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Incomplete Bessel, generalized incomplete gamma, or leaky aquifer functions

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Abstract

Functions characterized by the alternative appelations in the title hereof have application in areas as diverse as heat conduction, probability theory, electronic structure in periodic systems, and hydrology. These functions are regarded as difficult to evaluate and have been given attention by a number of investigators in all these fields. This communication ties together the previously disjoint literature, and presents several new expansions of these functions that are in various parameter ranges computationally more efficient than any of the previously proposed methods of evaluation. A new formula for computation of these functions from nearby tabulated values is also reported. The computational advantages of the new procedures are illustrated with examples.

MSC: 33B20; 33C10; 41A58

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1. Introduction

In the mid-1950s, Hantush and Jacob [13] showed that water levels in pumped aquifer systems with finite transmissivity and leakage could be analyzed in terms of an integral which they and subsequently other hydrologists called the *leaky aquifer function*. In a more general notation suitable for our present purposes, we write

$$K_\nu(x, y) = \int_1^\infty \frac{\mathrm{d}t}{t^{\nu+1}} \mathrm{e}^{-xt-y/t}, \tag{1}$$

with $K_0(x, y)$ the original leaky aquifer function and $K_n(x, y)$ (n a positive integer) representing generalizations useful in other hydrological systems [20]. Hydrologists [13,19,27] identified some methods for evaluating $K_n(x, y)$ for small non-negative integral n and for the ranges of x and y important to them, but did not undertake a systematic study. In the present communication we consider the entire range $x > 0$, $y \geqslant 0$, with ν values that are real but not necessarily integral. In the applications that were the target of a previous investigation by others [7], consideration was focused, in the notation of Eq. (1), on $\nu \leqslant 0$; in other applications we identify herein, integral and non-integral $\nu \geqslant 0$ also arise.

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Although we shall not discuss it in detail, we also note that many of the formulas presented here can be extended to substantial regions of the complex plane.

In 1981, Terras [26] explicitly identified $K_\nu(x, y)$ as an incomplete Bessel function of a type characterized in the treatise in [2]; Terras's definition actually took the form

$$K_\nu(x, y)_{\mathrm{Terras}} = \int_1^\infty t^{\nu-1}\, \mathrm{e}^{-xt-y/t}\, \mathrm{d}t = K_{-\nu}(x, y), \tag{2}$$

where the occurrence of ν is opposite in sign to its appearance in Eq. (1); in this work we use the definition in Eq. (1).

The appropriacy of the Bessel function nomenclature is obvious if one starts from the following formula [1] for the modified Bessel function (the Macdonald function):

$$K_\nu(z) = \frac{1}{2}\int_0^\infty \frac{\mathrm{d}t}{t^{\nu+1}}\mathrm{e}^{-(1/2)z(t+1/t)}. \tag{3}$$

If K_ν is made "incomplete" by increasing the lower limit of the integral to $(x/y)^{1/2}$, then setting $z = 2(xy)^{1/2}$, one recovers, after a change of the integration variable, an integral proportional to that in Eq. (1). A variant [22] of Eq. (3), with $t^{\nu-1}$ in place of $t^{-\nu-1}$, is a form that naturally relates to the formulas given by Terras and to that in Eq. (4) below.

Integrals of the form $K_\nu(x, y)$ also appear when Ewald-type summation acceleration procedures [9] are applied to electronic-structure calculations for systems described in terms of Gaussian-type atomic orbitals, with periodicity in one, two, or all three physical dimensions. For one-dimensional periodicity, the values of ν that occur will be integral and non-negative [8,10,11], ranging from zero to a maximum value that depends on the angular momenta of the orbitals. For periodicity in two dimensions, half-integral ν are encountered [15,18,23], while for full three-dimensional periodicity, integral ν again occur. It is largely because of the importance of $K_\nu(x, y)$ in this context that we choose to use the definition of Eq. (1) rather than that of Eq. (2).

