1}{y_0} \qquad \text{and} \qquad \tilde{r}_0^M = \frac{\tilde{y}_1^M}{\tilde{y}_0^M}.$$

Then

$$|r_0 - \tilde{r}_0^M| \le B_M \tag{25}$$

shows that accurate ratios $\tilde{r}_0^M$ are produced as $M \to \infty$. Now (16) yields

$$y_0 = \frac{x^{1-a}}{x + a - (1 + a/2)r_0},$$

and we compute y_0^M from this relation using $\tilde{r}_0^M$ in place of r_0,

$$y_0^M = \frac{x^{1-a}}{x + a - (1 + a/2)\tilde{r}_0^M}.$$

Therefore,

$$y_0 - y_0^M = y_0 y_0^M x^{a-1}(1 + a/2)(r_0 - \tilde{r}_0^M). \tag{26}$$

Solving for y_0^M and using (25), we get

$$y_0^M \leq \frac{y_0}{1 - y_0 x^{a-1}(1 + a/2)B_M},$$

and the relative error from (26) is bound by

$$\frac{|y_0 - y_0^M|}{y_0} \leq \frac{y_0 x^{a-1}(1 + a/2)B_M}{1 - y_0 x^{a-1}(1 + a/2)B_M}.$$

Now, the term involving B_M is intended to be small and $y_0 x^{a-1} = e^x E_a(x)$ can be approximated by the lower bound in (6). Since we are only interested in order-of-magnitude estimates and are willing to insert a multiplicative constant to keep inequality, we simplify this expression on the right and use the right-hand side of

$$\frac{|y_0 - y_0^M|}{y_0} \leq \frac{1 + a/2}{x + a} B_M \tag{27}$$

as an error test. Table II shows the smallest M for three tolerances.

While the asymptotic replacements did not always produce rigorous inequality, numerical experiments on the error reveal that (27) is indeed a bound which is fairly sharp near x = XCUT and becomes more conservative with increasing x. This simply means that more accuracy is obtained using (27) in an error test than can be expected.

Equation (17) with y_0 replaced by y_0^M gives

$$E_a(x) \doteq C_M \tilde{y}_0^M, \qquad E_{a+1}(x) \doteq C_M\left[\tilde{y}_0^M - \frac{(1 + a/2)\tilde{y}_1^M}{a}\right]$$

in terms of the computed quantities $\tilde{y}_0^M$ and $\tilde{y}_1^M$ from Miller's algorithm, where

$$C_M = \frac{e^{-x}}{a[\tilde{y}_0^M - (1 + a/2)\tilde{y}_1^M/a] + x\tilde{y}_0^M}. \tag{28}$$

One can see from these relations, as well as from (6), that exponential scaling is appropriate. This will increase the argument range of the subroutine variable x by many orders of magnitude at no overall increase in computation. To achieve this scaling, e^{-x} in (1) and (28) is replaced by 1, and series (2) is multiplied by e^x. The selection parameter KODE in EXPINT provides for this option. When scaling is not used, a nonfatal error flag IERR signals a potential underflow and returns zero values for $E_{N+k}(x)$, $k = 0, 1, \ldots, M - 1$.

The accuracy of y_0^M and y_1^M from the Miller algorithm can be further improved [4, p. 40] if we replace $\tilde{y}_{M+1}^M = 0$, which is supposed to approximate y_{M+1}/y_M, with

Table II. Starting Indices for Backward Recursion with Relative Errors $[(1 + a/2)/(x + a)]\, B_M \leq 10^{-3}, 10^{-8}, 10^{-14}$

x	n = 1	2	4	8	16	64	1024
0.5	9	9	7	5	3	2	1
	51	51	43	26	14	6	3
	145	145	129	85	39	13	6
1.0	6	6	6	4	3	2	1
	29	29	27	20	13	6	3
	79	79	75	59	34	13	6
2.0	4	4	4	4	3	2	1
	17	17	18	15	11	6	3
	44	44	44	39	29	13	6
4.0	3	3	3	3	3	2	1
	11	11	11	11	10	6	3
	26	26	27	26	22	12	6
8.0	2	2	3	3	3	2	1
	7	7	8	8	8	6	3
	16	16	17	18	17	12	6
16.0	2	2	2	2	2	2	1
	5	5	6	6	6	6	3
	10	10	11	12	13	11	6
32.0	2	2	2	2	2	2	1
	4	4	4	5	5	5	3
	7	7	8	9	9	9	6
64.0	2	2	2	2	2	2	1
	3	3	4	4	4	4	3
	6	6	6	7	7	8	6
256.0	1	1	1	1	1	1	1
	3	3	3	3	3	3	3
	4	4	4	5	5	6	6
512.0	1	1	1	1	1	1	1
	2	2	2	2	3	3	3
	4	4	4	4	4	5	5
1024.0	1	1	1	1	1	1	1
	2	2	2	2	2	3	3
	3	3	3	4	4	4	5

a more realistic value. This can be done in a convenient computational manner if we note that asymptotically $p_m \sim \alpha D_m$ and $y_m = \beta d_m$ from (21) and (22) are almost reciprocals. This reciprocal relation comes about if we use the uniform asymptotic expressions (23) for I_{a-1} and K_{a-1}. Thus we arrive at the approximation

$$\frac{y_{M+1}}{y_M} \sim \frac{d_{M+1}}{d_M} \sim \left(\frac{M+1}{M+1+a/2}\right)\left[\frac{M+1+a/2}{M+a/2}\right]^{(a-1)/2} \frac{\exp\{(a-1)\xi_M\}}{\exp\{(a-1)\xi_{M+1}\}} \sqrt{\frac{t_{M+1}}{t_M}}$$

