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On the Computation of Certain Integrals Containing the Modified Bessel Function $I_0(\xi)$

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Abstract. Efficient stratagems are developed for numerically evaluating one- and two-dimensional integrals over x, y with integrand $\exp(-x-y)I_0(2\sqrt{pxy})$. The integrals are expressed in terms of convergent series, which exhibit the correct limiting behavior, and which can be evaluated recursively. The performances of these stratagems are compared with numerical integration.

1. Introduction. This paper is concerned with the efficient evaluation of the following integrals, all involving the modified Bessel function, $I_0(\xi)$:

$$J(x, y) = \int_x^\infty e^{-(t+y)} I_0\left(2\sqrt{ty}\right) dt, \tag{1}$$

$$K(x, y) = \int_0^x e^{-(t+y)} I_0\left(2\sqrt{ty}\right) dt, \tag{2}$$

$$L(x, y, p) = (1-p)\int_0^y e^{pu-u} K(x, pu)\, du \tag{3}$$

$$= (1-p)\int_0^y du \int_0^x dt e^{-(u+t)} I_0\left(2\sqrt{put}\right), \tag{4}$$

where $p, x, y \geq 0$. These functions will be referred to as the J-, K-, and L-functions, respectively. The J- and K-functions are trivially related (see (18)).

The J- and/or K-functions are encountered in many contexts. These include: the study of exchange processes in columns (such as heat exchange [1], and ion exchange including chromatography [2]–[5]); dispersive exchange processes in hydrology and soil science [6]–[8]; a probabilistic analysis of targeted missile impacts [9], [5, Appendix]; in a solution to the telegraphy equation [5, Appendix], [10]; in a recently proposed filtration model of aerosol retention by a vegetative canopy 111], and in generalizations of such a model for other environmental-impact modelling applications [12].

Upon integrating (3) by parts, the L-function becomes expressible in terms of the K- or J-functions:

$$L(x, y, p) = (1 - e^{py-y}) + e^{py-y} J(x, py) - e^{px-x} J(px, y), \tag{5a}$$

$$= (1 - e^{py-y}) + e^{py-y} K(py, x) - e^{px-x} K(y, px). \tag{5b}$$

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Consequently, the analytic properties of $L(x, y, p)$ follow immediately from those of the J- or K-function; nevertheless, there seems to be some merit in retaining it as a function in its own right. The L-function was encountered, though not separately identified, by Brinkley [1, (22)]; it also arises naturally in a model of filtration [11], [12].

All of these functions commonly arise as solutions to the hyperbolic equations:

$$\frac{\partial}{\partial y}\phi_1(x, y) = \phi_2(x, y), \qquad \frac{\partial}{\partial x}\phi_2(x, y) = \phi_1(x, y),$$
$$\left(\frac{\partial^2}{\partial x \partial y} - 1\right)\phi_j(x, y) = 0, \qquad j = 1, 2. \tag{6}$$

The solutions to (6) satisfying the boundary conditions

$$\phi_1(x, 0) = A, \qquad \phi_2(0, y) = 0, \tag{7}$$

are

$$\phi_1(x, y) = AI_0\left(2\sqrt{xy}\right), \qquad \phi_2(x, y) = A\sqrt{x/y}\, I_1\left(2\sqrt{xy}\right). \tag{8}$$

The solutions satisfying the boundary conditions

$$\phi_1(x, 0) = 0, \qquad \phi_2(0, y) = Be^{y/\beta}, \tag{9}$$

are

$$\phi_1(x, y) = \beta Be^{\beta x + y/\beta} K(y/\beta, \beta x), \qquad \phi_2(x, y) = Be^{\beta x + y/\beta} J(\beta x, y/\beta). \tag{10}$$

The solution to (6) satisfying

$$\phi_1(x, 0) = Ce^{x/\alpha}, \qquad \phi_1(0, y) = Ce^{y/\beta} \tag{11}$$

is

$$\phi_1(x, y) = Ce^{x/\alpha + y/\beta}\{1 - L(x/\alpha, y/\beta, \alpha\beta)\}. \tag{12}$$

This last solution is trivial in the $\alpha\beta = 1$ limit. Luke [10] supplies several other partial differential equations with solutions expressible in terms of the J- and K-functions.