The functions under discussion have also been identified as generalizations of the incomplete gamma function in detailed work in [7,6]. These authors introduced the definition

$$\Gamma(\alpha, x; b) = \int_x^\infty t^{\alpha-1}\mathrm{e}^{-t-b/t}\, \mathrm{d}t \tag{4}$$

with obvious connections both to the conventional incomplete gamma function $\Gamma(\alpha, x)$ (as defined in [1, Formula 6.5.3]) and to the form in Eq. (1):

$$\Gamma(\alpha, x) = \Gamma(\alpha, x; 0), \tag{5}$$

$$K_\nu(x, y) = x^\nu\, \Gamma(-\nu, x; xy). \tag{6}$$

We note that the difference in the names assigned to $K_\nu(x, y)$ and $\Gamma(\alpha, x; b)$ was probably the reason there have been no previous communications connecting the above cited research communities.

These incomplete Bessel/generalized incomplete gamma functions have a deserved reputation as difficult to evaluate. Moreover, when used in electronic structure computations, the numerical requirements involved in their evaluation become extreme. Many millions of the integrals $K_\nu(x, y)$ must then be evaluated, with ν values ranging (for heavy atoms) from zero to 12 or more, and for a wide range of x and y. In addition, the evaluations must be carried out to high accuracy; depending on the application, six to 10 significant figures will be needed for the $K_\nu(x, y)$ of largest magnitude. To meet these requirements within reasonable computation times it will probably be necessary to use appropriate combinations of recurrence formulas, interpolation from tabulated values, and rapidly convergent expansions.

The present communication presents a number of new expansions of $K_\nu(x, y)$ that are more computationally efficient in various important parameter ranges than those previously proposed. Additionally, formulas are provided in which $K_\nu(x, y)$ is given, in the two-dimensional region in x, y near a point (x_0, y_0), as a one-dimensional sum involving $K_\mu(x_0, y_0)$. It is shown how, by optimum choices between new and existent methods, one can achieve efficient computation of $K_\nu(x, y)$ over a broad range of all three parameters ν, x, and y.

2. Functional relations and limiting values

Defining the two complementary variables $u=(xy)^{1/2}$ and $v=(x/y)^{1/2}$, and starting from Eq. (3) for $z=2u$, the integral may be broken into the two ranges $(0, v)$ and (v, ∞), thereby obtaining after appropriate rearrangements

$$K_\nu(x, y) + K_{-\nu}(y, x) = 2v^\nu K_\nu(2u). \tag{7}$$

This is a minor generalization of a formula in [19], and can also be regarded as a corollary to [7, Theorem 1]. Since good methods exist for evaluating $K_\nu(2u)$ [24] (see also Refs. [5,28]), Eq. (7) provides a practical procedure for interchange of the roles of x and y.

Integration by parts of the integral representation of $K_\nu(x, y)$ in Eq. (1) leads to the inhomogeneous recurrence formula

$$xK_{\nu-1}(x, y) + \nu K_\nu(x, y) - yK_{\nu+1}(x, y) = \mathrm{e}^{-(x+y)}, \tag{8}$$

reported in [27]. This is in [7, Theorem 4].

Differentiation of Eq. (1) with respect to x and y leads to the formulas

$$\frac{\partial K_\nu(x, y)}{\partial x} = -K_{\nu-1}(x, y), \tag{9}$$

$$\frac{\partial K_\nu(x, y)}{\partial y} = -K_{\nu+1}(x, y), \tag{10}$$

results equivalent to [7, Theorems 5 and 6], but with a more symmetric appearance because of the present choice of notation.

Setting $y=0$, we reach the obvious result

$$K_\nu(x, 0) = x^\nu \Gamma(-\nu, x) \tag{11}$$

$$= E_{\nu+1}(x), \quad \nu = -1,\ 0, 1, 2, \ldots, \tag{12}$$

$$K_{-\nu}(x, 0) = \alpha_{\nu-1}(x), \quad \nu = 1, 2, 3, \ldots, \tag{13}$$

where E_n is the exponential integral defined in [1, Formula 5.1.4] and α_n is defined in the immediately following Formula 5.1.5.

