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N.M. TEMME
NUMERICAL EVALUATION OF FUNCTIONS
ARISING FROM TRANSFORMATIONS OF FORMAL SERIES

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Abstract

An algorithm is given for the numerical evaluation of a class of functions of the confluent hypergeometric type. The method of computation is based on the well-known Miller algorithm and on asymptotic expansions.

1. Introduction

In 1953 A. van Wijngaarden wrote a paper on transformations of formal series, [5]. He discussed a general transformation of the asymptotic expansion of certain integrals for large parameter values. Special attention was paid to a transformation from which the following functions arose

$$(1\text{-}1) \qquad s_k(z) = z \int_0^\infty e^{-zt}\, t^k (1+t)^{-k-1}\, dt, \quad k = 0,1,2,\ldots, \ \mathrm{Re}\, z > 0.$$

This transformation can be described in different ways. One way is the following. If in the Laplace integral

$$(1\text{-}2) \qquad f(z) = z \int_0^\infty e^{-zt}\, F(t)\, dt$$

the function F is expanded in powers of t and the order of summation and integration is interchanged then a formal series

$$(1\text{-}3) \qquad f(z) \sim \sum_{k=0}^\infty F^{(k)}(0)\, z^{-k}$$

results. When, however, F(t) is expanded in the following way

$$(1\text{-}4) \qquad F(t) = \sum_{k=0}^\infty c_k\, t^k (1+t)^{-k-1}$$

then we obtain by termwise integration

$$(1\text{-}5) \qquad f(z) \sim \sum_{k=0}^\infty c_k\, s_k(z)$$

with s_k defined in (1-1). The series in (1-5) can be considered as a transformation of the series in (1-3).

In a forthcoming paper [3] Lauwerier will consider van Wijngaarden's transformation from a different point of view.

Van Wijngaarden announced the construction of tables for the functions $s_k(z)$ for complex values of z. The construction of these tables turned out to be a heavy task and the tables did not reach the stage of publication. Nowadays, with large scale computer systems at our disposal, tabular values are not as interesting as methods of computing.

The aim of this paper is to give information about the numerical evaluation of $s_k(z)$ for $|\arg z| < \pi$ and $k = 0,1,\ldots, K$, where K is some positive integer.

In the next section some elementary properties of the functions s_k are discussed. In fact s_k can be expressed as a confluent hypergeometric function (Whittaker function). In section 3 the asymptotic behaviour of s_k is determined. With these results the convergence of the algorithm in section 4 is proven. In section 5 the computation for small values of $|z|$ is discussed. Also in that case asymptotic expansions are of fundamental importance. Our methods of computation apply to a more general class of functions, in fact to the whole class of confluent hypergeometric functions to which the functions s_k belong. Information on that point will be given in section 7.

2. The functions $s_k(z)$

The functions $s_k(z)$, defined by (1-1) for Re $z > 0$, $k = 0,1,2,\ldots$, can be expressed in terms of confluent hypergeometric functions. Using the notation of Abramowitz and Stegun [1, chapter 13], we have

$$(2\text{-}1) \qquad s_k(z) = z\, k!\, U(k+1,1,z).$$

Relevant properties of $s_k(z)$ can be derived from well-known properties of $U(a,b,z)$.

Equation (1-1) defines $s_k(z)$ in the halfplane Re $z > 0$. The domain of definition can be extended to $|\arg z| < \frac{3\pi}{2}$ by rotating the path of integration. The function $s_k(z)$ is a many-valued function of z. We will consider its principal branch in the plane cut along the negative real axis, this branch being determined by the condition that $s_k(z)$ is real and positive if z is real and positive.

For convenience we will denote

(2-2) $$u_k(z) = s_k(z)/z,$$

$k = 0,1,2,\ldots$. Then u_k satisfies the confluent hypergeometric differential equation

(2-3) $$z\,u_k'' + (1-z)u_k' - (k+1)u_k = 0.$$

A second solution of this equation, linearly independent of u_k, is the function

(2-4) $$y_k(z) = M(k+1,1,z);$$

$y_0(z) = e^z$, $y_1(z) = (1+z)e^z$. $M(a,b,z)$ is known as Kummer's function. In the notation of hypergeometric functions the function $M(a,b,z)$ is defined by

(2-5) $$M(a,b,z) = {}_1F_1(a;b;z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)} \frac{\Gamma(b)}{\Gamma(b+n)} \frac{z^n}{n!} .$$

A corresponding series-representation for $s_k(z)$ can be derived from a known representation of $U(a,b,z)$ in [1; 13.1.6]. For $k = 0,1,2,\ldots$ we have

(2-6) $$s_k(z) = -\frac{z}{k!} \sum_{n=0}^{\infty} \frac{\Gamma(k+n+1)z^n}{n!\; n!} \{\ln z + \Psi(k+n+1) - 2\Psi(n+1)\},$$

where $\Psi(z) = \Gamma'(z)/\Gamma(z)$. The series converges for all z in the finite z plane.

