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Note

Algorithms for Some Integrals of Bessel Functions and Multivariate Gaussian Integrals

1. INTRODUCTION

In this paper we shall devise a Miller formula for evaluating the integral

$$Ki_1(x) = \int_x^\infty K_0(t)\, dt \qquad (x > 0), \tag{1}$$

and we shall devise a simple backwards recursion method for evaluating double integrals that have the canonical form

$$\alpha(r, s \mid x, y) = e^y \int_0^1 e^{-yu} \alpha(r, xu)\, u^{s-1}\, du, \tag{2}$$

where

$$\alpha(r, x) = e^x \int_0^1 e^{-xt} t^{r-1}\, dt, \tag{3}$$

with all arguments and parameters taken to be positive. The Bessel function integral has important applications in physics and is frequently tabulated. On the other hand, the double incomplete gamma integral has had its principal applications in statistics, but should be of interest to the scientific community. In our approach we draw most heavily upon our own two preceding papers [14, 15].

2. INTEGRALS OF BESSEL FUNCTIONS

Given the well-known Bessel function

$$K_\nu(x) = \int_0^\infty e^{-x \cosh u} \cosh \nu u\, du \qquad (x > 0) \tag{4}$$

one is able to derive an expansion

$$e^x \int_x^\infty t^{-\nu} K_\nu(t)\, dt = \pi^{1/2}\, 2^\nu \sum_{n=0}^\infty (-1)^n\, (\nu + \tfrac{1}{2})_n\, U(n + \tfrac{1}{2} + \nu, 2\nu, 2x), \tag{5}$$

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where $(a)_0 = 1$ and $(a)_n = a(a+1)(a+2)\cdots(a+n-1)$ when $n \geqslant 1$, and where $U(a, b, z)$ is the confluent hypergeometric function [1] with the integral representation

$$\Gamma(a)\, U(a, b, z) = e^z \int_1^\infty e^{-zt}(t-1)^{a-1}\, t^{b-a-1}\, dt, \tag{6}$$

which is valid for $z > 0$ and $a > 0$. One derives (5) by using the relation $K_\nu(x) = \pi^{1/2}(2x)^\nu e^{-x} U(\nu + \frac{1}{2}, 2\nu + 1, 2x)$ along with integration under the integral sign.

If one defines $Ki_n(x) = \int_x^\infty Ki_{n-1}(t)\, dt$ for $n \geqslant 1$, $Ki_0(x) = K_0(x)$, and $Ki_{-n}(x) = (-1)^n d^n/dx^n K_0(x)$ for $n \geqslant 1$ then one is able to extend our method in deriving (5) to get an expansion for $Ki_n(x)$. Indeed if we define $U(k) = U(k + \frac{1}{2}, 1 - n, 2x)$ for $k = 0, 1, 2, \ldots$ then one has the expansions

$$Ki_n(x) = \pi^{1/2} U(0) \left[1 + \sum_{k=1}^{\infty} (-1)^k \frac{(n)_k (\frac{1}{2})_k}{k!} \frac{U(1)}{U(0)} \frac{U(2)}{U(1)} \cdots \frac{U(k)}{U(k-1)}\right], \tag{7}$$

$$U(0) = (2x)^{-1/2} \left[1 + \sum_{k=1}^{\infty} \frac{(\frac{1}{2})_k (n + \frac{1}{2})_k}{k!} \frac{U(1)}{U(0)} \frac{U(2)}{U(1)} \cdots \frac{U(k)}{U(k-1)}\right]^{-1}. \tag{8}$$

Formulas of this type were termed Miller formulas in our preceding paper [15], where we also discussed the evaluation in detail. Our method entails the generation of successive quotients through the fractional linear transformations

$$\frac{U(k)}{U(k-1)} = \frac{4}{4(n + 2k + 2x) - (1 + 2k)(1 + 2k + 2n)\dfrac{U(k+1)}{U(k)}}, \tag{9}$$

which generate a continued fraction. When formulas (7) and (8) are written in terms of nested operations these quotients are folded into the nesting very efficiently. In that manner one has only to specify the truncation index of the series, which is also taken as the starting index of (9). Empirically computed starting indices for $Ki_1(x)$, the most important case, are tabulated in Table I.

In computer trials we were able to obtain accurate results for $Ki_n(x)$ $(n \geqslant 1)$. We verified the data for $Ki_1(x)$ by comparing with the tabulations in [1, 3, 8] and we verified our data for higher-order functions by making recursive checks. There is no uncertainty to the reliability of (8) because all terms are positive and because the proposition in [15] implies that the continued fraction is stable. On the other hand, series (7) is monotone in absolute value by the estimates in [15] and thus incurs essentially no error due to cancellation. In case of $Ki_1(x)$ this may be inferred from $\Gamma(a)\, U(a, b, x) \geqslant \Gamma(a+1)\, U(a+1, b, x)$. We tested our method for $Ki_n(x)$ in the intervals $1 \leqslant n \leqslant 100$ and $1 \leqslant x \leqslant 200$ with an appropriate starting index function.

