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ON THE NUMERICAL EVALUATION OF THE MODIFIED  
BESSEL FUNCTION OF THE THIRD KIND

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ON THE NUMERICAL EVALUATION OF THE MODIFIED BESSEL FUNCTION  
OF THE THIRD KIND

by

N.M. Temme

ABSTRACT

An algorithm is given for the numerical computation of the Bessel function  $K_\nu(z)$  for general  $\nu$  and  $z$ . For small  $|z|$  the Taylor expansion of the Bessel function  $I_\nu(z)$  is used, whereas for the remaining values the computation is based upon a combination of algorithms due to J.C.P. Miller and F.W.J. Olver. In both cases the function  $K_{\nu+1}(z)$  is obtained as well. ALGOL 60 procedures are given for the case of real  $\nu$  and  $z$ .

KEY WORDS & PHRASES: *modified Bessel function, gamma function, difference equations, Miller algorithm, ALGOL 60.*



## I. INTRODUCTION

I.1. *Definitions and relevant properties.* The modified Bessel function of the third kind can be defined by the integral

$$(1.1) \quad K_{\nu}(z) = \int_0^{\infty} e^{-z \cosh t} \cosh \nu t \, dt, \quad \operatorname{Re} z > 0.$$

Its definition can also be given by using the modified Bessel function of the first kind

$$(1.2) \quad I_{\nu}(z) = \left(\frac{1}{2}z\right)^{\nu} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}z\right)^{2k}}{\Gamma(\nu+k+1)k!}.$$

In terms of this function we have

$$(1.3) \quad K_{\nu}(z) = \frac{1}{2}\pi \frac{I_{-\nu}(z) - I_{\nu}(z)}{\sin \nu\pi}.$$

Since  $I_{-n}(z) = I_n(z)$ ,  $n = 0, 1, 2, \dots$ , the right-hand side of (1.3) appears in indeterminate form if  $\nu = n$ . However, the limit of this form as  $\nu \rightarrow n$  exists and agrees with  $K_n(z)$  given in (1.1). Clearly we have

$$(1.4) \quad K_{\nu}(z) = K_{-\nu}(z).$$

Furthermore, if  $z$  and  $\nu$  are real,  $z > 0$ ,

$$(1.5) \quad K_{\nu}(z) > 0, \quad K'_{\nu}(z) < 0.$$

The Bessel functions of half integral order can be expressed in terms of elementary functions. For  $\nu = \frac{1}{2}, 3/2$  we have

$$(1.6) \quad K_{\frac{1}{2}}(z) = (\pi/2z)^{\frac{1}{2}} e^{-z}, \quad K_{3/2}(z) = (\pi/2z)^{\frac{1}{2}} e^{-z} (1+1/z).$$

The functions  $I_{\nu}(z)$  and  $e^{i\nu\pi} K_{\nu}(z)$  are two solutions of the difference equation

$$(1.7) \quad y_{\nu+1} + (2\nu)/z y_{\nu} - y_{\nu-1} = 0.$$

Explicitly we have

$$(1.8) \quad I_{\nu+1}(z) + (2\nu/z) I_{\nu}(z) - I_{\nu-1}(z) = 0,$$

$$(1.9) \quad K_{\nu+1}(z) - (2\nu/z) K_{\nu}(z) - K_{\nu-1}(z) = 0.$$

Formula (1.9) can be used to compute  $K_{\nu+n}$  for  $n = 2, 3, \dots$  when  $K_{\nu}$  and  $K_{\nu+1}$  are given. In the forward direction the recurrence formula for  $K_{\nu}$  is numerically stable (see GAUTSCHI [5]).

From (1.2) and (1.3) the following asymptotic formulas are obtained. For small  $|z|$  we have

$$(1.10) \quad I_{\nu}(z) \sim (z/2)^{\nu}/\Gamma(\nu+1), \quad K_{\nu}(z) \sim \frac{1}{2}(z/2)^{-\nu}\Gamma(\nu), \quad \text{Re } \nu > 0.$$

These formulas also hold for the case that  $z$  is fixed and  $\nu \rightarrow \infty$ . Hence,  $I_{\nu}$  and  $e^{i\nu\pi}K_{\nu}$  are two linearly independent solutions of the difference equation (1.7).

When  $\nu$  is fixed and  $z \rightarrow \infty$  we have the well-known expansions

$$(1.11) \quad I_{\nu}(z) = (2\pi z)^{-\frac{1}{2}} e^z [1 + O(z^{-1})], \quad K_{\nu}(z) = (\pi/2z)^{\frac{1}{2}} e^{-z} [1 + O(z^{-1})],$$

the first relation holding for  $|\arg z| < \frac{1}{2}\pi$ , and the second one for  $|\arg z| < 3\pi/2$ .

