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Note

A Miller Algorithm for an Incomplete Bessel Function

1. Introduction

A canonical form of an incomplete Bessel function with various applications in physics is defined by the formula

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

with $x > 0$ and $y > 0$ and ν arbitrary. In this note we shall introduce a Miller algorithm for evaluating this function. A continued fraction for a quotient of confluent hypergeometric functions $U(a+1, b, x)/U(a, b, x)$ enters into our algorithm. We derive some mathematical estimates for the stability of this continued fraction. In the last section we shall demonstrate an occurrence of this function in the summation of potential lattice sums via the "method of theta functions."

2. Fundamental Formulas

It is easy to derive the expansion

$$K_\nu(x, y) = e^{-(x+y)}\,[U(1, \nu+1, x) + U(2, \nu+1, x)\, y + U(3, \nu+1, x)\, y^2 + \cdots], \tag{2}$$

where $U(a, b, x)$ is the confluent hypergeometric function in [1]. When $a > 0$ and $x > 0$ then one has the integral representation

$$\Gamma(a)\, U(a, b, x) = e^x \int_1^\infty e^{-xt}(t-1)^{a-1} t^{b-a-1}\, dt. \tag{3}$$

Formula (2) is the analytic continuation of $K_\nu(x, y)$ to the complex plane.

The function $K_\nu(x, y)$ can be related to the modified Bessel function $K_\nu(x)$ in two ways. We first recall the integral formula

$$K_\nu(x) = \frac{1}{2}\int_0^\infty e^{-(x/2)(t+1/t)}\, t^{\nu-1}\, dt \tag{4}$$

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from Lebedev [9]. Decomposition of the interval of integration then leads to the formula

$$K_\nu(x) = \tfrac{1}{2}[K_\nu(x/2, x/2) + K_{-\nu}(x/2, x/2)]. \tag{5}$$

We next demonstrate that $K_\nu(x, y)$ is an incomplete Bessel function in Agrest and Maximov [2]. If we denote (our notation)

$$L_\nu(x, z) = \frac{1}{2}\int_z^\infty e^{-(x/2)(t+1/t)}\, t^{\nu-1}\, dt, \tag{6}$$

then one has the relation

$$L_\nu(x, z) = \frac{1}{2} z^\nu K_\nu\left(\frac{xz}{2}, \frac{x}{2z}\right). \tag{7}$$

We next obtain an estimate of the rate of convergence of the series expansion (2). When ν is real and x, y are positive then one has

$$\sum_{k=n}^{\infty} U(k+1, \nu+1, x) y^k \leqslant U(1, \nu+1, x) \sum_{k=n}^{\infty} y^k/k!. \tag{8}$$

It follows that (2) converges at least as well as the exponential series $e^y = 1 + y + y^2/2! + \cdots$.

The basic formula of Agrest and Maximov [2] (a formula which is also mentioned in Faxen [6]) becomes, in our notation,

$$K_\nu(x, y) = e^{-x}[\varphi(\nu, x) - y\varphi(\nu-1, x) + y^2\varphi(\nu-2, x)/2! \mp \ldots], \tag{9}$$

where in our notation [12]

$$\varphi(\nu, x) = e^x \int_1^\infty e^{-xt} t^{\nu-1}\, dt. \tag{10}$$

The principal reason for deriving an alternative computational procedure for $K_\nu(x, y)$ comes from the severe cancellation instability of (9) when $y > 0$ gets large.

3. Derivation of a Miller Formula

A Miller algorithm is directly derivable from (3), but we shall introduce the notion of a *Miller formula*, which we define to be a series whose terms can be generated from the successive iterates of a continued fraction generated by backwards recursion. Gautschi [8] discusses Miller algorithms in the usual sense.