At $x=0$, $K_0(x, y)$ exhibits a logarithmic singularity, with behavior at $x \to 0^+$

$$K_0(x, y) \longrightarrow -\ln x - \ln y - 2\gamma - E_1(y) + \mathrm{O}(x), \tag{14}$$

where $\gamma = 0.57721\cdots$ is the Euler–Mascheroni constant. However, for $\nu > 0$, $K_\nu(0, y)$ remains nonsingular, given by

$$K_\nu(0, y) = y^{-\nu}\gamma(\nu, y). \tag{15}$$

Here $\gamma(\nu, y)$ is the incomplete gamma function defined in [1, Formula 6.5.2]. For $x=0$ and $\nu<0$, the integral representation of Eq. (1) fails, but Eq. (15) remains valid, exhibiting singularities only at negative integer values of ν.

For half-integer ν, $K_\nu(x, y)$ can be written as closed expressions involving the complementary error function. A formula for $\nu = \frac{1}{2}$ was given in [23] and used in [18]; extension to other half-integer ν appears in the study in [6].

3. Expansions of $K_\nu(x, y)$

Practical methods for the evaluation of $K_\nu(x, y)$ take different forms, depending upon the magnitudes of x and y and on their ratio.

Small y: As noted in almost all the cited literature, $K_\nu(x, y)$ has a reasonably convenient Maclaurin expansion in y; Chaudhry et al. [6] give this formula as their Eq. (2.1). The equivalent result in the present notation is

$$K_\nu(x, y) = \sum_{j=0}^{\infty} x^{\nu+j}\Gamma(-\nu-j, x)\frac{(-y)^j}{j!}. \tag{16}$$

For integral $v \geqslant -1$, Eq. (16) becomes

$$K_n(x, y) = \sum_{j=0}^{\infty} E_{n+j+1}(x) \frac{(-y)^j}{j!}. \tag{17}$$

While these expansions are convergent (for fixed x and v) for all y, the convergence rate becomes unacceptably slow as y increases, and other methods of computation are needed in practical applications.

Expansion in Legendre functions Q_m: An interesting expansion in Legendre functions of the second kind, motivated by the work in [21], was reported in [17]. Kryachko showed that a change of the integration variable in Eq. (1) from t to $z = (xt)^{1/2} - (y/t)^{1/2}$ caused $K_0(x, y)$ to assume the form

$$K_0(x, y) = 2\mathrm{e}^{-2\sqrt{xy}} \int_{x^{1/2}-y^{1/2}}^{\infty} \frac{\mathrm{e}^{-z^2}\,\mathrm{d}z}{\sqrt{z^2 + 4(xy)^{1/2}}}, \tag{18}$$

reminiscent of the integrand obtained in [6] for the discussion of an expansion of $\Gamma(\alpha, x; b)$ in terms of the error function.

Starting from Eq. (18), the Legendre expansion reads (for $x \geqslant y$)

$$K_0(x, y) = K_0(2\sqrt{xy}) - \mathrm{e}^{-(x+y)} \sum_{m=0}^{\infty} \frac{(x-y)^m}{m!} Q_m\left(\frac{x+y}{x-y}\right), \tag{19}$$

where Q_m is defined in [1, Formula 8.1.3]. Eq. (19) is convergent for all positive $x - y$. For $x = y$, the $m = 0$ term of the summation is to be replaced by its limit (zero), leaving $K_0(x, x) = K_0(2x)$, as expected from Eq. (7).

Differentiation of Eq. (19) with respect to y yields (for $x \geqslant y$)

$$K_1(x, y) = \left(\frac{x}{y}\right)^{1/2} K_1(2\sqrt{xy}) - \frac{\mathrm{e}^{-(x+y)}}{2y}\left[1 + \sum_{m=0}^{\infty}(x + y - m)\frac{(x-y)^m}{m!} Q_m\left(\frac{x+y}{x-y}\right)\right]. \tag{20}$$

We now make the new observation that use of the recurrence formula, Eq. (8), shows that an extension to $K_n(x, y)$ for general integers n will be of the form

$$K_n(x, y) = \left(\frac{x}{y}\right)^{n/2} K_n(2\sqrt{xy}) - \frac{\mathrm{e}^{-(x+y)}}{2y^n}\left[f_n + \sum_{m=0}^{\infty} g_{n,m}\frac{(x-y)^m}{m!} Q_m\left(\frac{x+y}{x-y}\right)\right], \tag{21}$$

with f_n and $g_{n,m}$ given recursively by the following equations:

$$f_{n+1} = xyf_{n-1} + nf_n + 2y^n, \quad f_0 = 0, \quad f_1 = 1, \tag{22}$$

$$g_{n+1,m} = xy\, g_{n-1,m} + n\, g_{n,m}, \quad g_{0,m} = 2, \quad g_{1,m} = x + y - m. \tag{23}$$