From the contiguous relations of the confluent hypergeometric functions we derive

(2-7) $$(k+1)\, s_{k+1}(z) - (2k+1+z)\, s_k(z) + k\, s_{k-1}(z) = 0.$$

This formula can also be obtained by partial integration of (1-1). The recurrence formula (2-7) can be considered as a homogeneous linear difference equation of the second order, of which of course u_k is also a solution, but u_k is not linearly independent of s_k. An independent solution turns out to be the function y_k defined in (2-4).

3. Asymptotic expansions

In this section we will study the asymptotic behaviour of s_k and y_k for large values of k and for various values of z, $|\arg z| < \pi$.

For small values of $|z|$, k fixed, the asymptotic behaviour follows from (2-5) and (2-6), viz.

(3-1) $$y_k(z) = 1 + O(z),$$

(3-2) $$s_k(z) = - z(\ln z + \Psi(k+1)) + O(|z^2 \ln z|).$$

For bounded values of $|z|$, say $|z| \leq M$, and large values of k we will use the differential equation (2-3) and a theorem due to Olver [4, 1956]. First we give a transformation of the dependent variable. If $u_k(z)$ is a solution of (2-3) then

(3-3) $$w(z) = z^{\frac{1}{2}} e^{-\frac{1}{2}z} u_k(z)$$

satisfies the equation

(3-4) $$w'' - \left(\frac{k+\frac{1}{2}}{z} - \frac{1}{4z^2} + \frac{1}{4}\right) w = 0.$$

The transformation of the independent variable

(3-5) $$z = t^2$$

and the substitution

(3-6) $$k + \tfrac{1}{2} = \tfrac{1}{4} \lambda^2$$

yield

$$w'' - \frac{1}{t} w' - [\lambda^2 - \frac{1}{t^2} + t^2]w = 0, \tag{3-7}$$

the differentiation in this equation being with respect to t.

For large values of λ and uniformly bounded values of $|t|$ the solutions of (3-7) will behave like the solutions of the so-called basic-equation

$$w'' - \frac{1}{t} w' - [\lambda^2 - \frac{1}{t^2}]w = 0. \tag{3-8}$$

The solutions of this equation are $t\, K_0(\lambda t)$ and $t\, I_0(\lambda t)$, where K_0 and I_0 are modified Bessel functions. By direct substitution in (3-7) it can be verified that the formal series

$$w_1(t) \sim t\, K_0(\lambda t) \sum_{n=0}^{\infty} \frac{A_n(t)}{\lambda^{2n}} - \frac{t}{\lambda} K_1(\lambda t) \sum_{n=0}^{\infty} \frac{B_n(t)}{\lambda^{2n}}, \tag{3-9}$$

$$w_2(t) \sim t\, I_0(\lambda t) \sum_{n=0}^{\infty} \frac{A_n(t)}{\lambda^{2n}} + \frac{t}{\lambda} I_1(\lambda t) \sum_{n=0}^{\infty} \frac{B_n(t)}{\lambda^{2n}}, \tag{3-10}$$

formally satisfy (3-7). The functions A_n and B_n are polynomials in t, recursively given by

$$\begin{cases} A_0(t) = 1, \\ 2B_n(t) = - A_n'(t) + \int_0^t \{x^2 A_n(x) - A_n'(x)/x\}dx, \\ 2A_{n+1}(t) = B_n(t)/t - B_n'(t) + \int_0^t x^2\, B_n(x)\, dx + a_{n+1}, \end{cases} \tag{3-11}$$

the integration constant a_{n+1} being arbitrary. The first few coefficients will be given in section 5. By application of Olver's theorem it can be shown that the series in (3-9), (3-10) are asymptotic expansions (in Poincaré's sense) of two linearly independent solutions w_1 and w_2 of (3-7) for large values of λ. These expansions hold uniformly in a closed bounded z-domain which includes the origin.

After these preliminary results we return to the functions u_k and y_k, introduced in the foregoing section. The functions

$$F(t) = e^{-\frac{1}{2}t^2} \; t \; u_k(t^2), \quad G(t) = e^{-\frac{1}{2}t^2} \; t \; y_k(t^2) \text{ are}$$

solutions of (3-7). Hence

$$F(t) = \alpha_1 \; w_1(t) + \alpha_2 \; w_2(t), \quad G(t) = \beta_1 \; w_1(t) + \beta_2 \; w_2(t),$$

where α_1, α_2, β_1, β_2 are independent of t. To evaluate these coefficients we need the following well-known properties of the Bessel functions.

(3-12) $$I_0(x) = 1 + O(x), \; K_0(x) = - \ln x + O(1), \; x \to 0;$$

(3-13) $$I_0(x) = (2\pi x)^{-\frac{1}{2}} \; e^x(1 + o(1)), \; K_0(x) = (\pi/2x)^{\frac{1}{2}} \; e^{-x}(1+o(1)), \; x \to \infty;$$

the formulas in (3-12) hold for arbitrary values of arg x, those of (3-13) hold for $|\arg x| < \frac{1}{2}\pi$.