Although analytic properties of the J-function have been well documented [5], [10], an algorithm for its efficient evaluation seems to be unavailable—except for an incomplete collection of analytical approximations of limited accuracy [13]. In the absence of such an algorithm, de Smedt and Wierenga [8] resorted to a truncation of the infinite summation:

$$J(x, y) = e^{-(x+y)} \sum_{n=0}^{\infty} \frac{y^n}{n!} \sum_{m=0}^{n} \frac{x^m}{m!}. \tag{13}$$

Such a series exhibits slow convergence for large arguments; moreover, it may be subject to underflow, even for modest argument values (e.g., for $x + y > 89$, $e^{-(x+y)} < 2^{-128}$).

The motivation for the current work is the validation of models of filtration [11], in which the search for optimal model parameters was hindered by the relatively slow numerical integration originally employed to compute the K- and L-functions. The superior algorithms subsequently developed, and reported herein, greatly assist such parameter searches.

Since the proposed strategems involve the Bessel functions $I_m(\xi)$, it is appropriate to first discuss their numerical evaluation.

2. Computation of the Modified Bessel Function, $I_m(\xi)$. The small-argument and asymptotic behavior of $I_m(\xi)$ are

$$I_m(\xi) = \left(\tfrac{1}{2}\xi\right)^m \sum_{k=0}^{\infty} \frac{\left(\tfrac{1}{2}\xi\right)^{2k}}{(k+m)!k!}, \tag{14}$$

$$I_m(\xi) \underset{\xi\to\infty}{\to} (2\pi\xi)^{-1/2} e^{\xi}. \tag{15}$$

Cody [14] has catalogued several computer codes for computing $I_m(\xi)$. Some are specific to $m = 0$ or 1, while others are appropriate for computing the sequence $I_m(\xi)$ for $m = 0, 1, \ldots, M$; the latter exploit the stable three-term backward-recursion relationship for contiguous values of m. In practice, $I_m(\xi)$ often occurs weighted exponentially (i.e., in the form $e^{-w}I_m(\xi)$), in which case efficiency is enhanced if the computer code returns the exponentially-scaled Bessel function, $e^{-\xi}I_m(\xi)$, without internal computation of the exponential function; it is natural to proceed in this way in the asymptotic domain where the behavior (15) dominates.

In the proposed stratagems for the large-ξ domain, we have chosen to employ the sequence $r_m(\xi)$ for $m = m_0, m_0 + 1, \ldots, M$ (where $m_0 = 0$ or 1) in place of the sequence $I_m(\xi)$. Here, $r_m(\xi)$ is the ratio of Bessel functions,

$$r_m(\xi) = I_{m+1}(\xi)/I_m(\xi); \tag{16}$$

it obeys the stable two-term backward-recursion relation,

$$r_{m-1}(\xi) = \{2m/\xi + r_m(\xi)\}^{-1}, \tag{17}$$

and the inequality $0 \leq r_m(\xi) < 1$. The implementation of such strategems calls for the computation of an initial ratio $r_M(\xi)$ and of a single Bessel function, usually $I_0(\xi)$ weighted exponentially, and for the recursive use of (17). The efficient computation of $r_M(\xi)$ has been the subject of several papers [15]–[17].

The performance of algorithms proposed herein were tested on a PDP-11/34 computer* (with 24-bit effective mantissa, 8-bit exponent, in single precision). In the large-ξ domain ($\xi \gtrsim 20$) Amos' iterative algorithm [15] is employed to compute $r_M(\xi)$ and Allen's formula [18] to compute $e^{-\xi}I_0(\xi)$. The latter formula comprises the product of the asymptote (15) and an eighth order polynomial in ξ^{-1}; its relative precision for $\xi > 3.75$ is better than 5×10^{-7} [19]. Rational approximations to $\xi^{1/2}e^{-\xi}I_0(\xi)$ for $\xi > 15$ have been developed by Blair and Edwards [20] to meet any desired precision, and these would also well serve the same task.