For later use, note that when $x = y$, Eq. (21) reads

$$K_n(x, x) = K_n(2x) - \frac{\mathrm{e}^{-2x} f_n}{2x^n}. \tag{24}$$

In addition, comparison with Eq. (7) shows that

$$K_{-n}(x, x) = K_n(2x) + \frac{\mathrm{e}^{-2x} f_n}{2x^n}, \tag{25}$$

equivalent to the observation (for $x = y$) that $f_{-n} = -x^{-2n} f_n$.

Continuing for $x = y$, we also note that the recurrence formula for f_n is equivalent to the explicit form

$$f_n = \sum_{j=0}^{n-1} \frac{(n-j-1)!}{j!}(2n-2j)_j\, x^j. \tag{26}$$

Here $(a)_p$ is the Pochhammer symbol, defined as $a(a+1)\cdots(a+p-1)$, with $(a)_0=1$. Eq. (26) may be verified by confirming that f_n as given therein satisfies both the recurrence formula and the starting values of f_0 and f_1 presented in Eq. (22).

y/x small: A formula which is useful when neither x nor y is small but their ratio is far from unity is an expansion given in [6] in terms of confluent hypergeometric functions. In the present notation, it reads

$$K_\nu(x,y)=\mathrm{e}^{-(x+y)}\sum_{n=0}^{\infty} y^n U(n+1,1-\nu,x), \tag{27}$$

where $U(a,b,z)$ is defined in [1, Formula 13.1.3]. This expansion is convergent for all y, and converges more rapidly than those which have been proposed in [14,16]. Good methods for evaluating $U(a,b,z)$ have been given in [25].

y/x near unity: Again using $u=(xy)^{1/2}$, $v=(x/y)^{1/2}$, we write $K_\nu(x,y)=v^\nu L(u,v)$, where

$$L(u,v)=\int_v^\infty \frac{\mathrm{e}^{-u(t+1/t)}}{t^{\nu+1}}\,\mathrm{d}t. \tag{28}$$

The Taylor series expansion of $L(u,v)$ about $v=1$ takes the form

$$L(u,v)=L(u,1)+\mathrm{e}^{-2u}\sum_{k=1}^{\infty} C_{k\nu}(u)(v-1)^k, \tag{29}$$

where

$$C_{k\nu}=-\frac{\mathrm{e}^{2u}}{k!}\left[\left(\frac{\partial}{\partial v}\right)^{k-1}\frac{\mathrm{e}^{-u(v+1/v)}}{v^{\nu+1}}\right]_{v=1}=\sum_{j=0}^{[(k-1)/2]}\frac{(-1)^{k-j}}{k}\frac{(\nu+j+1)_{k-2j-1}}{j!\,(k-2j-1)!}u^j. \tag{30}$$

Here $[p]$ stands for the integer part of p, and $(a)_p$ is the Pochhammer symbol, defined earlier herein. The proof of Eq. (30) is given in an Appendix.

Noting now that $L(u,1)=K_\nu(u,u)$, we reach

$$K_\nu(x,y)=v^\nu\left[K_\nu(u,u)+\mathrm{e}^{-2u}\sum_{k=1}^{\infty}C_{k\nu}(u)(v-1)^k\right]. \tag{31}$$

For integral ν, evaluation of $K_\nu(u,u)$ is most easily carried out using Eq. (24).