For real z and for all values of k considered we have $0 < u_k(z) < \frac{1}{z}$; this follows from (1-1) and (1-2). Hence $\alpha_2 = 0$ for all values of k. Because of the uniform property of the expansions (3-9) and (3-10) we may keep $\lambda = 2\sqrt{k+\frac{1}{2}}$ fixed and let $t \to 0$ through positive values. Since $y_k(z)$ is bounded if $z \to 0$ (see (3-1)) it is obvious that $\beta_1 = 0$. Finally, from (3-1), (3-2) and (3-12) it follows that $\alpha_1 = 2$, $\beta_2 = 1$. Moreover all integration constants in (3-11) have to vanish ($n = 0,1,2,\ldots$). Hence, using the various transformations we obtain

(3-14) $$s_k(z) \sim 2z \; e^{\frac{1}{2}z} \; \{K_0(\zeta) \sum_{n=0}^{\infty} \frac{A_n(\sqrt{z})}{(4k+2)^n} - \frac{K_1(\zeta)}{\sqrt{4k+2}} \sum_{n=0}^{\infty} \frac{B_n(\sqrt{z})}{(4k+2)^n}\},$$

(3-15) $$y_k(z) \sim e^{\frac{1}{2}z} \; \{I_0(\zeta) \sum_{n=0}^{\infty} \frac{A_n(\sqrt{z})}{(4k+2)^n} + \frac{I_1(\zeta)}{\sqrt{4k+2}} \sum_{n=0}^{\infty} \frac{B_n(\sqrt{z})}{(4k+2)^n}\},$$

for $k \to \infty$, where

(3-16) $$\zeta = 2\sqrt{z(k+\tfrac{1}{2})},$$

$\zeta > 0$ if $z > 0$. The expansions are uniformly valid with respect to z in a bounded domain of the z-plane, which contains the origin.
Corollary. For fixed values of $|z|$ it follows from (3-14), (3-15) and (3-13) that

(3-17) $$s_k(z) \sim \pi^{\frac{1}{2}} z^{3/4} k^{-1/4} e^{\frac{1}{2}z - 2\sqrt{zk}},$$

(3-18) $$y_k(z) \sim \tfrac{1}{2}\pi^{-\frac{1}{2}} (zk)^{-1/4} e^{\frac{1}{2}z + 2\sqrt{zk}}$$

as $k \to \infty$. The restrictions on z in (3-17) and (3-18) are

(3-19) $$|\arg z| < \pi,\ z \text{ fixed},\ z \neq 0.$$

It has to be pointed out that (3-17) and (3-18) are not valid for both k and z being large. Representations, which are valid for large k uniformly in $|z|$ for $|z| \geq \delta > 0$, can be derived by applications of theorem A in Olver [3, 1954]. This will now be done.

Again, the starting point is the differential equation (3-4). The transformation

(3-20) $$z = 2\lambda t,\ \lambda = 2k+1$$

yields

(3-21) $$\frac{d^2w}{dt^2} - (\lambda^2 \frac{t+1}{t} - \frac{1}{t^2})\, w = 0$$

and a further transformation

(3-22) $$w = (\frac{t}{1+t})^{1/4} v, \quad x = \ln(\sqrt{t} + \sqrt{1+t}) + \sqrt{t(1+t)}$$

results in

(3-23) $$\frac{d^2v}{dx^2} - \{\lambda^2 + f(x)\}\, v = 0.$$

The function f(x) cannot be given explicitly in terms of x, but in the variable t we have

$$f(x) = \frac{3+8t}{16t(1+t)^3} - \frac{1}{t(1+t)} ;$$

the relation between x and t is given in (3-22). According to Olver, for large values of λ the solutions of (3-23) behave like the solutions $e^{\pm\lambda x}$ of the basic-equation $v'' - \lambda^2 v = 0$. As a consequence, we have for two linearly independent solutions w_1 and w_2 of (3-21)

(3-24) $$w_1(t) \sim \left(\frac{t}{1+t}\right)^{\frac{1}{4}} \exp[\lambda\{\ln(\sqrt{t} + \sqrt{1+t}) + \sqrt{t(1+t)}\}],$$

(3-25) $$w_2(t) \sim \left(\frac{t}{1+t}\right)^{\frac{1}{4}} \exp[-\lambda\{\ln(\sqrt{t} + \sqrt{1+t}) + \sqrt{t(1+t)}\}]$$

as $\lambda \to \infty$.

Using Olver's theorem we can prove that this formulas hold uniformly in t in the domain $|t| \geq \delta$, $|\arg t| \leq \pi-\varepsilon$, where ε and δ are fixed positive numbers ($\varepsilon < \pi$).As in (3-9) and (3-10) we can construct asymptotic series which formally satisfy (3-23), but here we are interested in the first order approximation only..