*I.2. Contents of the paper.* We give algorithms for the computation of  $K_{\nu}(z)$  and  $K_{\nu+1}(z)$ . On account of (1.4) and (1.9) and the stability of (1.9) it suffices to consider values of  $\nu$  with  $-\frac{1}{2} \leq \text{Re } \nu \leq \frac{1}{2}$ . In section II we describe an algorithm for the computation of  $K_{\nu}(z)$  for small values of  $|z|$ . This algorithm is based on representations (1.3) and (1.2). Also the evaluation of the gamma function is discussed; some special approximations of this function are needed in the algorithm for small  $|z|$ .

Section III is devoted to the computation of  $K_{\nu}(z)$  for moderate or large values of  $|z|$ . In this case the algorithm is based on a combination of algorithms due to J.C.P. Miller and F.W.J. Olver.

In section IV the algorithms are described in terms of ALGOL 60 procedures.

There is a vast literature concerning the computation of this Bessel function (see for example LUKE [8] and [9]), especially for large values of  $|z|$ , whereas the computation for small values is rather neglected. Moreover, the methods are usually restricted to  $K_\nu(z)$  for integer values of  $\nu$ . The algorithms described in this paper may also be used for the class of confluent hypergeometric functions denoted by  $U(a,b,z)$ .

For the computation of the Bessel function  $I_\nu(z)$  the reader is referred to AMOS [2] and GAUTSCHI [5] and [6].

Thanks is due to Gert Jan Laan who tested the ALGOL 60 procedures.

## II. THE COMPUTATION FOR SMALL VALUES OF $|z|$

II.1. *Series representations.* Substitution of (1.2) into (1.3) leads to

$$(2.1) \quad K_\nu(z) = \sum_{k=0}^{\infty} c_k f_k,$$

$$(2.2) \quad f_0 = \frac{\pi}{2 \sin \nu\pi} \left\{ (z/2)^{-\nu} / \Gamma(1-\nu) - (z/2)^\nu / \Gamma(1+\nu) \right\}$$

and for general  $k$

$$(2.3) \quad f_k = \frac{\pi}{2 \sin \nu\pi} \left\{ (z/2)^{-\nu} / \Gamma(k+1-\nu) - (z/2)^\nu / \Gamma(k+1+\nu) \right\},$$

$$(2.4) \quad c_k = (z^2/4)^k / k!.$$

By using the well-known property of the gamma function  $\Gamma(z+1) = z\Gamma(z)$  we have for  $k = 1, 2, 3, \dots$  the recurrence relations

$$(2.5) \quad f_k = (k f_{k-1} + p_{k-1} + q_{k-1}) / (k^2 - \nu^2),$$

$$(2.6) \quad p_0 = \frac{1}{2} (z/2)^{-\nu} \Gamma(1+\nu), \quad p_k = p_{k-1} / (k-\nu),$$

$$(2.7) \quad q_0 = \frac{1}{2} (z/2)^\nu \Gamma(1-\nu), \quad q_k = q_{k-1} / (k+\nu).$$

In order to compute  $K_{\nu+1}(z)$  we write (using (1.3) and (1.8))

$$(2.8) \quad K_{\nu+1}(z) = \frac{2}{z} \frac{\nu\pi}{2 \sin \nu\pi} I_{-\nu}(z) + \frac{\pi}{2 \sin \nu\pi} (I_{\nu+1}(z) - I_{-\nu+1}(z)).$$

By substitution of (1.2) we obtain

$$(2.9) \quad K_{\nu+1}(z) = \frac{2}{z} \sum_{k=0}^{\infty} c_k (p_k - k f_k).$$

If an algorithm for the gamma function is available  $f_0$ ,  $p_0$  and  $q_0$  can be computed, and the remaining values  $f_k$ ,  $p_k$  and  $q_k$  can be obtained by recursion.

It should be pointed out that we wish to compute  $K_\nu$ ,  $K_{\nu+1}$  for  $-\frac{1}{2} \leq \text{Re } \nu \leq \frac{1}{2}$ , and inspection of (2.2) shows that, if  $\nu \rightarrow 0$ , an indeterminate form appears in  $f_0$  (and in all  $f_k$  but by using (2.5) only  $f_0$  has to be considered). Analytically,  $f_0$  can be defined in the limit  $\nu = 0$ . However, for small  $|\nu|$  numerical evaluation of  $f_0$  from representation (2.2) will cause a loss of correct significant digits. If  $|\nu|$  is small,  $f_0$  might be expanded in a series  $\sum a_k(z) \nu^k$ ; in fact this method is suggested by GOLDSTEIN & THALER [7]). This series converges for  $|\nu| < 1$  (because of the singularity at  $\nu = 1$ ), but the coefficients  $a_k(z)$  are not easily obtained. Moreover, for small  $|z|$  convergence of the series is rather poor.