We note that $L(u,v)$ has no singularities except possibly at $v=0$, so Eq. (31) will always converge for $0<v<2$. However, if $v>1$, a series that converges more rapidly than Eq. (31) can be obtained by interchanging the roles of x and y via Eq. (7), then evaluating $K_{-\nu}(y,x)$.

x and y small: In addition to the formulas presented above, an expansion of $K_0(x,y)$ in both x and y leads initially to

$$\begin{aligned}K_0(x,y)&=\sum_{n=0}^{\infty}E_{n+1}(x)\frac{(-y)^n}{n!}\\&=\sum_{n=0}^{\infty}\left[\frac{(-x)^n}{n!}[-\ln x+\psi(n+1)]-\sum_{m=0}^{\infty}{}'\,\frac{(-x)^m}{(m-n)m!}\right]\frac{(-y)^n}{n!}\\&=\sum_{n=0}^{\infty}\frac{(xy)^n}{n!\,n!}[-\ln x+\psi(n+1)]-\sum_{m,n=0}^{\infty}{}'\,\frac{(-1)^{n+m}x^m y^n}{(m-n)m!\,n!}.\end{aligned} \tag{32}$$

The prime on the sums over m indicate that the term $m=n$ is to be omitted from the summation, and $\psi(n+1)$ is the digamma function as given in [1, Formula 6.3.2]: $\psi(1)=-\gamma$, $\psi(n+1)=\psi(n)+1/n\ (n\geqslant 1)$.

We now invoke [1, Formula 9.6.10], which for the present purposes can be written as

$$I_j(2\sqrt{xy}) = (xy)^{j/2} \sum_{n=0}^{\infty} \frac{(xy)^n}{n!\,(n+j)!}, \tag{33}$$

and will also use [1, Formula 9.6.13], written as follows and rearranged as shown:

$$K_0(2\sqrt{xy}) = \left[-\frac{1}{2}(\ln x + \ln y) - \gamma\right] I_0(2\sqrt{xy}) + \frac{xy}{1!\,1!} + \left(1+\frac{1}{2}\right)\frac{(xy)^2}{2!\,2!} + \left(1+\frac{1}{2}+\frac{1}{3}\right)\frac{(xy)^3}{3!\,3!} + \cdots \tag{34}$$

$$= -\frac{1}{2}(\ln x + \ln y) I_0(2\sqrt{xy}) + \sum_{j=1}^{\infty} \psi(j+1)\frac{(xy)^j}{j!\,j!}. \tag{35}$$

Observing that the $\ln x$ term of Eq. (32) reduces by virtue of Eq. (33) to $-\ln x\, I_0(2\sqrt{xy})$, the use of Eq. (35) permits Eq. (32) to be brought to the form

$$K_0(x,y) = K_0(2\sqrt{xy}) - \frac{1}{2}\ln\left(\frac{x}{y}\right) I_0(2\sqrt{xy}) - {\sum_{m,n=0}^{\infty}}' \frac{(-1)^{n+m} x^m y^n}{(m-n)m!\,n!}. \tag{36}$$

Finally, we rearrange the summation of Eq. (36). For the range $m > n$, replace the m summation by a sum over $j = m - n$, with $1 \leqslant j < \infty$; for $n > m$, replace the n summation by a sum over $j = n - m$, also with $1 \leqslant j < \infty$. The result of these manipulations is

$$
\begin{aligned}
{\sum_{m,n=0}^{\infty}}' \frac{(-1)^{n+m} x^m y^n}{(m-n)m!\,n!} &= \sum_{j=1}^{\infty} \frac{(-1)^j}{j}\left[\sum_{n=0}^{\infty} \frac{x^j (xy)^n}{(n+j)!\,n!} - \sum_{m=0}^{\infty} \frac{y^j (xy)^m}{m!\,(m+j)!}\right] \\
&= \sum_{j=1}^{\infty} \frac{(-1)^j}{j} \frac{(x^j - y^j)}{(xy)^{j/2}} I_j(2\sqrt{xy}).
\end{aligned} \tag{37}
$$

Inserting Eq. (37) and using $u = \sqrt{xy}$, $v = \sqrt{x/y}$, the final result is

$$K_0(x,y) = K_0(2u) - \ln v\, I_0(2u) - \sum_{j=1}^{\infty} \frac{(-1)^j}{j}(v^j - v^{-j}) I_j(2u). \tag{38}$$

Since the ratio $I_{j+1}(2u)/I_j(2u)$ approaches u/j in the limit $j \gg u$, Eq. (38) will be absolutely convergent for all finite nonzero v. The actual convergence rate will be optimum for v close to unity.

An expansion parallel to Eq. (38) for $K_\nu(x,y)$ of nonzero ν is more complicated and will not be pursued here.