To give the results for y_k and s_k we proceed as in the foregoing case. First we remark that

$$z^{\frac{1}{2}} e^{-\frac{1}{2}z} u_k(z) = (2\lambda t)^{-\frac{1}{2}} e^{-\lambda t} s_k(2\lambda t) = F(t),$$

$$z^{\frac{1}{2}} e^{-\frac{1}{2}z} y_k(z) = (2\lambda t)^{\frac{1}{2}} e^{-\lambda t} y_k(2\lambda t) = G(t)$$

(where $\lambda = 2k+1$) are solutions of (3-20). Hence

$$F(t) = \alpha_1 w_1(t) + \alpha_2 w_2(t), \; G(t) = \beta_1 w_1(t) + \beta_2 w_2(t),$$

where α_1, α_2, β_1, β_2 are independent of t. To evaluate these coefficients we use (3-17) and (3-18). If in (3-20) z is fixed and λ is large then t is small. In this case it follows from (3-24) and (3-25)

$$w_1(t) \sim t^{\frac{1}{4}}\ e^{2\lambda\sqrt{t}} \sim z^{\frac{1}{4}}\ 2^{-\frac{1}{2}}\ k^{-\frac{1}{4}}\ e^{2\sqrt{kz}},$$

$$w_2(t) \sim t^{\frac{1}{4}}\ e^{-2\lambda\sqrt{t}} \sim z^{\frac{1}{4}}\ 2^{-\frac{1}{2}}\ k^{-\frac{1}{4}}\ e^{-2\sqrt{kz}}$$

as $k \to \infty$. Taking into account (3-17) and (3-18) we have $\alpha_1 = \beta_2 = 0$ and $\alpha_2 = \sqrt{2\pi}$, $\beta_1 = 1/\sqrt{2\pi}$. Hence

$$s_k(z) = \sqrt{2\pi z}\, e^{\frac{1}{2}z}\ w_2(t)\ ,$$

$$y_k(z) = 1/\sqrt{2\pi z}\, e^{\frac{1}{2}z}\ w_1(t)$$

and, using (3-24) and (3-25) we have

(3-26) $$s_k(z) \sim (2\pi z\ \text{th}\ \alpha)^{\frac{1}{2}} \exp\{\tfrac{1}{2}z - (k+\tfrac{1}{2})(2\alpha + \text{sh}\ 2\alpha)\}\ ,$$

(3-27) $$y_k(z) \sim (\text{th}\ \alpha/2\pi z)^{\frac{1}{2}} \exp\{\tfrac{1}{2}z + (k+\tfrac{1}{2})(2\alpha + \text{sh}\ 2\alpha)\}$$

as $k \to \infty$, where α is defined by

(3-28) $$z = 4(k+\tfrac{1}{2})\ \text{sh}^2\alpha;$$

$\text{sh}\ \alpha$ is real and positive if z is positive. In (3-26), (3-27) the restrictions on z are

(3-29) $$|\arg z| \leq \pi-\varepsilon,\ 0 < \varepsilon < \pi,\ |z| \geq \delta > 0.$$

In (3-26) and (3-27) we can fix k and let $z \to \infty$. Taking limiting forms of the functions of α for large α we obtain

$$s_k(z) \sim \frac{k!}{z^k}$$

$$y_k(z) \sim \frac{z^k e^z}{k!}\ ,$$

as $z \to +\infty$, k fixed. These formulas correspond to well-known results of the confluent hypergeometric functions. The formula for s_k can be derived direct from (1-1). The formula for y_k then follows from (3-26), (3-27), $y_k(z)\ s_k(z) \sim \text{th}\ \alpha\ e^z \sim e^z$.

The formulas (3-17) and (3-26) may also be derived from (1-1) by using saddle point techniques.

The asymptotic expansion in (3-14) will be used for the numerical evaluation of $s_k(z)$ for large values of k (and small values of $|z|$). See section 5. Formula (3-17) gives information about the rate of convergence of series with $s_k(z)$, for instance series of type (1-5).

4. Method of computation

The recurrence relation (2-7) is an important tool for generating a sequence of values $s_k(z)$ for fixed z and k = 0,1,2,..., K. If the values of $s_k(z)$ are known for two consecutive values of k, then the functions may be computed for other values of k by successive application of the recurrence relation.

In [2], Gautschi investigates the problem of numerical instability for general three-term recurrence relations. In this connection he introduces the concepts of minimal solution and dominant solution of a recurrence relation. Starting from two initial values, an application of the recurrence relation in the forward direction (i.e. in the direction of increasing order) yields a disastrous build-up of errors for the minimal solution, whereas the computation of the dominant solution remains numerically stable.