Approximate starting index. The function $n(x) = [10 + 92/x]$ is a good approximation for the starting indices in Table I. In computer checks on the Burroughs

TABLE I[a]

x	$e^x Ki_1(x)$	$n(x)$	x	$e^x Ki_1(x)$	$n(x)$
20.0	2.7212024643(−1)	11	3.0	6.1960339780(−1)	36
16.0	3.0215888406(−1)	12	2.5	6.6300151284(−1)	44
12.0	3.4506429758(−1)	14	2.0	7.1762950619(−1)	52
8.0	4.1388069462(−1)	18	1.8	7.4386972345(−1)	58
7.0	4.3871053502(−1)	20	1.6	7.7344800413(−1)	62
6.0	4.6869289171(−1)	24	1.4	8.0719042891(−1)	74
5.0	5.0593097082(−1)	24	1.2	8.4626097487(−1)	86
4.0	5.5399411680(−1)	30	1.1	8.6829966674(−1)	94
3.5	5.8397138419(−1)	32	1.0	8.9237516814(−1)	102

[a] Starting indices $n(x)$ for computation to 11 significant digits.

B7800, this index function yielded $e^x Ki_1(x)$ to eleven significant digits (machine precision) in single-precision arithmetic in the domain $x \geqslant 1$. Programs in ALGOL are available on request. Starting index functions for more or fewer significant digits are easily designed. In the region $0 < x < 1$ our algorithm is slow, but here the usual series expansion is accurate.

Iterated integrals. In order to generate higher-order integrals one can make use of the recursive formula

$$nKi_{n+1}(x) = x(Ki_{n-2}(x) - Ki_n(x)) + (n-1)\,Ki_{n-1}(x), \tag{10}$$

which is proved in Bickley and Nayler [3] and Blair *et al.* [4], with an application in [2]. It suffices to have available high-precision values $Ki_1(x)$, $Ki_0(x) = K_0(x)$, and $Ki_{-1}(x) = K_1(x)$ to generate higher integrals, but this recursion does become unstable for large x. Fortunately, our algorithm for $Ki_1(x)$ also contains sufficient data for constructing $K_1(x)$ and $K_0(x)$ with no additional effort, as may be seen from the formulas

$$\begin{aligned} e^x K_0(x) &= \pi^{1/2}(2x)^{-1}\,U(0)(\tfrac{1}{2} + 2x - \tfrac{3}{4}U(1)/U(0)), \\ e^x K_1(x) &= \pi^{1/2}(2x)^{-1}\,U(0)(\tfrac{3}{2} + 2x - \tfrac{3}{4}U(1)/U(0)), \end{aligned} \tag{11}$$

where $U(k) = U(k + \frac{1}{2}, 0, 2x)$. Other high-precision algorithms for $K_0(x)$ and $K_1(x)$ are discussed by Temme [13] and Terras [15]. Our suggested approach is much more accurate than the usual series method [1,3]. Moreover, our algorithm for $Ki_1(x)$ is reasonably rapid when $x \geqslant 1$, and our ALGOL code is very short. In the event that the repeated integrals of low order need to accessed frequently, we recommend use of the rational approximations in [4], which have the advantage of speed.

Additional formulas of interest are

$$e^x Ki_n(x) = \pi^{1/2}\, 2^{-n} \sum_{k=0}^{\infty} 2^{-k} \frac{(n)_k}{k!}\, U(\tfrac{1}{2}, 1-n-k, 2x), \tag{12}$$

$$e^x \int_x^{\infty} t^{-\nu} K_\nu(t)\, dt = \pi^{1/2}\, 2^{\nu-1} \sum_{k=0}^{\infty} 2^{-k} U(\nu + \tfrac{1}{2}, 2\nu - k, 2x), \tag{13}$$

which converge approximately as $\sum_{k\geqslant 0} 2^{-k}$. Because our most general Miller formula for $U(a, b, x)$ is always stable when $b \leqslant a + 1$ and $x \geqslant 1$, we were able to experiment with (12), in addition to our Miller formulas, in computing $Ki_n(x)$ for large parameters n.