3. The *J*- and *K*-functions. Analytic properties cited below are taken from Goldstein [5] and/or Luke [10]. The complementarity relation

$$J(x, y) + K(x, y) = 1 \tag{18}$$

can be used to relate the properties of the *J*- and *K*-functions. Throughout this

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* The particular computer is equipped with the extended multiplication instruction set (EIS) as a hardware feature, but not with the floating-point multiplication instruction set (FIS).

section we adopt the abbreviations

$$\xi = 2\sqrt{xy}\,, \qquad \eta = \sqrt{y/x}\,. \tag{19}$$

We note the following interrelationship and limiting values:

$$J(x, y) = K(y, x) + e^{-(x+y)}I_0(\xi), \tag{20}$$

$$K(0, y) = 0, \quad J(x,0) = e^{-x}, \quad \lim_{y\to\infty} K(x, y) = 0. \tag{21}$$

For small values of the arguments, $J(x, y)$ can be efficiently evaluated by summing to convergence the following adaptation of the series (13):

$$J(x, y) = e^{-x} + e^{-(x+y)} \sum_{n=1}^{\infty} \frac{y^n}{n!} \sum_{m=1}^{n} \frac{x^m}{m!}. \tag{22a}$$

This series has the virtue that the $y \to 0$ behavior is reproduced in the leading term. The analogous series for $K(x, y)$ is

$$K(x, y) = e^{-(x+y)} \sum_{n=1}^{\infty} \frac{x^n}{n!} \sum_{m=0}^{n-1} \frac{y^m}{m!}. \tag{22b}$$

Convergence is assisted by using (22a) and (22b) for the parameter domains $x > \max(y, 1)$ and $x \leqslant \max(y, 1)$, respectively, and invoking (18) as necessary.

Consider the large-ξ domain, in which expressions exhibiting the appropriate asymptotic behavior are required.

From (20) it is evident that any expression for $K(x, y)$ in terms of x and y has a closely analogous counterpart for $J(x, y)$ in terms of y and x. Such counterparts are supplied here, and consideration is otherwise restricted to an algorithm for $K(x, y)$ with $x \leqslant y$; a corresponding algorithm for $J(x, y)$ with $x \geqslant y$ follows analogously, thereby completing the parameter space $x, y \geqslant 0$ by virtue of (18). The subtraction implied by invoking (18) incurs no loss of precision, because $K(x, y) \gtrsim \frac{1}{2}$ for $x > y$ and $J(x, y) > \frac{1}{2}$ for $x \leqslant y$ in the domain $\xi \gtrsim 15$.

The following expansions cited by Goldstein [5] and Luke [10] converge to the correct asymptotes, unless η is near unity:

$$J(x, y) = e^{-(x+y)} \sum_{m=0}^{\infty} \eta^m I_m(\xi), \qquad \eta < 1, \tag{23a}$$

$$K(x, y) = e^{-(x+y)} \sum_{m=1}^{\infty} \eta^{-m} I_m(\xi), \qquad \eta > 1. \tag{23b}$$

This can be seen by noting the m-independence of $I_m(\xi)$ in the asymptotic region, where expansions (23) then become

$$J(x, y) \underset{\xi\to\infty}{\to} e^{-(x+y)}(1 - \eta)^{-1} I_0(\xi), \qquad \eta < 1,$$

$$K(x, y) \underset{\xi\to\infty}{\to} e^{-(x+y)}(\eta - 1)^{-1} I_0(\xi), \qquad \eta > 1,$$

consistently with Goldstein's cited asymptotes [5, (74), (75)]. That the two expressions (23) are compatible with (18) follows from the generating function for modified Bessel functions [19]:

$$I_0(\xi) + \sum_{m=1}^{\infty} (\eta^m + \eta^{-m}) I_m(\xi) \equiv e^{\xi(\eta+\eta^{-1})/2}. \tag{24}$$

For small values of η^{-1}, one can truncate the series (23b) appropriately, and compute $K(x, y)$ by accumulating terms in order of decreasing m. For this purpose, the series can be expressed in the recursive form

$$K(x, y) \simeq e^{-(x+y)} \sum_{m=1}^{M} \eta^{-m} I_m(\xi) \tag{25}$$

$$= e^{-(x+y)} S_0 I_0(\xi), \tag{26a}$$

where

$$S_{M+1} = 0, \qquad S_m = \eta^{-1} r_m(\xi) S_{m+1} + 1. \tag{26b}$$

To effect this recursion, one is required to calculate the number of terms M, the initial ratio $r_{M-1}(\xi)$, and $I_0(\xi)$; the rapid recursive processes (17) and (26) then follow. The calculation of $r_{M-1}(\xi)$ and $I_0(\xi)$ is discussed in Section 2. A lower bound on the number of terms, M, can be estimated by utilizing the inequality $r_m(\xi) < 1$ (which is fairly tight if $\xi \gtrsim m$) to bound the following remainder function (the difference between (23b) and its approximation (25)):

$$\begin{aligned} R_M(x, y) = e^{-(x+y)} \sum_{m=M+1}^{\infty} \eta^{-m} I_m(\xi) &< e^{-(x+y)} \sum_{m=1}^{\infty} \eta^{-(m+M)} I_m(\xi) \\ &= \eta^{-M} K(x, y). \end{aligned} \tag{27}$$