A Bessel function expansion: Another expansion in Bessel functions can be obtained easily by rewriting Eq. (1) as

$$K_\nu(x,y) = \int_1^{\infty} \frac{e^{-(x+y)t}\, e^{y(t-1/t)}}{t^{\nu+1}}\, dt. \tag{39}$$

Now identifying the second exponential as the generating function for $J_n(2y)$ [1, Formula 9.1.41], Eq. (39) becomes

$$
\begin{aligned}
K_\nu(x,y) &= \sum_{n=-\infty}^{\infty} \left(\int_1^{\infty} t^{n-\nu-1} e^{(x+y)t}\, dt\right) J_n(2y) \\
&= (x+y)^{\nu}\Gamma(-\nu, x+y) J_0(2y) + \sum_{n=1}^{\infty} [(x+y)^{\nu-n}\Gamma(n-\nu, x+y) \\
&\quad + (-1)^n (x+y)^{\nu+n}\Gamma(-n-\nu, x+y)] J_n(2y).
\end{aligned} \tag{40}
$$

Eq. (40) is absolutely convergent for all positive x and y, but for most of this range the convergence is less rapid than for one or more of the methods presented previously.

4. Interpolation methods

Here we consider evaluations that obtain $K_\nu(x_0+x, y_0+y)$ using data from a nearby point (x_0, y_0). The key result needed for this purpose is an expansion formula, which for $xy > 0$ takes the form

$$K_\nu(x_0+x, y_0+y) = K_\nu(x_0, y_0) I_0(2\sqrt{xy}) + \sum_{j=1}^{\infty} (-1)^j [y^j K_{\nu+j}(x_0, y_0) + x^j K_{\nu-j}(x_0, y_0)](xy)^{-j/2} I_j(2\sqrt{xy}). \tag{41}$$

This formula is also applicable when $xy < 0$, but the appearance of imaginary quantities can be avoided by converting Eq. (41) to the form

$$K_\nu(x_0+x, y_0+y) = K_\nu(x_0, y_0) J_0(2\sqrt{-xy}) + \sum_{j=1}^{\infty} (-1)^j [y^j K_{\nu+j}(x_0, y_0) + x^j K_{\nu-j}(x_0, y_0)](-xy)^{-j/2} J_j(2\sqrt{-xy}). \tag{42}$$

A main virtue of Eqs. (41) and (42) is that the two-dimensional array of derivatives arising in the Taylor expansion of K_ν about (x_0, y_0) is reduced, by virtue of Eqs. (9) and (10), to a one-dimensional array consisting of $K_{\nu\pm j}(x_0, y_0)$. For the same reason, a single one-dimensional array suffices to permit interpolation for all $K_\nu(x, y)$ of an integer-spaced set of ν values.

To prove Eqs. (41) and (42), note that because $(\partial/\partial x)^\sigma (\partial/\partial y)^\tau K_\nu(x_0, y_0) = (-1)^{\sigma+\tau} K_{\nu+\tau-\sigma}(x_0, y_0)$, the Taylor expansion takes the form

$$K_\nu(x_0+x, y_0+y) = \sum_{\sigma,\tau} (-1)^{\sigma+\tau} K_{\nu+\tau-\sigma}(x_0, y_0) \frac{x^\sigma y^\tau}{\sigma!\,\tau!}. \tag{43}$$

Writing the summations in terms of new indices $j = \tau - \sigma$ and $k = \min(\tau, \sigma)$, with ranges $-\infty < j < \infty$, $0 \leqslant k < \infty$, one can reach

$$K_\nu(x_0+x, y_0+y) = \sum_{j=-\infty}^{\infty} (-1)^j x^{(j-|j|)/2} y^{(j+|j|)/2} K_{\nu+j}(x_0, y_0) \sum_{k=0}^{\infty} \frac{(xy)^k}{k!\,(k+|j|)!}. \tag{44}$$

Invoking [1, Formula 9.6.10], the k summation can be identified as $(xy)^{-|j|/2} I_{|j|}(2\sqrt{xy})$. Combining terms of the same $|j|$ value, it is now straightforward to confirm Eq. (41).