In order to avoid these troubles we propose the following representation of  $f_0$

$$(2.10) \quad f_0 = \frac{\nu\pi}{\sin \nu\pi} [\Gamma_1(\nu) \cosh \mu + \Gamma_2(\nu) \ln(2/z) \sinh(\mu)/\mu],$$

where

$$(2.11) \quad \begin{cases} \Gamma_1(\nu) = [1/\Gamma(1-\nu) - 1/\Gamma(1+\nu)]/(2\nu) \\ \Gamma_2(\nu) = [1/\Gamma(1-\nu) + 1/\Gamma(1+\nu)]/2, \end{cases}$$

and  $\mu = \nu \ln(2/z)$ . The cancellation for small  $\nu$  may now occur in  $\Gamma_1$  and  $\sinh$  but for these functions the cancellation is better controlled than in  $f_0$ .

For the computation of  $\Gamma_1$  and  $\Gamma_2$  the reader is referred to subsection II.3.

II.2. *Stability of computation.* If  $|z|$  is not too large the series in (2.1) and (2.9) converge rapidly. The convergence is of the same rate as that of



(1.2). For large values of  $|z|$  the method described above is not attractive. Many terms in the series are needed. But there is another important reason. For large values of  $|z|$ , the Bessel functions behave as indicated in (1.11). Hence, if  $|z|$  is not small the subtraction in (1.3) will again cause a large relative error. This time the loss of significant digits cannot easily be avoided. A rough indication of the loss of digits, say  $q$ , can be obtained from

$$10^q \sim \frac{1}{2} e^{2 \operatorname{Re} z}.$$

Hence, for  $\operatorname{Re} z > 5$  at least 4 digits are lost.

For the case of real  $z$  and  $\nu$ ,  $z > 0$ ,  $|\nu| \leq \frac{1}{2}$ , the loss of relative accuracy can be elaborated somewhat further. In this case  $K_\nu(z)$  is positive, see (1.5). If  $f_0 > 0$ , then, as follows from (2.5), (2.6) and (2.7), all terms in (2.1) are positive, and the summation in (2.1) is stable.

But  $f_0$  is negative if  $z$  is large. The equation  $f_0 = 0$  defines a curve in the  $(z, \nu)$ -plane given by

$$z(\nu) = 2[\Gamma(1+\nu)/\Gamma(1-\nu)]^{1/(2\nu)},$$

with  $z(0) = 1.1229\dots$  and  $z(\frac{1}{2}) = 1$ . Some computations show  $z(\frac{1}{2}) \leq z(\nu) \leq z(0)$  for  $-\frac{1}{2} \leq \nu \leq \frac{1}{2}$ . It follows that if  $0 < z \leq 1$ ,  $-\frac{1}{2} \leq \nu \leq \frac{1}{2}$ ,  $K_\nu(z)$  can be safely computed by using (2.1).

As for  $K_{\nu+1}(z)$ , the situation is more complicated. If  $f_0 \geq 0$ , then all  $p_k$  and  $f_k$  in (2.9) are non-negative. By using (2.5), (2.6) and (2.7), it follows that for  $k \geq 1$

$$p_k - kf_k = (\nu p_{k-1}^{-k} f_{k-1}^{-k} q_{k-1}) / (k^2 - \nu^2).$$

If  $-\frac{1}{2} \leq \nu < 0$ , then the right-hand side is negative and so all terms in (2.9) except  $p_0$  are negative. But  $K_{\nu+1}(z) > 0$  and, in summing the series, cancellation may occur.

However, for small values of  $z$  we have from (1.2), (1.10) and (2.6)

$$K_{\nu+1}(z) \sim p_0 \sim z^{-1} \frac{\nu\pi}{\sin \nu\pi} I_{-\nu}(z).$$

So, for small  $z$ ,  $p_0$  dominates the remaining terms in (2.9), which are  $o(1)$

for  $z \rightarrow 0$ . Hence it may be expected that for  $z$  sufficiently small, no cancellation in (2.9) will occur.

From numerical experiments it follows that

$$p_0 > 2 \left| \sum_{k=1}^{\infty} c_k (p_k^{-k} f_k) \right|$$

for  $0 < z \leq 1$  and  $-\frac{1}{2} \leq \nu \leq \frac{1}{2}$ . As a consequence, for these values of  $z$  and  $\nu$ ,  $K_{\nu+1}(z)$  can be safely computed by using (2.9).

As indicated in subsection II.1, if  $\frac{1}{2} < \nu \leq 1$ , then the functions  $K_{\nu-1}(z)$  and  $K_{\nu}(z)$  are computed.  $K_{\nu+1}(z)$  follows then from (see (1.9))

$$K_{\nu+1}(z) = (2\nu)/z K_{\nu}(z) + K_{\nu-1}(z)$$

in which both terms on the right are positive.

II.3. *The computation of the gamma function.* Since in the literature no approximations for the odd and even parts (with respect to  $\nu$ ) of the function  $1/\Gamma(1-\nu)$  are available, a description of our method is given here for the case of real  $\nu$ .