If a relative precision, ρ, is demanded of $K(x, y)$, then M can be selected such that η^{-M} is not larger than ρ. If an absolute precision, α, is specified, η^{-M} should not be larger than $\alpha / K_U(x, y)$, where $K_U(x, y)$ is an upper bound of $K(x, y)$. Such an upper bound may be deduced from (23b):

$$K(x, y) < e^{-(x+y)} I_0(\xi) \sum_{m=1}^{\infty} \eta^{-m} = (\eta - 1)^{-1} e^{-(x+y)} I_0(\xi).$$

When η is near unity, the series (23) are inappropriate. A more appropriate series follows from invoking the "multiplication theorem" [19] to expand $I_m(\xi)$ of (23) in terms of $I_{m+n}(\xi_0)$, where ξ_0 is the smaller of $2x$ and $2y$:

$$\eta^m I_m(\xi) = \sum_{n=0}^{\infty} \frac{(x - y)^n}{n!} I_{m+n}(2y), \qquad x > y, \tag{28a}$$

or

$$\eta^{-m} I_m(\xi) = \sum_{n=0}^{\infty} \frac{(y - x)^n}{n!} I_{m+n}(2x), \qquad x < y. \tag{28b}$$

Substitution of (28b) into (23b), and rearrangement of the summations, produce

$$K(x, y) = e^{-(x+y)} \sum_{n=0}^{\infty} \frac{(y - x)^n}{n!} \sum_{m=n+1}^{\infty} I_m(2x).$$

The infinite sum over m can be replaced with a finite sum, by invoking the standard normalization result,

$$2 \sum_{m=1}^{\infty} I_m(\xi) + I_0(\xi) \equiv e^{\xi}, \tag{29}$$

(which is actually a special case of (24)), to produce

$$K(x, y) = K(x, x) - e^{-(x+y)} \sum_{n=1}^{\infty} \frac{\Delta^n}{n!} \sum_{m=1}^{n} I_m(\xi_0), \tag{30}$$
$$K(x, x) = \tfrac{1}{2}\{1 - e^{-\xi_0} I_0(\xi_0)\}.$$

Here $\xi_0 = 2x$ and $\Delta = y - x$.

To evaluate (30), the sum over n is truncated to $n < N$ and then evaluated recursively

$$\sum_{n=1}^{N-1} \frac{\Delta^n}{n!} \sum_{m=1}^{n} I_m(\xi_0) = A_0 I_0(\xi_0),$$

where

$$A_N = B_N = 0, \quad A_n = \frac{\Delta}{n+1} r_n(\xi_0)(A_{n+1} + B_{n+1}), \quad B_n = \frac{\Delta}{n+1} B_{n+1} + 1,$$

are $r_n(\xi_0)$ obeys the backward recursion relation (17). Again, the computation of $r_N(\xi_0)$ and $I_0(\xi_0)$ proceeds as described in Section 2. It remains only to estimate a lower bound on N by bounding the remainder function

$$R_N(x, y) \equiv e^{-(x+y)} \sum_{n=N}^{\infty} \frac{\Delta^n}{n!} \sum_{m=1}^{n} I_m(\xi_0). \tag{31}$$

Extending the sum over m upwards toward ∞, and making use of (23), produces the inequality

$$R_N(x, y) < e^{x-y} K(x, x) \sum_{n=N}^{\infty} \frac{\Delta^n}{n!}. \tag{32}$$