The Miller formula for our function is given by

$$K_\nu(x, y) = e^{-(x+y)} U(1, \nu+1, x) \times \left[1 + y \frac{U(2, \nu+1, x)}{U(1, \nu+1, x)} + y^2 \frac{U(2, \nu+1, x)\, U(3, \nu+1, x)}{U(1, \nu+1, x)\, U(2, \nu+1, x)} + \cdots \right]. \tag{11}$$

The quotients that appear in this series are related by the fractional linear transformation

$$\frac{U(a, b, x)}{U(a-1, b, x)} = \frac{1}{(2a + x - b) - a(1 + a - b)\, U(a+1, b, x)/U(a, b, x)} \tag{12}$$

which gives rise to the continued fraction

$$\frac{U(a, b, x)}{U(a-1, b, x)} = \frac{1|}{|(2a + x - b)} - \frac{a(1 + a - b)|}{|(2a + 2 + x - b)} - \frac{(a+1)(2 + a - b)|}{|(2a + 4 + x - b)} - \cdots - \frac{(a+n)(2 + a + n - b)|}{|(2a + 2n + x - b)\omega}, \tag{13}$$

where $\omega = U(a+n+1, b, x)/U(a+n, b, x)$. With the initialization $\omega = 0$ one obtains a *convergent* of the infinite continued fraction, and n is called a *starting index*. Convergence of such continued fractions is demonstrated in Perron [10] for $x > 0$. Save for stability problems, a choice of sufficiently large starting index n will yield quantities which approximate $U(a, b, x)/U(a-1, b, x)$ to any desired degree of accuracy.

In the next section we derive the simple estimate $U(a+1, b, x)/U(a, b, x) < 1/(a + x)$, which is valid whenever $a > 0$ and $x > 0$. Term-by-term comparison then yields

$$1 + y \frac{U(2)}{U(1)} + y^2 \frac{U(2)}{U(1)} \frac{U(3)}{U(2)} + \cdots \leqslant 1 + y \frac{1}{(1+x)} + y^2 \frac{1}{(1+x)(2+x)} + \cdots, \tag{14}$$

where $U(n) = U(n, \nu+1, x)$. This estimate shows that the rate of convergence of (11) is frequently better than that of the exponential series. Moreover, it is relatively easy to determine a truncation index for (11) by using (14).

The leading factor $U(1, \nu+1, x)$ in (11) may be evaluated in various ways. For one thing the function $U(a, b, x)$ itself has a Miller formula. One has

$$U(a, b, x) = x^{-a} \left[1 + \frac{ac}{1} \frac{U(a+1, b, x)}{U(a, b, x)} + \frac{a(a+1)\, c(c+1)}{1 \cdot 2} \frac{U(a+1, b, x)}{U(a, b, x)} \frac{U(a+2, b, x)}{U(a+1, b, x)} + \cdots \right]^{-1}, \tag{15}$$

where $c = 1 + a - b$. In thin disguise this Miller formula is precisely the one devised by Temme [11] for evaluating $K_\nu(x)$.

Another method for evaluating the leading factor comes about by noting that $U(1, \nu + 1, x) = \varphi(\nu, x)$ in terms of our notation (10).

This function has the well-known Legendre continued fraction

$$\varphi(\nu, x) = \frac{1|}{|x} + \frac{(1-\nu)|}{|1} + \frac{1|}{|x} + \frac{(2-\nu)|}{|1} + \frac{2|}{|x} + \frac{(3-\nu)|}{|1} + \frac{3|}{|x} + \cdots. \tag{16}$$

A manuscript which details a careful stability analysis of this continued fraction may be obtained from the author on request. The Legendre continued fraction converges rapidly when $x > 0$ is not small and is stable if $\nu < 1$. In computer evaluation, both Miller formulas are amenable to the method of nested operations for evaluating truncated series. We abbreviate $U(n) = U(n, \nu + 1, x)$ to obtain

$$\begin{aligned} &1 + y\frac{U(2)}{U(1)} + \cdots + y^n \frac{U(2)}{U(1)}\frac{U(3)}{U(2)} \cdots \frac{U(n+1)}{U(n)} \\ &\quad = 1 + y\frac{U(2)}{U(1)}\left(\cdots\left(1 + y\frac{U(n)}{U(n-1)}\left(1 + y\frac{U(n+1)}{U(n)}\right)\right)\cdots\right). \end{aligned} \tag{17}$$