The starting point is the expansion

$$(2.12) \quad 1/\Gamma(\nu) = \sum_{k=1}^{\infty} c_k \nu^k, \quad |\nu| < \infty.$$

The first 26 coefficients  $c_k$  are tabulated in ABRAMOWITZ & STEGUN [1] (16 digits), and the first 41 in WRENCH [15] (31 digits). From (2.12) and  $\Gamma(\nu+1) = \nu\Gamma(\nu)$  we easily obtain

$$(2.13) \quad 1/\Gamma(1-\nu) = \sum_{n=0}^{\infty} (-1)^n c_{n+1} \nu^n.$$

From this representation the odd and even parts may be obtained and so the values of  $\Gamma_1(\nu)$  and  $\Gamma_2(\nu)$  defined in (2.11). In the Bessel function algorithm we need  $\Gamma_1$  and  $\Gamma_2$  for  $-\frac{1}{2} \leq \text{Re } \nu \leq \frac{1}{2}$ . To give a satisfactory numerical approximation on the real interval  $[-\frac{1}{2}, \frac{1}{2}]$ , we expand  $1/\Gamma(1-\nu)$  in the Chebyshev polynomials  $T_n(x) = \cos(n \arccos(x))$ ,

$$(2.14) \quad 1/\Gamma(1-\nu) = \sum_{n=0}^{\infty} (-1)^n c_{n+1} 2^{-n} (2\nu)^n = \sum_{n=0}^{\infty} a_n T_n(2\nu).$$

(The notation  $\Sigma'$  means that the first term in the series is to be halved).

The coefficients  $a_n$  in (2.14) can be computed by rearranging the Taylor series in (2.14). This method is described in CLENSHAW [4]. The powers of  $(2\nu)$  are replaced by their expansions in Chebyshev polynomials, and the series is rearranged in the form  $\Sigma' a_n T_n(2\nu)$ . The first few coefficients  $a_n$  are given in TABLE I. A check on these coefficients can be performed by evaluating (2.14) for  $\nu = 0, \frac{1}{2}, -\frac{1}{2}$ . We must have

$$\sum_{n=0}^{\infty} (-1)^n a_{2n} = 1, \quad \sum_{n=0}^{\infty} a_n = \pi^{-\frac{1}{2}}, \quad \sum_{n=0}^{\infty} (-1)^n a_n = 2\pi^{-\frac{1}{2}}.$$

The functions  $\Gamma_1$  and  $\Gamma_2$  defined in (2.11) may now be written as

$$\nu\Gamma_1(\nu) \simeq \sum_{n=0}^6 a_{2n+1} T_{2n+1}(2\nu), \quad \Gamma_2(\nu) \simeq \sum_{n=0}^7 a_{2n} T_{2n}(2\nu),$$

and an appropriate summation method (see CLENSHAW [4]) gives  $\Gamma_1$  and  $\Gamma_2$ .

TABLE I

n	$a_{2n}$			$a_{2n+1}$		
0	+ 1.84374	05873	00906	- 0.28387	65422	76024
1	- 0.07685	28408	44786	+ 0.00170	63050	71096
2	+ 0.00127	19271	36655	+ 0.00007	63095	97586
3	- 0.00000	49717	36704	- 0.00000	08659	20800
4	- 0.00000	00331	26120	+ 0.00000	00017	45136
5	+ 0.00000	00002	42310	+ 0.00000	00000	09161
6	- 0.00000	00000	00170	- 0.00000	00000	00034
7	- 0.00000	00000	00001			

### III. THE COMPUTATION FOR LARGE OR MODERATE VALUES OF $|z|$

For large  $|z|$  we have the well-known asymptotic expansion

$$K_\nu(z) \sim (\pi/2z)^{\frac{1}{2}} e^{-z} \sum_{m=0}^{\infty} (\nu, m) (-2z)^{-m},$$

where  $(\nu, m)$  is Hankel's symbol given by

$$(3.1) \quad (\nu, m) = (m!)^{-1} \Gamma(\frac{1}{2} + \nu + m) / \Gamma(\frac{1}{2} + \nu - m) \\ = (\pi m!)^{-1} (-1)^m \cos \nu \pi \Gamma(\frac{1}{2} + \nu + m) \Gamma(\frac{1}{2} - \nu + m).$$

The series diverges for all finite values of  $|z|$ , but it can be used very successfully if  $|z|$  is large. To give an indication, for real  $z$ ,  $z > 15$ , the asymptotic series can be used to give an approximation, which is correct up to 13 significant digits. For intermediate values of  $|z|$  we have to resort to other techniques. In this section we will discuss a method which enables computation of  $K_\nu(z)$  for  $|z| \geq 1$ .

III.1. *The Miller algorithm.* We need some properties of the confluent hypergeometric functions. We use the notation of ABRAMOWITZ & STEGUN [1].