The determination of N to assure a specified precision is simplified, even if N is thereby overestimated, by using the inequality $n!N! < (n + N)!$ to write

$$\sum_{n=N}^{\infty} \frac{\Delta^n}{n!} < \frac{\Delta^N}{N!} e^{\Delta},$$

whereupon

$$R_N(x, y) < \frac{(y - x)^N}{N!} K(x, x), \qquad x < y. \tag{33}$$

An alternative upper bound on $R_N(x, y)$ is obtained by writing $I_m(\xi_0) < I_0(\xi_0)$ in (31). This produces the inequality

$$R_N(x, y) < \Delta e^{-(x+y)} I_0(\xi_0) \sum_{n=N-1}^{\infty} \frac{\Delta^n}{n!} \tag{34}$$

$$< \frac{(y - x)^N}{(N-1)!} e^{-2x} I_0(2x), \qquad x < y. \tag{35}$$

A specified absolute precision, α, can be met by selecting N such that at least one of the upper bounds (33), (35) is smaller than α; for a specified relative tolerance, ρ, at least one should be smaller than $\rho K_L(x, y)$, where $K_L(x, y)$ is a lower bound of $K(x, y)$. Such a lower bound is deducible by writing (30) as

$$K(x, y) = K(x, x) - R_1(x, y),$$

and utilizing bounds (32), (34); thus

$$K(x, y) > \max\{e^{x-y}K(x, x), K(x, x) - (y - x)e^{-2x}I_0(2x)\}.$$

Performance. One of the small-ξ expansions (22) is employed wherever $\xi \leq \xi_c$. Otherwise, $K(x, y)$ for $x \leq y$ is computed via the more economical of the two truncated expansions, (25) or (30)—expansions in η^{-1} or Δ, respectively. We have chosen to judge the relative economy of these expansions by the number of terms, M or N, in their truncated expansions. A simple test to determine approximately the relative magnitude of M and N appears in the appendix; the test usually avoids computing both M and N and always avoids computing N unnecessarily. A large-ξ delimiter of $\xi_c = 20$ is also recommended in the appendix.

A numerical experiment is devised to compare the performance of four contending algorithms for $K(x, y)$. The first of the four algorithms is that proposed herein; the second employs the series expansions (22a), (22b) in the parameter domains $x \leq y$ and $x > y$, respectively; the remaining two employ numerical integration, one by an adaptive Simpson's rule, the other by a doubly-adaptive Clenshaw-Curtis quadrature. The adaptive Simpson's rule found to provide the best performance is the AECL routine COSIMP [21] with a modified error accumulation which reduces the number of integrand evaluations. The doubly-adaptive Clenshaw-Curtis quadrature is a FORTRAN translation of Oliver's ALGOL procedure ADAPQUAD [22], augmented to accommodate an optional relative precision in a manner based upon (but more flexible than) the proposal of O'Hara and Smith [23, Appendix]. Both numerical integrators evaluate (2) directly if $x \leq y$; but for $x > y$ it is more efficient to reexpress $K(x, y)$ in terms of $K(y, x)$ (via Eqs. (18), (20)). Thus, in either case, the integral is over the range $[0, \min(x, y)]$, which in practice is scaled to $[0, 1]$ and the precomputed additive term (for $x > y$) added directly to the integrand. Allen's formulae [18], [19] are used to compute $I_0(z)$ for $0 \leq z \leq \xi$.

The numerical experiment determines the mean functional evaluation time for $K(x, y)$ over identical geometric grids of x and y (35 values of each) such that $\xi_c \leq \xi \leq 80$. Those times are recorded in Table 1, corresponding to a demanded relative accuracy of $\rho = 10^{-5}$, and to the same supplemented by a demanded absolute accuracy of $\alpha = 10^{-5}$. The superiority of the proposed algorithm is clearly exposed. The relative inferiority of numerical integration arises because of the requirement to compute $I_0(z)$ (weighted exponentially) at each integrand evaluation; in fact Allen's formula as used here is quite efficient for this purpose, but would unnecessarily limit the precision achievable in some computing environments. In contrast, the proposed algorithm computes only one exponentially-weighted Bessel function (either $I_0(\xi)$ or $I_0(\xi_0)$)—except in marginal parameter domains, where both are calculated—together with the ratio $r_M(\xi)$ or $r_N(\xi_0)$; all are computed in the asymptotic region ($\xi, \xi_0 \gtrsim 20$), where their evaluations are straightforward.

The adaptive Simpson's rule displays superiority over the doubly-adaptive Clenshaw-Curtis quadrature as a numerical integrator; this is despite the former requiring $\sim 10\%$ more integrand evaluations, on the average (typically 20 to 50 per integral for the performance test undertaken). This presumably reflects the relatively complex arithmetic within the latter integrator's overhead (e.g., in the computation of Chebyshev series—each of which may have complexity comparable to that of an

integrand evaluation). The required Clenshaw-Curtis roots and weights contribute insignificantly to this overhead, as they are computed only once throughout each test.