Next we abbreviate $U(n) = U(n + a, b, x)$ to obtain

$$\begin{aligned} &1 + \frac{ac}{1!}\frac{U(1)}{U(0)} + \cdots + \frac{(a)_n(c)_n}{n!}\frac{U(1)}{U(0)}\frac{U(2)}{U(1)} \cdots \frac{U(n)}{U(n-1)} \\ &\quad = 1 + \frac{ac}{1}\frac{U(1)}{U(0)}\left(1 + \frac{(a+1)(c+1)}{2}\frac{U(2)}{U(1)}\right. \\ &\quad \left.\times\left(\cdots\left(1 + \frac{(a+n-1)(c+n-1)}{n}\frac{U(n)}{U(n-1)}\right)\right)\cdots\right), \end{aligned} \tag{18}$$

where $(a)_n = a(a+1)\cdots(a+n-1)$. These two formulas together with (12) allow one to make an extremely rapid evaluation of the Miller formulas (11) and (15) after one has devised a suitable approximation for the starting index n, which takes into account the continued fraction approximation as well as the series truncation.

To give an idea of the running time of the algorithm we tabulate in Table I the empirically determined starting index $n(x)$ for evaluating $K_0(x, x) = K_0(2x)$. Computation was carried out in floating point arithmetic accurate to 11 decimal digits on a Burroughs B7800 computer. Except for rounding errors in the last digit, the results agreed with tabulated values for $K_0(2x)$ in [1].

In the next section we shall explain why our algorithm for $K_\nu(x, y)$ will be reliable when $\nu \leqslant 2$ and $x > 0$ and $y > 0$. However, upward recursion is stable when $\nu > 0$.

$$K_{\nu+1}(x, y) = \frac{1}{x}e^{-(x+y)} + \frac{\nu}{x}K_\nu(x, y) + \frac{y}{x}K_{\nu-1}(x, y). \tag{19}$$

TABLE I[a]

x	$n(x)$	x	$n(x)$	x	$n(x)$
0.2	170	2.0	38	12.0	26
0.3	130	3.0	30	14.0	26
0.4	108	4.0	26	16.0	28
0.5	80	5.0	26	18.0	30
0.6	74	6.0	24	20.0	30
0.7	74	7.0	24	22.0	32
0.8	68	8.0	26	24.0	34
0.9	62	9.0	26	26.0	34
1.0	56	10.0	26	28.0	34

[a] Starting index function $n(x)$ for computing $K_0(x,x)$ to 11 decimal digits.

The Bessel function $K_{i\nu}(x)$. It is worthwhile noting that these Bessel functions of pure imaginary parameter, which occur in Lebedev [9] and elsewhere in mathematical physics, have few effective expansions. Our method with $K_{i\nu}(x)=[K_{i\nu}(x/2,x/2)+K_{-i\nu}(x/2,x/2)]/2$ is no exception. However, one has $K_{i\nu}(x)=\pi^{1/2}\,e^{-x}(2x)^{i\nu}U(i\nu+\frac{1}{2},2i\nu+1,2x)$. A while ago the author communicated to Cartier [4] that the Miller formula (15) is effective in this case. This colleague has continued to collect a lot of information on effective algorithms for this Bessel function.

4. STABILITY ANALYSIS

If correctly computed iterates $U(n+1,\ \nu+1,x)/U(n,\nu+1,x)$ are entered in our formula (11) with $y>0$ then one is summing only positive terms and one has to contend only with the accumulation of rounding error, which is quite innocuous.

On the other hand, it is well known that continued fractions can be quite treacherous and sporadic in their behavior. Thus in order to guarantee the numerical effectiveness of our Miller formula (11) we shall make some mathematical assertions regarding the stability of the continued fraction that enters into our algorithm. One is able to assert stability by making some restrictive assumptions regarding parameters. This result will demonstrate that our algorithm for $K_\nu(x,\ y)$ is numerically stable when $\nu<2$, $x>0$, and $y>0$.

Let T be a differentiable function of a single variable. One defines $\theta_T(\omega)=\omega T'(\omega)/T(\omega)$. The function T is *stable* at ω if $|\theta_T(\omega)|\leqslant 1$.