5. Numerical illustrations

There is no unique set of optimum computational procedures for the $K_\nu(x, y)$, as the choice depends, *inter alia*, upon the accuracy required, and also whether that accuracy is relative or absolute. Also, different methods become optimum if values are needed, for given x and y, for a set of integer-spaced ν values, as opposed to a situation in which only one ν value is required. Moreover, nearly all of the expansions presented above involve special-function evaluations, and advances in the efficiency of those evaluations may impact assessments of computational efficiency.

To illustrate the relative efficiency of the various methods, we consider four cases, with a required absolute accuracy of $\pm 10^{-10}$, computed in 8-byte floating point arithmetic (about 16 significant decimal digits):

Case 1. $x = 0.01$, $y = 4.00$, $\nu = 0(1)9$: A good approach is to use upward recursion in ν starting from $K_0(x, y)$ and $K_1(x, y)$. To obtain these starting values we use Eq. (7) to interchange x and y, obtaining

$$K_0(x, y) = 2K_0(2\sqrt{xy}) - K_0(y, x), \tag{45}$$

$$K_1(x, y) = 2\left(\frac{x}{y}\right)^{1/2} K_1(2\sqrt{xy}) - K_{-1}(y, x). \tag{46}$$

Table 1
$K_n(0.01, 4.00)$: "This research", computed in 8-byte floating point arithmetic by the procedure described in the text. "Accurate values", obtained by numerical integration of Eq. (1)

n	This research	Accurate values
0	2.22531 07612 66468	2.22531 07612 66469
1	0.21389 41668 22939	0.21389 41668 22940
2	0.05450 34697 99701	0.05450 34697 99701
3	0.02325 31215 07707	0.02325 31215 07708
4	0.01304 27509 96080	0.01304 27509 96080
5	0.00856 75349 90649	0.00856 75349 90649
6	0.00620 86768 06601	0.00620 86768 06601
7	0.00480 10852 38177	0.00480 10852 38177
8	0.00388 40720 49626	0.00388 40720 49627
9	0.00324 67980 03148	0.00324 67980 03149

Table 2
Alternative expansions of $K_2(4.95, 5.00)$. $n_{\max}$ is the maximum index value used in the expansion

Method	$n_{\max}$	Value
Accurate		0.00001 22499 87981
Q_n expansion, Eq. (21)	1	0.00001 22499 87980
U expansion, Eq. (27)	10	0.00001 22499 60637
$v-1$ expansion, Eq. (31)	2	0.00001 22499 86022

The Bessel functions $K_0(2\sqrt{xy})$ and $K_1(2\sqrt{xy})$ can be computed as described in [24,5,28]; $K_0(y, x)$ and $K_{-1}(y, x)$ are obtained using Eq. (17). To apply that equation, one needs $E_0(y)$, which is simply e^{-y}/y, and $E_n(y)$ for $n \geqslant 1$, which can be computed by the methods given in [3,4].

The recurrence in v is carried out using Eq. (8), which, though not entirely stable, yields the presently required accuracy. The result of the procedure outlined above is shown in Table 1, which provides a comparison with values obtained by an entirely accurate, but unacceptably slow numerical integration.

Case 2. $x = 4.95$, $y = 5.00$, $v = 2$: Possible evaluation methods include that of Ref. [6], namely Eq. (27), and two procedures new to the present work, Eqs. (21) and (31). The procedure of Eq. (27) has the advantage that it only requires one significant special-function evaluation, namely that of the confluent hypergeometric function $U(1, 1 - v, x)$; this is true because $U(0, 1 - v, x) = 1$ and $U(n, 1 - v, x)$ for $n > 1$ can be generated with sufficient accuracy by upward recursion in n. However, for the illustrated parameter values the series in Eq. (27) converges very slowly.

The procedure of fastest convergence is the expansion in Legendre Q_n, Eq. (21), which requires the evaluation of one K_v and the fairly easily computable Q_n. It should be noted that the easiest approach to the Q_n is by upward application of the well-known recurrence formula. As has been pointed out in [12] and since by many others, upward recurrence of this function is unstable and must be used with caution. However, the instability will not introduce computational problems in circumstances (as in this example) where the desired convergence of the Q_n expansion is reached before the Q_n values become too inaccurate.