TABLE 1

Mean evaluation times of $K(x, y)$

Algorithm	Mean time (*ms*)	
	$\rho = 10^{-5}$	$\alpha = \rho = 10^{-5}$
As proposed	95	90
Expansion (22)	146	146
Ad. Simpson[a]	295	202
D-ad. C-C[b]	394	310

[a]A modified version of COSIMP [21].
[b]An augmented doubly-adaptive Clenshaw-Curtis algorithm [22].

4. The *L*-Function. Since $L(x, y, p)$ is a symmetric function of x and y, there is no loss of generality in assuming throughout that $x \geqslant y$. We adopt the abbreviations

$$\xi = 2\sqrt{pxy}\,, \tag{36a}$$

$$\eta_1 = \sqrt{py/x}\,, \qquad \eta_2 = \sqrt{px/y} = p/\eta_1, \tag{36b}$$

noting that $\eta_1 < \min(\eta_2, \eta_2^{-1}) < 1$.

One can easily verify the useful relationship

$$L(x, y, p) = (1 - e^{py-y})(1 - e^{px-x}) - e^{(p-1)(x+y)}L(px, py, p^{-1}), \tag{37}$$

as a result of which analytic properties of $L(x, y, p)$ with $p > 1$ can be deduced from those with $p < 1$. Consequently, we restrict consideration here to $p \leqslant 1$, though the strategem so developed is suitable also for $p > 1$ if the transformation $(x, y, p) \rightarrow (px, py, p^{-1})$ is made and the subtraction in (37) accommodated analytically.

The following properties follow immediately from Eqs. (3)–(5):

$$L(x, 0, p) = 0, \qquad L(x, y, 0) = (1 - e^{-x})(1 - e^{-y}), \tag{38a}$$

$$\lim_{x \to \infty} L(x, y, p) = 1 - e^{py-y}, \qquad L(x, y, 1) = 0. \tag{38b}$$

In principle, $L(x, y, p)$ can be evaluated by subsituting into (5) the appropriate expansions for the J- or K-function. In practice, some care must be taken to avoid loss of precision upon subtraction (particularly for p near unity), and some economy is obtained by noting that both K- (or J-) functions share the same ξ-value.

The substitution of (22a) into (5a) produces the small-ξ expansion

$$L(x, y, p) = (1 - e^{py-y})(1 - e^{-x}) - e^{-(x+y)} \sum_{n=2}^{\infty} \frac{y^n}{n!} \sum_{m=1}^{n-1} \frac{(p^m - p^n)x^m}{m!}. \tag{39}$$

The leading term of (39) is within $\sim 10\%$ of the value of $L(x, y, p)$ everywhere in the parameter domain $x \geqslant y$, $p \leqslant 1$, and is exact in the $\xi = 0$ or $p = 1$ limits.

An expansion alternative to (39) is more appropriate for small p:

$$L(x, y, p) = (1 - e^{py-y})(1 - e^{px-x}) - e^{-(x+y)}(e^{px} - 1)(e^{py} - 1) + e^{-(x+y)} \sum_{n=1}^{\infty} \frac{p^n}{n!} \left\{ \sum_{m=1}^{n} \frac{x^m y^n + x^n y^m}{m!} - \frac{(xy)^n}{n!} \right\}. \tag{40}$$

Expansion (40) exhibits faster convergence than (39) for $p < y/x$. Moreover, in the parameter domain $p > x/y > 1$, it is essential to employ (40) in place of (39) for the computation of $L(px, py, p^{-1})$.

Consider the large-ξ domain, for which the cases $\eta_2 < 1$ and $\eta_2 > 1$ require separate consideration.