The Bessel function  $K_\nu(z)$  can be written as

$$(3.2) \quad K_\nu(z) = \pi^{\frac{1}{2}} (2z)^\nu e^{-z} U(\nu + \frac{1}{2}, 2\nu + 1, 2z).$$

where  $U(a, b, z)$  is a confluent hypergeometric function, which for  $\text{Re } z > 0$  and  $\text{Re } a > 0$  may be defined by

$$(3.3) \quad \Gamma(a) U(a, b, z) = \int_0^{\infty} e^{-zt} t^{a-1} (1+t)^{b-a-1} dt.$$

The function

$$(3.4) \quad k_n(z) = (-1)^n (\nu, n) U(\nu + \frac{1}{2} + n, 2\nu + 1, 2z), \quad n = 0, 1, 2, \dots,$$

with  $(\nu, n)$  given in (3.1), satisfies the following recurrence relation

$$(3.5) \quad k_{n+1}(z) - b_n k_n(z) + a_n k_{n-1}(z) = 0$$

with

$$(3.6) \quad a_n = [(n-\frac{1}{2})^2 - \nu^2]/(n^2+n), \quad b_n = 2(n+z)/(n+1), \quad n = 1, 2, \dots$$

The function

$$(3.7) \quad y_n(z) = \Gamma(n+\nu+\frac{1}{2}) {}_1F_1(\nu+\frac{1}{2}+n; 2\nu+1, 2z)/n!$$

also satisfies (3.5).  ${}_1F_1(a; b; z)$  is the hypergeometric function defined by

$$(3.8) \quad {}_1F_1(a; b; z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)} \frac{\Gamma(b)}{\Gamma(b+n)} \frac{z^n}{n!}.$$

The functions  $k_n$  and  $y_n$  are two linearly independent solutions of the difference equation (3.5), as follows from the behaviour of these solutions for large values of  $n$ , viz.

$$(3.9) \quad k_n(z) \sim \pi^{-\frac{1}{2}} \cos \nu\pi \, 2^{\frac{1}{4}} n^{-\frac{1}{2}} z^{-\nu-\frac{1}{4}} \exp[z-2(2nz)^{\frac{1}{2}}],$$

$$(3.10) \quad y_n(z) \sim \pi^{-\frac{1}{2}} 2^{-\nu-\frac{3}{4}} n^{-\frac{1}{2}} z^{-\nu-\frac{1}{4}} \Gamma(2\nu+1) \exp[z+2(2nz)^{\frac{1}{2}}],$$

$$(3.11) \quad k_n(z)/y_n(z) \sim 2^{\nu+1} \cos \nu\pi \exp[-4(2nz)^{\frac{1}{2}}]/\Gamma(2\nu+1).$$

Formulas (3.9) and (3.10) may be derived from results in BUCHHOLTZ [3].

Buchholtz derived his results for real  $z/n$  by using saddle point techniques. We can show, however, by using other methods (see SLATER [13] and TEMME [14]) that (3.9), (3.10) and (3.11) are valid under the following restrictions

$$(3.12) \quad n \rightarrow \infty, \quad z \text{ fixed}, \quad z \neq 0, \quad |\arg z| < \pi.$$

We will now describe our method of computing  $k_0$  and  $k_1$  defined in (3.4). If these functions are evaluated then the Bessel functions  $K_\nu$  and  $K_{\nu+1}$  can be computed from

$$K_\nu(z) = \pi^{\frac{1}{2}} (2z)^\nu e^{-z} k_0(z),$$

$$K_{\nu+1}(z) = K_\nu(z) [\nu+z+\frac{1}{2}-k_1(z)/k_0(z)]/z.$$

The latter equation may be derived from (3.2) and (3.4) and some contiguous relations of the confluent hypergeometric functions (cf. ABRAMOWITZ & STEGUN [1, 13.4.16 and 13.4.18]).

The functions  $k_0$  and  $k_1$  may be computed with Miller's algorithm. We use Gautschi's version of this algorithm, the details of which can be found in [5]. As normalization relation we use

$$(3.13) \quad \sum_{n=0}^{\infty} k_n(z) = (2z)^{-\nu-\frac{1}{2}},$$

which relation follows from (3.3) and (3.4) and substitution of the integral representation of  $k_n$  in (3.13).

In Miller's algorithm a positive integer  $N$  is selected and a sequence  $\bar{k}_0^{(N)}, \bar{k}_1^{(N)}, \dots, \bar{k}_N^{(N)}$  is computed by using (3.5) in backward direction with initial values  $\bar{k}_{N+1}^{(N)} = 0, \bar{k}_N^{(N)} = 1$ . By normalizing  $\bar{k}_0^{(N)}$  and  $\bar{k}_1^{(N)}$  with (3.13)  $k_0^{(N)}$  and  $k_1^{(N)}$  are computed. Then

$$(3.14) \quad \lim_{N \rightarrow \infty} k_n^{(N)} = k_n(z), \quad n = 0, 1.$$

Using the asymptotic estimates (3.8) and (3.9) we can readily show that the conditions of theorems in [5] are fulfilled, from which the validity of (3.14) follows. (The algorithm can be used for the computation of  $k_n$  for larger values of  $n$ , but here we only need to consider  $n = 0, 1$ ). In [14] we applied this algorithm for the computation of  $s_k(z) = z k! U(k+1, 1, z)$ . In fact it may be used for general  $U(a+n, b, z)$ ,  $n = 0, 1, 2, \dots$ , if  $|z|$  is not too small.