If the recurrence relation

(4-1) $$y_{n+1} + a_n\, y_n + b_n\, y_{n-1} = 0$$

has two linearly independent solutions f_n and g_n having the property

(4-2) $$\lim_{n\to\infty} f_n/g_n = 0$$

then f_n is called a minimal solution and g_n is called the dominant solution of (4-1). From (3-17) and (3-18) it follows

(4-3) $$\frac{s_k(z)}{y_k(z)} \sim 2\, z\pi e^{-4\sqrt{zk}},$$

$k \to \infty$, under the conditions in (3-19). Consequently, in our case, $s_k(z)$ is a minimal solution of (2-7) and $y_k(z)$ is a dominant solution.

Gautschi's paper concentrates mainly on the development of an algorithm for the computation of minimal solutions. This algorithm is based on Miller's method which enables computation without any knowledge of starting values for large k.

To describe the algorithm for the computation of the minimal solution $f_n (n = 0,1,\ldots,N)$ of (4-1) let

(4-4) $$\sum_{m=0}^{\infty} \lambda_m f_m = t, \qquad t \neq 0,$$

(4-5) $$r_n = f_{n+1}/f_n,$$

(4-6) $$t_n = f_n^{-1} \sum_{m=n+1}^{\infty} \lambda_m f_m,$$

where t and $\lambda_0, \lambda_1, \ldots$ are given quantities and the series (3-4) is known to converge. At first we suppose that r_n and t_n are known for some value $n = \nu \geq N$. From (4-1) and (4-5) there follows

(4-7) $$r_{n-1} = -b_n/(a_n+r_n), \; n = \nu, \nu-1, \ldots, 1,$$

and from (4-6) and (4-7)

(4-8) $$t_{n-1} = r_{n-1}\,(\lambda_n+t_n), \; n = \nu, \nu-1, \ldots, 1.$$

Hence r_n and t_n can be obtained recursively for $0 \leq n < \nu$; in particular we have, using (4-4)

(4-9) $$t_0 = f_0^{-1}\,(t - \lambda_0 f_0),$$

and so

(4-10) $$f_0 = t/(\lambda_0 + t_0),$$

giving the initial value of the minimal solution. The remaining values can be obtained from

(4-11) $$f_n = r_{n-1}\, f_{n-1}, \; n = 1,2,\ldots, N.$$

When the algorithm is executed with the (incorrect) starting values $r_\nu^{(\nu)} = 0$, $t_\nu^{(\nu)} = 0$, we have the following set of recursions

(4-12) $$\begin{cases} \left.\begin{array}{l} r_\nu^{(\nu)} = 0, \quad r_{n-1}^{(\nu)} = -\, b_n/(a_n + r_n^{(\nu)}) \\ t_\nu^{(\nu)} = 0, \quad t_{n-1}^{(\nu)} = r_{n-1}^{(\nu)}\,(\lambda_n + t_n^{(\nu)}) \end{array}\right\} \quad n = \nu, \nu-1, \ldots, 1, \\ f_0^{(\nu)} = t/(\lambda_0 + t_0^{(\nu)}), \quad f_n^{(\nu)} = r_{n-1}^{(\nu)}\, f_{n-1}^{(\nu)}, \quad n = 1, 2, \ldots, N. \end{cases}$$

Gautschi showed that the set of recursions (4-12) is numerically stable and that

(4-13) $$\lim_{\nu\to\infty} f_n^{(\nu)} = f_n \qquad (n = 0,1,\ldots, N)$$

if and only if

(4-14) $$\lim_{\nu\to\infty} \frac{f_{\nu+1}}{g_{\nu+1}} \sum_{m=0}^{\nu} \lambda_m\, g_m = 0,$$

where g_n is a dominant solution of (4-1).

Under the restrictions on z given in (3-29) the functions $s_k(z)$ $(k = 0,1,\ldots, K)$ can be computed with Gautschi's algorithm (4-12). For the series in (4-4) the following series can be used

(4-15) $$\sum_{k=0}^{\infty} s_k(z) = 1.$$

This formula may be proved by substitution of (1-1).

Hence

$$t = \lambda_n = 1, \; a_n = -(2n+1+z)/(n+1), \; b_n = n/(n+1),$$

(cf. (4-1) and (2-7)). We can choose ν so large that

$$(4\text{-}16) \qquad \left| \frac{f_k^{(\nu)} - s_k(z)}{s_k(z)} \right| < \varepsilon, \; \varepsilon > 0, \; k = 0,1,\ldots, K,$$

if and only if condition (4-14) is fulfilled.

In our case it reads

$$(4\text{-}17) \qquad \lim_{\nu\to\infty} \frac{s_{\nu+1}(z)}{y_{\nu+1}(z)} \sum_{m=0}^{\nu} y_m(z) = 0$$

for the values of z specified in (3-19).

To verify condition (4-17) we compute the finite sum in this formula. We have

$$(4\text{-}18) \qquad \sum_{m=0}^{\nu} y_m(z) = (\nu+1)(y_{\nu+1}(z) - y_\nu(z))/z.$$

This formula can be derived by using (2-7) and mathematical induction with respect to ν. With (4-18), (4-3), and (3-18) it is easy to prove that (4-17) holds for $|\arg z| < \pi$, $z \neq 0$, z fixed.