In the evaluation we made use of the upward recursion

$$\begin{aligned}(n+1+a)\, U(a, -n-1, x) \\ = (n+1)\, U(a, -n, x) + x(U(a, 1 \llcorner n, x) - U(a, -n, x)),\end{aligned}$$

which is stable when x is not too much larger than n. In this manner we obtained satisfactory results for $Ki_n(x)$ $(1 \leqslant x \leqslant n)$ with n large.

3. Integrals of Incomplete Gamma Functions

For the functions $\alpha(s, y)$ and $\alpha(r, s \mid x, y)$ one has the recursive relations

$$\alpha(s, y) = (1 + y\alpha(s+1, y))/s, \tag{14}$$

$$\alpha(r, s \mid x, y) = (\alpha(s, y) + x\alpha(r+1, s+1 \mid x, y))/r. \tag{15}$$

These recursions generate the series

$$\alpha(s, y) = \frac{1}{s} + \frac{y}{s(s+1)} + \frac{y^2}{s(s+1)(s+2)} + \cdots, \tag{16}$$

$$\begin{aligned}\alpha(r, s \mid x, y) = \frac{1}{r}\alpha(s, y) + \frac{x}{r(r+1)}\alpha(s+1, y) \\ + \frac{x^2}{r(r+1)(r+2)}\alpha(s+2, y) + \cdots .\end{aligned} \tag{17}$$

One may also obtain (17) from (2) through substitution of the series for $\alpha(r, xu)$. Formula (17) yields the easily computed double series

$$\alpha(r, s \mid x, y) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{x^m y^n}{r(r+1)\cdots(r+m)(s+m)(s+m+1)\cdots(s+m+n)} \tag{18}$$

but there is a much more efficient way to sum (17). One uses nested operations to write

$$\begin{aligned}\frac{1}{r}\alpha(s,y)+\frac{x}{r(r+1)}\alpha(s+1,y)+\cdots+\frac{x^n}{r(r+1)\cdots(r+n)}\alpha(s+n,y)\\ =\frac{1}{r}\left(\alpha(s,y)+\frac{x}{r+1}\left(\alpha(s+1,y)\right.\right.\\ \left.\left.+\cdots+\frac{x}{r+n-1}\left(\alpha(s+n-1,y)+\frac{x}{r+n}\alpha(s+n,y)\right)\cdots\right)\right).\end{aligned}\tag{19}$$

In our preceding paper [14] we analyzed in detail the backward recursion (14). We discovered that the situation is quite analogous to the continued fraction recursion (9). If one starts out with the arbitrary assignement $\alpha(s+n+1,y)=0$, then the successive iterates $\alpha(s+n,y)$, $\alpha(s+n-1,y),\ldots,\alpha(s,y)$ are increasingly more accurate approximations to the correct values of the integrals. We gave a relative error estimate for the accuracy of the approximation and tabulated the necessary starting indices for some parameters. The algebra of the computation of the nesting yields

$$\alpha(s+m,y)=(1+y\alpha(s+m+1,y))/(s+m),\tag{20}$$

$$\alpha(r+m,s+m\mid x,y)=(\alpha(s+m,y)+x\alpha(r+m+1,s+m+1\mid x,y))/(r+m)\tag{21}$$

for $m=n,n-1,\ldots,1$. These equations are just versions of (14) and (15) and thus we have shown that simultaneous backwards recursion with (14) and (15) will compute $\alpha(r,s\mid x,y)$. The starting index is easily determined from

$$\sum_{m=0}^{n}\frac{x^m}{r(r+1)\cdots(r+m)}\alpha(s+m,y)=\alpha(r,s\mid x,y)(1-\theta_n(x,y)),\tag{22}$$

where

$$\theta_n(x,y)=\frac{x^{n+1}}{r(r+1)\cdots(r+n)}\frac{\alpha(r+n+1,s+n+1\mid x,y)}{\alpha(r,s\mid x,y)}.$$

It is useful to note that $\alpha(r,s\mid x,y)\leqslant\alpha(r,x)\,\alpha(s,y)$ is a close estimate when $r>x$ and $s>y$.

Applications. Our integrals have been analyzed in well-known special cases. One has the double integral of Rosser [11]

$$G(z,p)=\int_0^z e^{-p^2y^2}\,dy\int_0^y e^{-x^2}\,dx.\tag{23}$$

Reduction to our canonical form yields

$$G(z,p)=\frac{z^2}{4}\exp(-(p^2+1)\,z^2)\;\alpha\left(\frac{1}{2},1\,|\,z^2,(p^2+1)\,z^2\right). \tag{24}$$

Rosser develops a formula which is essentially equivalent to (17), but use of the backwards recursion is not considered. The formula also extends to complex p and z, but will suffer from cancellation error when z^2 or $(p^2+1)\,z^2$ is large in magnitude and does not lie close to the real positive axis.