III.2. *Determination of the starting index*  $N$ . The relative error  $\varepsilon$  of  $k_n^{(N)}$  with respect to  $k_n(z)$  can be expressed by

$$(3.15) \quad k_n^{(N)} = k_n(z) (1+\varepsilon),$$

where  $\varepsilon$  depends on  $N, z, n$  and  $\nu$ . On account of (3.14),  $|\varepsilon|$  is small for large

N. For numerical applications it is necessary to have an idea how large the starting index of the Miller algorithm  $N$  has to be, in order to have a satisfactorily small  $|\varepsilon|$ .

As in GAUTSCHI [5], the determination of  $N$  can be based on asymptotic formulas for the functions  $y_n$  and  $k_n$ . A more satisfactory approach, however, is pointed out by OLVER & SOOKNE [12]. Their method is based on results of OLVER in [10] and [11]. Beginning with  $p_0 = 0$ ,  $p_1 = 1$ , Olver computes a solution  $p_n$  of (3.5) for  $n = 1, 2, \dots$ . Also computed is a sequence  $\{e_n\}$  defined by

$$e_0 = 1, \quad e_n = a_n e_{n-1}$$

where, in our case,  $a_n$  is given by (3.6), giving

$$e_n = (-1)^n (\nu, n) / (n+1)!$$

Next, the following quantity is introduced

$$E_N = \sum_{k=N}^{\infty} e_k / (p_k p_{k+1}), \quad N \geq 1.$$

and the selection of the starting index  $N$  depends on the construction of a bound of  $E_N$ .

In order to construct this bound we consider henceforth real values of  $z$  and  $\nu$ . As remarked in subsection I.2, it suffices to consider values of  $\nu$  in  $[-\frac{1}{2}, \frac{1}{2}]$ . Furthermore, we suppose  $z \geq 1$ . Under these conditions we have  $b_n \geq 1 + a_n$ , from which easily follows  $p_{n+1} \geq p_n$  for  $n \geq 0$ . Moreover,  $e_n \geq 0$  for  $n \geq 0$ . Hence,  $E_N$  is dominated as follows

$$(3.16) \quad E_N \leq \sum_{n=N}^{\infty} p_n^{-2} e_n = \pi^{-1} \cos \nu \pi \sum_{n=N}^{\infty} p_n^{-2} \Gamma(\frac{1}{2} + \nu + n) \Gamma(\frac{1}{2} - \nu + n) / [n! (n+1)!].$$

The series can be bounded by using the following lemma.

LEMMA. Let  $a$ ,  $b$  and  $z$  be real numbers such that  $b \geq a+1 > 0$  and  $z > 0$ . Then

$$\Gamma(z+a) / \Gamma(z+b) \leq z^{a-b}.$$

PROOF. From the integral (cf. [1,6.2.1])

$$\Gamma(b-a) \Gamma(z+a)/\Gamma(z+b) = \int_0^{\infty} e^{-(z+a+1)t} t^{b-a-1} [(1-e^{-t})/t]^{b-a-1} dt$$

we obtain, by using  $e^{-(a+1)t} \leq 1$ ,  $(1-e^{-t})/t \leq 1$  ( $t \geq 0$ ),

$$\Gamma(b-a) \Gamma(z+a)/\Gamma(z+b) \leq \int_0^{\infty} e^{-zt} t^{b-a-1} dt$$

from which the lemma follows.  $\square$

Applying the lemma to (3.16) we obtain

$$(3.17) \quad E_N \leq \pi^{-1} \cos v\pi \sum_{n=N}^{\infty} 1/(n^2 p_n^2).$$

The function  $p_n$  is a solution of (3.5). It can be written as a linear combination of  $y_n$  and  $k_n$ ;  $p_n$  and  $y_n$  have for large  $n$  the same asymptotic behaviour up to a factor independent of  $n$ . Considering (3.10) and comparing the series in (3.17) with the integral

$$\int_N^{\infty} n^{-1} \exp[-4(2nz)^{\frac{1}{2}}] dn$$

we observe that it is plausible to replace (3.17) by

$$(3.18) \quad E_N \leq 2\pi^{-1} \cos v\pi (2z)^{-\frac{1}{2}} N^{-3/2} p_N^{-2}.$$

To the first order of small quantities, the relative error in the Miller algorithm is in our case (cf. OLVER[10,(11.11)])

$$(3.19) \quad \sigma_N = E_N \sum_{n=0}^N p_n + \sum_{n=N+1}^{\infty} p_n E_n.$$

Hence, by using (3.18) and the same argumentation for both series in (3.19) as was used for (3.17), we obtain for  $\sigma_N$  the bound

$$(3.20) \quad \pi^{-1} z^{-1} \cos v\pi N^{-1} p_N^{-1}.$$



The least value of  $N \geq 1$  for which (3.20) is smaller than the prescribed relative accuracy will be taken as the starting index for the Miller algorithm.