$$\sim \frac{(M+1)(M+a)}{(M+1+a/2)^2} \frac{t_{M+1}}{t_M} \frac{D_M(x)}{D_{M+1}(x)}$$

where the subscripts M and $M+1$ denote corresponding evaluations of t and ξ in (23) with $z_M = 2\sqrt{x(M+a/2)}$. Now, $p_M \sim \alpha D_M$ for $M \to \infty$, and we use $\tilde{y}_M^M = 1$ together with

$$\tilde{y}_{M+1}^M = \frac{(M+1)(M+a)}{(M+1+a/2)^2}\sqrt{\frac{(a-1)^2+4x(M+a/2)}{(a-1)^2+4x(M+1+a/2)}}\,\frac{p_M}{p_{M+1}}$$

to start backward recursion after M is determined by means of a tolerance test on (27). This modification for $\tilde{y}_{M+1}^M \neq 0$ adds up to three extra digits of accuracy over the same computation when $\tilde{y}_{M+1}^M = 0$. The effect is most dramatic when x is close to XCUT and a is large but diminishes as x increases. In order to take advantage of this extra accuracy, it was determined experimentally that error tolerances TOL less than or equal to 10^{-3} could be increased by a factor of nearly 90 and still give the requested accuracy with smaller values of M. To be slightly conservative, we use a factor of 20 in the error test.

If $N = 1$, we generate $E_2(x)$ and use (1) to compute $E_1(x)$, $x >$ XCUT.

The implementation of the recursion relations and the error test can be simplified to minimize the number of multiplications, divisions, and square roots. We compute a_m by means of

$$a_M \equiv \frac{m(m+a-1)}{(m+a/2)(m+1+a/2)} = \frac{d_m}{d_m + c_m + m + a^2/4}$$

where $c_m = m + a/2$, $d_m = m(m+a-1)$ are computed recursively by additions in the form

$$c_0 = \frac{a}{2}, \qquad c_m = c_{m-1} + 1, \qquad m = 1, 2, \ldots$$

$$d_1 = a, \qquad d_m = d_{m-1} + c_{m-1} + c_{m-1}, \qquad m = 2, 3, \ldots.$$

The quantities

$$f_m = \frac{1}{\sqrt{(a-1)^2 + 4x(m+a/2)}}, \qquad m = 1, 2, \ldots, M,$$

occur in the error term (27). Recursively, we have

$$f_m = R_{m-1} f_{m-1} = R_{m-1} R_{m-2} \cdots R_0 f_0, \qquad R_m = \frac{f_m}{f_{m+1}}$$

where

$$R_m = \sqrt{\frac{(a-1)^2 + 4x(m+a/2)}{(a-1)^2 + 4x(m+a/2+1)}} \sim 1 - \frac{2x}{(a-1)^2 + 4x(m+a/2+1)}.$$

Thus f_m can be updated by one multiplication and one division. Since the error test from (27) can be arranged into the form

$$\frac{e_M(M+1+a/2)f_M}{\mathrm{TOL}} \cdot \frac{1+a/2}{x+a} < p_M^2,$$

we can compute every factor on the left, except $M + 1 + a/2$, by forward recursion at the same time the $\{p_m\}$ sequence is being generated,

$$g_0 = (a-1)^2 + 4x\left(\frac{a}{2}\right), \qquad g_m = g_{m-1} + 4x, \qquad m = 1, 2, 3, \ldots,$$

$$F_0 = \frac{(1 + a/2)f_0}{(x+a)\cdot\mathrm{TOL}}, \qquad F_m = F_{m-1}a_{m-1}(1 - 2x/g_m).$$

Similarly, for y_{M+1}^M, we have a reduction in computation by replacing R_M with three terms of the series and expressing other factors in terms of available quantities,

$$y_{M+1}^M = \frac{d_{M+1}}{d_{M+1} + M + 1 + a^2/4} \cdot \frac{P_M}{P_{M+1}} \cdot \left[1 - \frac{2x}{g_M} + \frac{3}{8}\left(\frac{2x}{g_M}\right)^2\right].$$

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REFERENCES

1. Abramowitz, M., and Stegun, I.A. *Handbook of Mathematical Functions* (Appl. Math. Ser. 55), Nat. Bureau Standards, Washington, D.C., Dec 1965.
2. Gautschi, W. Algorithm 471. Exponential integrals. *Commun. ACM 16*, 12 (Dec. 1973), 761-763.
3. Gautschi, W. An evaluation procedure for incomplete gamma functions. MRC Tech. Summary Rep. 1717, Math. Res. Ctr., Madison, Wis., Feb. 1977.
4. Gautschi, W Computational aspects of three-term recurrence relations. *SIAM Rev. 9* (1967), 24-82.
5. Gautschi, W. Recursive computation of certain integrals *J. ACM 8*, 1 (Jan. 1961), 21-40.
6. Olver, F W.J Numerical solution of second-order linear difference equations. *Nat. Bureau Standards J. Res , B Math , Math Phys 71B* (1967), 111-129.
7. Olver, F.W.J , and Sookne, D.J. Note on backward recurrence algorithms. *Math. Comput. 26* (1972), 941-947.
8. Slater, L J. *Confluent Hypergeometric Functions.* Cambridge Univ. Press, Cambridge, England, 1960.
9. Temme, N.M. Numerical evaluation of functions arising from transformations of formal series. *J. Math. Anal Appl, 51* (1975), 678-694.
10. Temme, N M. On the numerical evaluation of the modified Bessel function of the third kind. *J. Comput Phys. 3* (1975), 324-337.

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