In the large-η_2 domain, $\eta_1 < \eta_2^{-1} < 1$, two substitutions of (23b) into (5b) produce

$$L(x, y, p) = (1 - e^{py-y}) - e^{-(x+y)} \sum_{m=1}^{\infty} (\eta_2^{-m} - \eta_1^m) I_m(\xi). \tag{41}$$

The nullity of $L(x, y, 1)$ is apparent. Note that the leading term in (41) is the $x \to \infty$ asymptote, relative to which the subtracted term is small ($\lesssim 10\%$). The analogous expression in the small-η_2 domain, $\eta_1 < \eta_2 < 1$, which is incompatible with $p \to 1$, is

$$L(x, y, p) = 1 - e^{py-y} - e^{px-x} + e^{-(x+y)} \left\{ I_0(\xi) + \sum_{m=1}^{\infty} (\eta_1^m + \eta_2^m) I_m(\xi) \right\}, \tag{42}$$

which is symmetric in x, y. In each of (41) and (42), the series can be truncated to $m < M$ and summation effected by backward recursion in a manner similar to (25) ff.

If either or both of η_1 and η_2 is near unity, it is convenient to symmetrize (5) to produce

$$L(x, y, p) = 1 - \tfrac{1}{2}(e^{py-y} + e^{px-x}) - e^{py-y} \delta K(x, py) - e^{px-x} \delta K(y, px), \tag{43}$$

where

$$\delta K(x, y) \equiv \tfrac{1}{2}\{K(x, y) - K(y, x)\}. \tag{44}$$

If η_1 is small, we have

$$\delta K(x, py) = \tfrac{1}{2}\{1 - e^{-(x+py)} I_0(\xi)\} - e^{-(x+py)} \sum_{m=1}^{\infty} \eta_1^m I_k(\xi), \tag{45}$$

in which the summation can be truncated, as before. Otherwise, one can deduce from (30) and its analogue for $x > y$

$$\delta K(x, y) = e^{-(x+y)} \sum_{n=1}^{\infty} \frac{(x-y)^n}{n!} \sum_{m=0}^{n}{}'' I_m(2y), \qquad x \geqslant y, \tag{46}$$

where the double prime denotes that the first and last terms in the sum (i.e., $m = 0, n$) are to be halved. The summations of (46) can be truncated and the remainder bounded as in (32)–(35). The truncated summation can then be cast in

the convenient backward-recursive form:

$$\sum_{n=1}^{N-1} \frac{\Delta^n}{n!} \sum_{m=0}^{n}{}'' I_m(\xi_0) = A_0 I_0(\xi_0),$$

$$A_N = B_N = 0,$$

$$A_n = \frac{\Delta}{n+1}\{r_n(\xi_0)A_{n+1} + \tfrac{1}{2}(1 + r_n(\xi_0))B_{n+1}\},$$

$$B_n = \frac{\Delta}{n+1}B_{n+1} + 1.$$

Several factors of the form $(1 - e^{-w})$ are encountered in these formulae. In order to avoid a loss of precision when w is small, it is prudent to employ an approximation—such as one presented by Hart et al. [24]—which explicitly exhibits a factor of w at small w.

Performance. The series (39) or (40) are implemented whenever $\xi \leqslant \xi_c$. Criteria to determine which of the expansions (41)–(46) to proceed with when $\xi > \xi_c$ are more complex than those for $K(x, y)$ in the appendix, and are omitted here. It is sufficient to note that the universal choice $\xi_c = 28$ optimized typical functional evaluation times.

The performance of our algorithm, vis-à-vis the series expansions (39), (40) and numerical integration, was tested using a numerical experiment similar to that for $K(x, y)$. Table 2 reports the mean of 1296 evaluation times, over an arithmetic grid of nine p-values in the range [0.05, 0.95] and, for each p-value, identical geometric grids of x and y (12 values of each) such that $\xi_c \leqslant \xi \leqslant 80$. For numerical integration purposes $L(x, y, p)$ is recast as

$$L(x, y, p) = (1 - e^{-qy}) - \int_0^y \{q + p(1 - e^{q(u-y)})\}e^{-(u+x)}I_0\left(2\sqrt{pux}\right) du,$$

where $q = 1 - p$; the entire right-hand side is then rewritten as an integral over the range [0, 1].

The superiority of the algorithm proposed herein is again in evidence, although to a lesser degree than for $K(x, y)$. This is because the additive leading terms in each expansion dominate $L(x, y, p)$. Accordingly, typical evaluation times are also smaller than for $K(x, y)$.

TABLE 2

Mean evaluation times of $L(x, y, p)$

Algorithm	Mean time (*ms*)	
	$\rho = 10^{-5}$	$\alpha = \rho = 10^{-5}$
As proposed	74	74
Expansions (39), (40)	107	106
Ad. Simpson*	108	106
D-ad. C-C*	256	255

* As in footnotes, Table 1.