REMARK. It may be noted that (3.20) vanishes for  $\nu = \pm \frac{1}{2}$ . As follows from (3.4) and (3.1), the functions  $k_n$  also vanish for  $n \geq 1$ , while  $k_0(z)$  equals 1 or  $1/(2z)$  if  $\nu = -\frac{1}{2}$  or  $\nu = +\frac{1}{2}$ , respectively. If the choice of  $N$  is based upon (3.20), small values of  $N$  will result in  $\nu$ -neighbourhoods of  $\pm \frac{1}{2}$ . This phenomenon will not disturb the actual algorithm. As can be verified, see the ALGOL procedure *besska*, in the limit  $\nu = \pm \frac{1}{2}$  the correct values are computed.

#### IV. ALGOL 60 PROCEDURES

The algorithms described in sections II and III are given as an ALGOL 60 procedure for real values of the parameters. For convenience we write  $z = x$  and  $\nu = a$ . The procedure *besska* computes for  $x > 0$  and  $a \in \mathbb{R}$  the Bessel functions  $K_a(x)$  and  $K_{a+1}(x)$ ; *besska* makes use of two nonlocal procedures *sinh* and *recipgamma*. The latter computes  $1/\Gamma(1-a)$  and the functions  $\Gamma_1(a)$  and  $\Gamma_2(a)$  defined in (2.11) for  $-\frac{1}{2} \leq a \leq \frac{1}{2}$ .

By choosing  $\epsilon$  the procedure *besska* can be used up to any (relative) tolerance. The two procedures *recipgamma* and *sinh* are supplied with fixed relative accuracy (about  $10^{-14}$ ). By only modifying these two procedures, the set of three procedures presented here can be adapted to any computer and to any accuracy.

The procedures are tested on the CD CYBER 73 of SARA, Amsterdam. For

$$x^{\pm} = 1 \pm 2^{-47}$$

we computed the numerical values of the expressions

$$d_0 = \{K_a(x^-) - K_a(x^+)\} / K_a(x^-),$$

$$d_1 = \{K_{a+1}(x^-) - K_{a+1}(x^+)\} / K_{a+1}(x^-).$$

In TABLE II we give  $d_0, d_1$ , the maximum number of terms ( $n$ ) used in (2.1), and the starting index  $N$  for the Miller algorithm.

TABLE II

eps		5.0 <sub>10</sub> -06	5.0 <sub>10</sub> -09	5.0 <sub>10</sub> -12	5.0 <sub>10</sub> -14
a					
0.0	d0	1.4 <sub>10</sub> -06	6.1 <sub>10</sub> -10	7.4 <sub>10</sub> -13	8.4 <sub>10</sub> -15
	d1	1.4 <sub>10</sub> -06	6.1 <sub>10</sub> -10	7.1 <sub>10</sub> -13	3.5 <sub>10</sub> -14
	(n,N)	( 6, 22)	( 8, 50)	( 9, 89)	(10,122)
0.2	d0	1.6 <sub>10</sub> -06	5.7 <sub>10</sub> -10	6.6 <sub>10</sub> -13	4.2 <sub>10</sub> -15
	d1	1.6 <sub>10</sub> -06	5.7 <sub>10</sub> -10	6.4 <sub>10</sub> -13	2.0 <sub>10</sub> -14
	(n,N)	( 6, 21)	( 8, 49)	( 9, 88)	(10,120)
0.4	d0	1.6 <sub>10</sub> -06	5.2 <sub>10</sub> -10	6.0 <sub>10</sub> -13	1.6 <sub>10</sub> -14
	d1	1.6 <sub>10</sub> -06	5.2 <sub>10</sub> -10	5.8 <sub>10</sub> -13	2.5 <sub>10</sub> -14
	(n,N)	( 6, 18)	( 8, 44)	( 9, 81)	(10,112)
0.6	d0	1.6 <sub>10</sub> -06	5.2 <sub>10</sub> -10	6.0 <sub>10</sub> -13	7.4 <sub>10</sub> -15
	d1	1.6 <sub>10</sub> -06	5.2 <sub>10</sub> -10	5.9 <sub>10</sub> -13	1.4 <sub>10</sub> -14
	(n,N)	( 7, 18)	( 8, 44)	( 9, 81)	(10,112)
0.8	d0	1.6 <sub>10</sub> -06	5.7 <sub>10</sub> -10	6.6 <sub>10</sub> -13	0.0 <sub>10</sub> +00
	d1	1.6 <sub>10</sub> -06	5.7 <sub>10</sub> -10	6.5 <sub>10</sub> -13	1.7 <sub>10</sub> -14
	(n,N)	( 6, 21)	( 8, 49)	( 9, 88)	(10,120)
1.0	d0	1.4 <sub>10</sub> -06	6.1 <sub>10</sub> -10	6.8 <sub>10</sub> -13	7.1 <sub>10</sub> -14
	d1	1.4 <sub>10</sub> -06	6.1 <sub>10</sub> -10	6.8 <sub>10</sub> -13	7.0 <sub>10</sub> -14
	(n,N)	( 6, 22)	( 8, 50)	( 9, 89)	(10,122)

```

real procedure recip gamma(x,odd,even); value x; real x,odd,even;
begin integer i; real alfa, beta, x2; array b[1:12];
  b[ 1]:= -.28387 65422 76024; b[ 2]:= -.07685 28408 44786;
  b[ 3]:= +.00170 63050 71096; b[ 4]:= +.00127 19271 36655;
  b[ 5]:= +.00007 63095 97586; b[ 6]:= -.00000 49717 36704;
  b[ 7]:= -.00000 08659 20800; b[ 8]:= -.00000 00331 26120;
  b[ 9]:= +.00000 00017 45136; b[10]:= +.00000 00002 42310;
  b[11]:= +.00000 00000 09161; b[12]:= -.00000 00000 00170;
  x2:= x x x x 8; alfa:= -.00000 00000 00001; beta:= 0;
  for i:= 12 step -2 until 2 do
    begin beta:= -(alfa x 2 + beta); alfa:= -beta x x2 - alfa + b[i] end;
  even:= (beta/2 + alfa) x x2 - alfa + .92187 02936 50453;
  alfa:= -.00000 00000 00034; beta:= 0;
  for i:= 11 step -2 until 1 do
    begin beta:= -(alfa x 2 + beta); alfa:= -beta x x2 - alfa + b[i] end;
  odd:= (alfa + beta) x 2; recip gamma:= odd x x + even
end recip gamma;