The positive integer ν in (4-12), which indicates the starting-point of the backward recurrence, can be chosen so that (4-16) is fulfilled. The number ν depends on ε, z and K; ν is large if $|z|$ is small, even $\nu \to \infty$ if $z \to 0$. This can be recognized by observing that for $z \to 0$ the series in (4-15) converges poorly. Besides, and this is the main point, the dominance of y_k over s_k becomes rather weak, as can be seen from (4-3).

Therefore, for small values of $|z|$ the algorithm becomes less attractive, and as a consequence, for small values of $|z|$ we need accurate starting values of $s_k(z)$ for two consecutive values of k.

Throughout this paper we will fix the dividing-line in the z-plane for the two methods at $|z| = 1$. An optimal choice of a boundary may be found by numerical methods. From our experience, $|z| = 1$ is a convenient choice.

5. The computation for $|z| < 1$, $z \neq 0$

The algorithm describes in (4-12) provides us with a numerical procedure for the computation of $s_k(z)$ $(k = 0,1,\ldots, K)$ which converges and which is numerically stable for every z in the z-plane satisfying $|\arg z| < \pi$, $z \neq 0$. However for small values of $|z|$, the number ν may be considerably large when (4-16) has to be satisfied and therefore the procedure converges slowly, unless correct values of $r_\nu^{(\nu)}$ and $t_\nu^{(\nu)}$ are substituted in (4-12). In that case we need two starting values $s_\nu(z)$ and $s_{\nu+1}(z)$, $\nu \geq N$.

The series-representation (2-6) converges for all finite values of z. However, when k is a large integer cancellation of significant digits occurs when the series is summed numerically. Besides, convergence is rather poor when k is large.

Since $s_\nu(z)$ has to be evaluated for large values of ν it is more attractive to use an asymptotic expansion of $s_\nu(z)$ valid for large values of ν, while small values of $|z|$ do not invalidate the approximation. In section 3 we derived an expansion satisfying these requirements, namely (3-14). This expansion gives an excellent approximation for $s_k(z)$ for large k and fixed values of $|z|$, while the approximation is becoming better according as $|z|$ becomes smaller.

The first few values of the polynomials A_n and B_n are

$$A_0(t) = 1,$$

$$A_1(t) = t^2(t^4-12)/72,$$

$$A_2(t) = t^4(5t^8-1128t^4+27216)/1\ 55520,$$

$$A_3(t) = t^2(35t^{16}-31500t^{12}+58\ 59216t^8-2067\ 63840t^4+5486\ 74560)/11757\ 31200,$$

$$A_4(t) = t^4(5t^{20}-11472t^{16}+70\ 68384t^{12}-13282\ 03008t^8+$$
$$+6\ 51177\ 79200t^4-49\ 98537\ 21600)/33\ 86105\ 85600,$$

$$B_0(t) = t^3/6,$$

$$B_1(t) = t(5t^8-432t^4+2160)/6480,$$

$$B_2(t) = t^3(7t^{12}-3528t^8+2\ 98224t^4-30\ 48192)/65\ 31840,$$

$$B_3(t) = t(5t^{20}-7560t^{16}+27\ 76896t^{12}-2642\ 28480t^8$$
$$+47953\ 03680t^4-65840\ 94720)/70543\ 87200.$$

By substitution of polynomial representations of A_n and B_n in (3-11) recurrence relations for the coefficients of these polynomials may be derived in order to compute A_n and B_n for other values of n.

Some remarks on the computation of the modified Bessel functions $K_0(\zeta)$ and $K_1(\zeta)$ will follow in section 7.

6. The estimation of ν

In this section we give an estimate of the starting value ν to be used in algorithm (4-12), given the relative accuracy desired. Gautschi [2] obtained an approximation for the relative error which in our notation reads as follows (see Gautschi's discussions around 3.18 and 5.11 in [2])

(6-1) $$\frac{f_k^{(\nu)} - s_k(z)}{s_k(z)} \approx s_{\nu+1}(z) - \frac{s_{\nu+1}(z)\, y_k(z)}{y_{\nu+1}(z)\, s_k(z)},$$

ν large, $k = 0,1,\dots, K$.

Our aim is to determine ν such that

(6-2) $$\left|\frac{f_k^{(\nu)} - s_k(z)}{s_k(z)}\right| < \varepsilon$$

holds for $k = 0,1,\dots, K$, $|z| \geq 1$, $|\arg z| < \pi$, where ε is the relative accuracy desired. Since $|y_k(z)/s_k(z)|$ ultimately grows rapidly with k, see (4-3), it is plausible to expect that when (6-2) holds for $k = K$ it will also be valid when $k < K$, particularly when K is large. We therefore consider the simplified problem of bounding

(6-3) $$\left| s_{\nu+1}(z) - \frac{s_{\nu+1}(z)\, y_K(z)}{y_{\nu+1}(z)\, s_K(z)} \right|.$$

We assume K, and thus ν, so large that the functions in (6-3) may be replaced by approximations of these functions holding for large values of ν and K.
The asymptotic expressions in (3-17) and (3-18) are not suitable for large $|z|$, therefore it is necessary to use the more intricate formulas (3-26) and (3-27).