5. Summary. We have deduced and presented suitable series expansions for $K(x, y)$, with $x \leqslant y$, and for $L(x, y, p)$ in the asymptotic domain; complementary expansions for $J(x, y)$ with $x > y$ follow analogously to those for $K(x, y)$. These expansions supplement the small-argument expansions (22), (39), (40).

The practical term-by-term evaluation of the series expansion must be performed in the backward direction, necessitating the determination of a truncation point. The expansions may then be summed, and recursive expressions to accomplish this have been presented. They require the evaluation of a Bessel function ratio, $r_M(\xi)$ of (16), and of an exponentially-weighted Bessel function, $e^{-w}I_0(\xi)$; here, ξ is always in the asymptotic region (i.e., $I_0(\xi)$ is dominated by the behavior (15)), where the evaluations are relatively straightforward [14]–[20].

The proposed algorithm is significantly more efficient than either direct numerical integration or small-argument expansions extended to domains stable against underflow. This should greatly benefit the modelling of exchange and filtration processes [1]–[8], [11], [12], for which searches in model-parameter space necessitate successive functional evaluations. In particular, for models of dispersive exchange processes [6]–[8], multiple evaluations of the J- and/or K-functions are required to accomplish numerical integration at each parameter vector in the search; a fast algorithm for these evaluations then becomes imperative in an extensive parameter search.

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Appendix. This appendix presents a scheme for assessing approximately, with minimal computational overhead, the relative magnitude of M and N (respectively, the number of terms retained in the truncated series (25) and (30) for $K(x, y)$ to meet a demanded precision).

An approximate equality of the two remainder functions (27) and (33) yields

$$\eta^{-M} \simeq \frac{\Delta^N}{N!} \simeq \left(\frac{e\Delta}{N}\right)^N, \tag{A1}$$

which is of similar order to the specified precision. In deducing (A1), multipliers independent of M or N have been dropped, and the last expression follows from Stirling's approximation to $N!$. The reliability of (A1) should therefore improve with increasing M and N. The break-even point for the two expansions (i.e., $M = N$) satisfies approximately $e\Delta \simeq M\eta^{-1}$. For values of $e\Delta$ smaller or larger than $M\eta^{-1}$, expansions in Δ or in η^{-1} (respectively) are likely to be the more appropriate. The following two easily-proven lemmas interpret (A1) as an exact equality and permit the implementation of this consideration.

LEMMA 1. *Define*

$$E(M_c) \equiv (M_c!)^{1/M_c}. \tag{A2}$$

If $\Delta < \eta^{-1}E(M_c)$, *then* $N < \max(M, M_c)$.

LEMMA 2. *If*

$$M - M_0 < e\Delta \quad or \quad \eta^{-M} < \left(\frac{e\Delta}{M - M_0} \right)^{M - M_0}, \tag{A3}$$

then $M < N + M_0$.

The proof of Lemma 2 invokes Stirling's approximation for $(M - M_0)!$; its converse also holds to within the accuracy of this approximation.

The recommended strategy for computing $K(x, y)$ for $\eta > 1$, $\xi > \xi_c$ is: if $\Delta < \eta^{-1}E(M_c)$—for a supplied value of $E(M_c)$—then proceed via an expansion in Δ; otherwise compute M (appropriate to an expansion in η^{-1}) and proceed via this expansion if (A3) is satisfied (for a supplied value of M_0), or via an expansion in Δ otherwise. The rationale is that, if M, $N < M_c$, the overhead to ascertain the more appropriate expansion is unwarranted; and if, having computed M, an expansion in Δ is the more appropriate, the presence of M_0 compensates for the overhead in also computing N.

Optimum universal choices for ξ_c, M_c, and M_0 would depend upon the distribution of encountered parameter values, x and y, upon the precision demanded, and upon the computing environment. We here propose such choices, determined by minimizing the mean evaluation time of $K(x, y)$ on a PDP-11 computer for identical geometric grids of x and y, and for a demanded relative precision of 10^{-5}:

$$\xi_c = 20, \quad M_0 = 50, \quad M_c = 20, \quad E(M_c) = 8.3.$$

None of these choices are critical: changes of $\sim 10\%$ affect mean evaluation times by $\lesssim 1\%$.

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