```

real procedure sinh(x); value x; real x;

begin real ax, y;  
 ax:= abs(x);  
if ax < .3 then  
begin y:= if ax < .1 then x × x else x × x/9;  
 x:= (((1/5040 × y + 1/120) × y + 1/6) × y + 1) × x;  
 sinh:= if ax < .1 then x else x × (1 + 4 × x × x/27)  
end else  
begin ax:= exp(ax); sinh:= sign(x) × .5 × (ax-1/ax) end  
end sinh;

procedure besska(a,x,eps,ka,ka1); value a,x,eps; real a,x,eps,ka,ka1;  
begin real a1,b,c,d,e,f,g,h,p,pi,q,s; integer n,na; boolean rec,rev;

x:= abs(x); pi:= 4 × arctan(1);  
 rev:= a < -.5; if rev then a:= -a-1;  
 rec:= a > .5; if rec then begin na:= entier(a+.5); a:= a - na end;  
if a = -.5 then f:= g:= sqrt(pi/x/2) × exp(-x) else  
if x < 1 then  
begin b:= x/2; d:= -ln(b); e:= a × d; c:= a × pi;  
 c:= if abs(c) < 10<sup>-15</sup> then 1 else c/sin(c);  
 s:= if abs(e) < 10<sup>-15</sup> then 1 else sinh(e)/e;  
 e:= exp(e); a1:= (e + 1/e)/2; g:= recip gamma(a,p,q) × e;  
 ka:= f:= c × (p × a1 + q × s × d); e:= a × a;  
 p:= .5 × g × c; q:= .5/g; c:= 1; d:= b × b; ka1:= p;  
for n:= 1, n + 1 while h/ka + abs(g)/ka1 > eps do  
begin f:= (f × n + p + q)/(n × n - e); c:= c × d/n;  
 p:= p/(n - a); q:= q/(n + a); g:= c × (p - n × f);  
 h:= c × f; ka:= ka + h; ka1:= ka1 + g  
end;  
 f:= ka; g:= ka1/b  
end else  
begin c:= .25 - a × a; g:= 1; f:= 0; e:= x × cos(a × pi)/pi/eps;  
for n:= 1, n + 1 while h × n < e do  
begin h:= (2 × (n + x) × g - (n - 1 + c/n) × f)/(n + 1);  
 f:= g; g:= h  
end;  
 p:= q:= f/g; b:= x + x; e:= b - 2;  
for n:= n, n - 1 while n > 0 do  
begin p:= (n - 1 + c/n)/(e + (n + 1) × (2 - p)); q:= p × (q + 1) end;  
 f:= sqrt(pi/b) × exp(-x)/(1 + q); g:= f × (a + x + .5 - p)/x  
end;  
if rec then  
begin x:= 2/x;  
for n:= 1 step 1 until na do  
begin h:= f + (a + n) × x × g; f:= g; g:= h end  
end;  
if rev then begin ka1:= f; ka:= g end else  
begin ka:= f; ka1:= g end  
end besska;

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