Applications of (3-26) and (3-27) to (6-3) gives (if a few unimportant coefficients have been omitted)

(6-4) $$\left|\frac{f_k^{(\nu)} - s_k(z)}{s_k(z)}\right| \leq e^{\mathrm{Re}\{\frac{1}{2}z-\nu f(\alpha)\}} + e^{2\mathrm{Re}\{K\, f(\beta)-\nu f(\alpha)\}},$$

$$f(\alpha) = 2\alpha + \mathrm{sh}\, 2\alpha,$$

$$\mathrm{sh}^2\alpha = z/4\nu,\ \mathrm{sh}\,\alpha > 0 \text{ if } z > 0,$$

$$\mathrm{sh}^2\beta = z/4K,\ \mathrm{sh}\,\beta > 0 \text{ if } z > 0.$$

The positive integer ν can be chosen so large (if z, K and ε are known) that simultaneously

(6-5) $$e^{\mathrm{Re}\{\frac{1}{2}z-\nu f(\alpha)\}} < \tfrac{1}{2}\varepsilon, \quad e^{2\mathrm{Re}\{Kf(\beta)-\nu f(\alpha)\}} < \tfrac{1}{2}\varepsilon.$$

The proper value of ν can be found by inverting the function $\mathrm{Re}\{\nu f(\alpha)\}$. Somer properties of this function will now be given.

Let

$$\mathrm{sh}^2\alpha = z/4\nu = re^{i\theta}/4\nu, \; r > 0, \; -\pi < \theta < \pi,$$

$$\alpha = \gamma + i\delta, \; \gamma > 0, \; -\frac{\pi}{2} < \delta < \frac{\pi}{2} .$$

Then, by eleminating δ,

(6-6) $$\mathrm{Re}\{\nu f(\alpha)\} = \frac{r}{2\mathrm{sh}^2\, 2\gamma} [2\gamma\{\mathrm{ch}\, 2\gamma+\cos\theta\} + \mathrm{sh}\, 2\gamma\{1+\cos\theta\;\mathrm{ch}\, 2\gamma\}]$$

and

(6-7) $$\nu = \frac{r}{2\;\mathrm{sh}^2\, 2\gamma} \{\mathrm{ch}\, 2\gamma+ \cos\theta\}.$$

Denoting (6-6) by $\phi(\gamma)$ then

$$\lim_{\gamma\to 0} \phi(\gamma) = \infty, \quad \lim_{\gamma\to\infty} \phi(\gamma) = \tfrac{1}{2}\, r \cos\theta$$

and

$$\phi'(\gamma)= -\frac{2\gamma r}{\mathrm{sh}^3\, 2\gamma} \{\mathrm{ch}^2\, 2\gamma+2 \cos\theta\;\mathrm{ch}\, 2\gamma+1\}.$$

Thus, $\phi(\gamma)$ is a monotone decreasing function of γ and the equation

(6-8) $$\phi(\gamma) = p$$

has a unique solution $\gamma = \phi^{-1}(p)$ for all $p > \frac{1}{2}\, r \cos\theta$.

The inequalities in (6-5) are equivalent with $\phi(\gamma) > \frac{1}{2} r \cos\theta + \ln(2/\varepsilon)$, $\phi(\gamma) > \phi(\lambda) + \frac{1}{2}\ln(2/\varepsilon)$ where λ is implicitly given by (cf. (6-7))

(6-9) $$K = \frac{r}{2\,\mathrm{sh}^2\, 2\lambda}\{\mathrm{ch}\, 2\lambda + \cos\theta\}.$$

This equation may be inverted to give λ explicitly, viz.

(6-10) $$\lambda = \tfrac{1}{2}\,\mathrm{arc\,ch}\,(y + \sqrt{y^2+2y\cos\theta+1}),$$

where $y = r/4K$.

If we set

(6-11) $$\gamma = \phi^{-1}\{\max(\tfrac{1}{2} r\cos\theta+\ln(2/\varepsilon),\ \phi(\lambda)+\tfrac{1}{2}\ln(2/\varepsilon))\}$$

then the number ν given by (6-7) may be used for starting the algorithm described in (4-12).