Almost as rapidly convergent is the procedure of Eq. (31), which, via Eq. (24), also requires one K_v evaluation. The overall conclusion is that for the illustrated parameter values, the Legendre expansion, Eq. (21), is the most efficient. Values and expansion lengths are presented in Table 2.

Case 3. $x = 10$, $y = 2$, $v = 6$: Here Eq. (27) is best. The accurate value of $K_6(10., 2.)$ is 0.00023 44186 32699; from Eq. (27) with $n_{\max} = 5$, we get 0.00023 44186 19816.

Case 4. $x = 3.1$, $y = 2.6$, $v = 5$: This example demonstrates the efficacy of the interpolation formula, Eq. (41). We assume the availability of a precomputed table of $K_n(3.0, 2.5)$ for a sufficient range of n. Then, carrying the summation of Eq. (41) through $j = 5$, we obtain $K_5(3.1, 2.6) \approx 0.00052\,85043\,21353$; the accurate value is 0.00052 85043 25244.

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Appendix A. Proof of Eq. (30)

Eq. (30) of the main text involves evaluation of an expression of the form

$$F_{n,v}(u, v) = \left(\frac{\partial}{\partial v}\right)^n \frac{\mathrm{e}^{-u(v+1/v)}}{v^v}, \tag{47}$$

for the special value $v = 1$. Noting that $\partial \mathrm{e}^{-u(v+1/v)}/\partial v = -(1 - v^{-2})u\mathrm{e}^{-u(v+1/v)}$ and that a subsequent differentiation of $(1 - v^{-2})$ yields a factor v^{-3}, we see that a contribution to $F_{n,v}(u, v)$ that involves j differentiations of the factor $\mathrm{e}^{-u(v+1/v)}$ and single differentiations of m factors $(1 - v^{-2})$ must also involve $n - j - m$ differentiations of a power of v, so that the net power of v in that contribution will be $-v - 3m - (n - j - m)$. These observations lead to the conclusion that $F_{n,v}(u, v)$ can be written as

$$F_{n,v}(u, v) = \sum_{jm} A^n_{jm} u^j \left(1 - \frac{1}{v^2}\right)^{j-m} v^{j-2m-n-v}\, \mathrm{e}^{-u(v+1/v)}, \tag{48}$$

with $0 \leqslant j \leqslant n$ and $0 \leqslant m \leqslant \min(j, n - j)$. Differentiating Eq. (48) with respect to v and setting the result equal to the expansion for $F_{n+1,v}(u, v)$, we find that A^n_{jm} satisfies (for $n \geqslant 0$) the recurrence formula

$$A^{n+1}_{jm} = 2(j - m + 1)A^n_{j,m-1} - A^n_{j-1,m} + (j - 2m - n - v)A^n_{jm}, \tag{49}$$

where any A^n_{jm} with indices not satisfying the conditions given above is to be assigned the value zero. In addition, we verify directly from Eqs. (47) and (48) that $A^0_{00} = 1$.

We now assert that the solution of this recurrence system is

$$A^n_{jm} = \frac{(-1)^{n-m}\, n!\, (v + m)_{n-j-m}}{m!\, (j - m)!\, (n - j - m)!}, \tag{50}$$

where $(v + m)_{n-j-m}$ is a Pochhammer symbol. The correctness of Eq. (50) can be confirmed by verifying that it satisfies Eq. (49) and yields the starting value $A^0_{00} = 1$.

It is straightforward to specialize Eq. (48) to $v = 1$. The only contributing value of m is then $m = j$, and we have (because now $2j$ must not exceed n)

$$F_{n,v}(u, 1) = \sum_j^{[n/2]} A^n_{jj}\, u^j\, \mathrm{e}^{-2u} = \sum_j^{[n/2]} \frac{(-1)^{n-j}\, n!\, (v + j)_{n-2j}}{j!\, (n - 2j)!}\, u^j\, \mathrm{e}^{-2u}, \tag{51}$$

with $[n/2]$ denoting the integer part of $n/2$. Making the final observation $C_{kv} = -(\mathrm{e}^{2u}/k!)F_{k-1,v+1}(u, 1)$, we recover the right-hand member of Eq. (30).

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