In addition to the above, Zelen and Severo reporting in [1] consider the closely related probabilistic integral of a Gaussian density in the plane over the triangle $\{(x,y)\,|\,0\leqslant y\leqslant ax,\,0\leqslant x\leqslant h\}$ given by

$$V(h,ah)=(2\pi)^{-1}\int_0^h dx\int_0^{ax} dy\exp\left(-\left(\frac{x^2+y^2}{2}\right)\right). \tag{25}$$

After reduction to our canonical form one has

$$V(h,ah)=\frac{ah^2}{8\pi}\exp\left(-\left(\frac{h^2(1+a^2)}{2}\right)\right)\alpha\left(\frac{1}{2},1\,\middle|\,\frac{1}{2}a^2h^2,\frac{1}{2}h^2(1+a^2)\right). \tag{26}$$

In [1] the formulas for computing $V(h,ah)$ are quite different from our own and depend on another integral which is evaluated in terms of repeated derivatives of the one-dimensional Gaussian density. One has the relation $V(\sqrt{2zp},\sqrt{2z})=(p/\pi)\,G(z,p)$ when $p>0$ and $z>0$. Yet another quite efficient way to evaluate $V(h,ah)$ is developed in Nicholson [9] and Owen [10].

For repeated evaluation we note the Taylor expansions

$$\begin{aligned}\alpha(r,s\,|\,x+h,y+h)&=e^h\sum_{n=0}^{\infty}\alpha(r+n,s+n\,|\,x,y)\,h^n/n!,\\ \alpha(r,s\,|\,x,y+h)&=e^h\sum_{n=0}^{\infty}\alpha(r,s+n\,|\,x,y)\,h^n/n!\end{aligned} \tag{27}$$

and note the recursion $(s-r)\,\alpha(r,s\,|\,x,y)=(y-x)\,\alpha(r,s+1\,|\,x,y)+\alpha(r,x)-\alpha(s,y)$, which is downward stable when $s>r$ and $y>x$.

A multidimensional integral. The two-dimensional integral (2) has several possible generalizations. We shall mention one. If one defines

$$\begin{aligned}&\alpha(s_1,s_2,\ldots,s_n\,|\,x_1,x_2,\ldots,x_n)\\ &\quad=e^{x_n}\int_0^1 e^{-x_nt}t^{s_n-1}\alpha(s_1,s_2,\ldots,s_{n-1}\,|\,x_1t,x_2t,\ldots,x_{n-1}t)\,dt\end{aligned} \tag{28}$$

inductively for $n \geqslant 2$ and for positive arguments and parameters, then one can obtain the recursive relation

$$s_1 \alpha(s_1, s_2, \ldots, s_n \mid x_1, x_2, \ldots, x_n)$$
$$= \alpha(s_2, s_3, \ldots, s_n \mid x_2, \ldots, x_n) + x_1 \alpha(s_1 + 1, s_2 + 1, \ldots, s_n + 1 \mid x_1, \ldots, x_n). \tag{29}$$

It is easy to see that the function $\alpha(s_1, s_2, \ldots, s_n \mid x_1, x_2, \ldots, x_n)$ can be computed through simultaneous backwards recursion in a manner which generalizes (20) and (21). This function also has a multidimensional series analogous to (18). Brute force summation of this series to a given accuracy requires on the order of $O(N^n)$ operations, whereas the backwards recursion method requires $O(Nn)$ operations, which grows only linearly with dimension. We note that in Schavitt [12] use of the series for $\alpha(s, x)$ led to the solution of other multidimensional integral problems.

We can relate some iterated integrals of the one-dimensional Gaussian density to our integrals (28). Let $Z(t) = (2\pi)^{-1/2} \exp(-t^2/2)$. Define $L_0(x) = Z(x)$ and define

$$L_n(x) = \int_0^x L_{n-1}(t)\, dt \qquad (n \geqslant 1). \tag{30}$$

One has

$$L_n(x) = (2/n)^{-n} Z(x)\, \alpha\left(\frac{1}{2}, 1, \ldots, \frac{n}{2} \,\middle|\, \frac{1}{2}x^2, \frac{1}{2}x^2, \ldots, \frac{1}{2}x^2\right), \tag{31}$$

when $n \geqslant 1$. If $n \geqslant 0$ then one has the recursive relation

$$(n+1) L_{n+2}(x) = L_n(x) + x L_{n+1}(x) - (2\pi)^{-1/2} x^n / n!. \tag{32}$$

We checked our formula for $V(h, ah)$ by using simultaneous backwards recursion with $\alpha(r, s \mid x, y)$ on a programmable calculator and found agreement with the tabulations of Nicholson [9].

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