We wil now consider the stability of the fractional linear transformation

$$T(\omega)=\frac{1}{(2a+x-b)-a(1+a-b)\omega}, \tag{20}$$

which is relevant to the discussion because $T(U(a+1,b,x)/U(a,b,x)) = U(a,b,x)/U(a-1,b,x)$. We have the stability factor relation

$$\theta_T(U(a+1,b,x)/U(a,b,x)) = \frac{U(a+1,b,x)}{U(a,b,x)} \frac{U(a,b,x)}{U(a-1,b,x)} a(1+a-b). \quad (21)$$

LEMMA. *If $a > 0$ and $b < a+1$ then*

$$\frac{U(a+1,b,x)}{U(a,b,x)} \leqslant \min\left\{\frac{1}{(a+1-b+x)}, \frac{1}{(a+x)}\right\}. \quad (22)$$

Proof. One is able to deduce these estimates from $U(a+1,b,x)/U(a,b,x) = [(a+1-b+xU(a+1,b+1,x)/U(a+1,b,x)]^{-1}$ and $U(a+1,b,x)/U(a,b,x) = 1/a - U(a,b-1,x)/aU(a,b,x)$ along with (12).

PROPOSITION. *If $a > 0, b < a+1$, and $x \geqslant 1$ then one has*

$$0 \leqslant \theta_T(U(a+1,b,x)/U(a,b,x)) < 1. \quad (23)$$

A continued fraction is *stable* if each individual fractional linear transformation in backwards recursion is stable at its corresponding argument. One is able to check on a computer that a continued fraction which meets our stability test will execute accurately.

COROLLARY. *If $v < 2$ and $x \geqslant 1$ or if $x > 1+v$ then*

$$\frac{U(2,v+1,x)}{U(1,v+1,x)} = \frac{1|}{|(3+x-v)} - \frac{2(2-v)|}{|(5+x-v)} - \frac{3(3-v)|}{|(7+x-v)} - \cdots \quad (24)$$

is stable.

A computer check turned up some significant instability only in the case when $v > 0$ was very large and $x > 0$ was very small.

5. THE PARALLEL PLATE POTENTIAL

The potential generated by a charge q at (x, y, z) between conducting plates perpendicular to the x-axis at $x = 0$ and $x = a$, as measured at (u, v, w) between the plates, is represented by the absolutely convergent series

$$\begin{aligned} &\Phi(x, y, z \mid u, v, w) \\ &= q \sum_{n=-\infty}^{\infty} (\|(x-u+2an, y-v, z-w)\|^{-1} - \|(-x-u+2an, y-v, z-w)\|^{-1}), \end{aligned} \quad (25)$$

where $\|(u, v, w)\| = (u^2+v^2+w^2)^{1/2}$. Matters are so delicate that one cannot even distribute summation over the subtraction. The convergence is slow. We note that this formula is a special case of an exhaustive study of such lattice sums appearing in Terras and Swanson [13, 14]. The method of theta functions is further developed in [1].

In a recent paper Fong and Kittel [7] derived a rapidly convergent series for this potential. One has

$$\Phi(x, y, z \mid u, v, w) = \frac{4q}{a} \sum_{n=1}^{\infty} \sin(\pi n x/a) \sin(\pi n u/a)\, K_0(\pi n \rho/a), \tag{26}$$

where $\rho^2 = (y-v)^2 + (z-w)^2$. This formula converges slowly when ρ is small and is singular at $\rho = 0$. For this reason one seeks additional rapidly convergent expansions. When one imitates Ewald's "method of theta functions" [3, 5] one obtains a formula which is not singular for $\rho = 0$. One has

$$\begin{aligned}\Phi(x, &y, z \mid u, v, w) \\ &= 2q\sqrt{R} \sum_{n=-\infty}^{\infty} \sum_{\lambda=1,-1} \lambda F(\pi \|(2na + \lambda x - u,\ y - v,\ z - w)\|^2 R) \\ &\quad + 2qa^{-1} \sum_{n=1}^{\infty} \sin(\pi n x/a) \sin(\pi n u/a)\, K_0(\pi (n/2a)^2 R^{-1}, \pi \rho^2 R),\end{aligned} \tag{27}$$

where $R > 0$ is an arbitrary parameter and where

$$F(x) = \int_1^{\infty} e^{-xt^2}\, dt = \frac{1}{2}\int_1^{\infty} e^{-xt} t^{-1/2}\, dt = \frac{1}{2} e^{-x} \varphi(1/2, x). \tag{28}$$

In writing a computer code we took $R = a^{-2}$. The truncations $\sum_{n=-4}^{4} \sum_{\lambda=1,-1}$ and $\sum_{n=1}^{4}$ yielded data to 11 decimal digits.

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