For real values of z approximations of ϕ^{-1} are easily obtained. By inverting (6-8) for large values of p we have

(6-12) $$\phi^{-1}(p) \simeq \frac{r}{p}\left(1 + \frac{1}{45}\left(\frac{r}{p}\right)^4\right),\quad p/r \to \infty,$$

and by inverting for values of p close to $\frac{1}{2}z$ we obtain

(6-13) $$\phi^{-1}(p) \simeq \gamma_0\left(1 + \frac{2q}{q + \gamma_0(q^2+1)}\right),\quad q \to 1,\ q > 1,$$

where $q = 2p/r$, $\gamma_0 = \frac{1}{2}\ln\left(\frac{q+1}{q-1}\right)$. Using (6-12) for $q \geq 2$ and (6-13) for $1 < q < 2$, we have a suitable approximation of $\phi^{-1}(p)$ for all $p > 1$.

For real values of z ($\theta = 0$, $z = r$) we will give the successive steps in the computation of ν. The three quantities z, K and ε are given.

1) compute λ from (6-10); $\lambda = \ln(\sqrt{y} + \sqrt{y+1})$; $y = z/4K$;
2) compute $\phi(\lambda) = z(2\lambda + \mathrm{sh}\, 2\lambda)/4\,\mathrm{sh}^2\lambda$;
3) compute $p = \max\{\frac{1}{2}z + \ln(2/\varepsilon),\ \phi(\lambda) + \frac{1}{2}\ln(2/\varepsilon)\}$;
4) compute $\gamma = \phi^{-1}(p)$ from (6-12) or (6-13);
5) compute ν from (6-7).

The estimated value of ν can be compared with the smallest value of ν empirically found, for a given set of values z, K and ε. Emperical values were found by running algorithm (4-12) with $\nu = K + 15$, $K + 20$, $K + 25, \ldots$ until for the first time the K + 1 values $f_k^{(\nu)}$, $(k = 0,1,\ldots, K)$ agreed within a relative accuracy of ε with the respective values of $f_k^{(\nu-5)}$.

In the following table we give some values of the starting number ν for $\varepsilon = 10^{-10}$. The empirical values may be compared with the values between brackets which are obtained from the asymptotic relations. For small values of K the estimated values appear to be less accurate.

z \ K	15	30	50	80	100
1.0	155(147)	155(146)	160(168)	210(221)	245(253)
3.0	60(53)	80(79)	110(110)	150(152)	180(180)
5.0	45(42)	65(66)	95(94)	135(134)	160(160)
10.0	35(33)	55(54)	80(80)	115(117)	140(141)
25.0	30(26)	45(44)	70(68)	105(102)	125(125)
50.0	30(22)	45(40)	65(63)	95(96)	120(117)
80.0	30(21)	45(38)	65(60)	95(92)	115(114)

If $|z| < 1$ the choice of ν depends on the number of terms used in the asymptotic series (3-14). We used this expansion with n = 4 for the A-series and with n = 3 for the B-series and $\nu \geq \max(K,100)$. In this way we found nine correct significant digits in $s_k(z)$, $k = 0,1,\ldots, K$.

7. Generalizations

When instead of (1-2) integrals of the type

$$f(z) = z \int_0^\infty t^\alpha e^{-zt} F(t)dt$$

are considered, $-1 < \text{Re}\,\alpha < 0$, the analysis proceeds in the same manner. The function F(t) is expanded as in (1-4) and the functions $s_k^{(\alpha)}$, now depending on α, can be written as

$$s_k^{(\alpha)}(z) = z \int_0^\infty e^{-zt} t^{k+\alpha}(1+t)^{-k-1} dt =$$

$$= z\,\Gamma(k+\alpha+1)\, U(k+\alpha+1,\alpha+1,z).$$

These functions may be computed by using analogous methods as described in sections 4 and 5. In fact it is possible to evaluate the whole class of hypergeometric functions $u_k = U(a+k,b,z)$, $k = 0,1,\ldots$ in this way. The asymptotic properties of u_k and s_k are not essentially different, since it suffices to consider $0 \le a \le 1$, $0 \le b \le 1$. (For $n = 0,1,2,\ldots$ the functions $U(a,b+n,z)$ can be computed with starting values for $n = 0,1$; in this case computation in the forward direction is numerically stable). The asymptotic series for u_k (analogous to the representation is s_k in (3-14)) follows from Olver's paper. The coefficients A_n and B_n will depend on a and b. The Bessel functions have to be replaced by K_{b-1} and K_b.

The Bessel functions $K_a(z)$ may also be computed by the methods of section 4, at least if $|z|$ is not too small, say $|z| \ge 1$. Namely, we can write $K_a(z)$ as a confluent hypergeometric function,

$$K_a(z) = \pi^{\frac{1}{2}} (2z)^a e^{-z} U(a+\tfrac{1}{2},2a+1,2z).$$

For small values of $|z|$ the calculation can be attempted by using the well-known formula

$$K_a(z) = \frac{\pi}{2} \frac{I_{-a}(z) - I_a(z)}{\sin a\pi} .$$

In a forthcoming publication we will work out some new ideas on the numerical evaluation of the Bessel function $K_a(z)$.

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