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# COMPUTATIONAL ASPECTS OF THREE-TERM RECURRENCE RELATIONS*

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**Introduction.** Recurrence relations are one of the basic mathematical tools of computation. There is hardly a computational task which does not rely on recursive techniques, at one time or another. The widespread use of recurrence relations can be ascribed to their intrinsic constructive quality, and the great ease with which they are amenable to mechanization. On the other hand, like most recursive processes, recurrence relations are susceptible to error growth. Each cycle of a recursive process not only generates its own rounding errors, but also inherits the rounding errors committed in all the previous cycles. If conditions are unfavorable, the resulting propagation of error may well be disastrous. It is this aspect of recurrence relations—the possibility and the prevention of numerical instability—that will be of concern to us.

The problem of numerical instability has been studied extensively for difference equations arising in the numerical solution of ordinary and partial differential equations. In the seemingly much simpler context of a single linear difference equation, the problem has received only sporadic attention, even though such difference equations, particularly of the second order, occur prominently in many branches of pure and applied mathematics. We mention, e.g., the recurrence relations satisfied by large classes of special functions of mathematical physics and statistics, the three-term recurrence relations that lie at the heart of continued fraction theory and the theory of orthogonal polynomials, and the miscellaneous recurrence relations one encounters when constructing series expansions, asymptotic or otherwise, to solutions of linear differential equations. We believe, therefore, that a systematic review of some of the computational problems attending recurrence relations might be of value. In the following we attempt to present such a survey, restricting attention to the special case of three-term recurrence relations.

The kind of instability we are concerned with, may be described as follows. Consider a three-term recurrence relation of the form

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots, \tag{0.1}$$

where $a_n$, $b_n$ are given sequences of real or complex numbers, and $b_n \neq 0$. The general solution of (0.1) can be spanned by any pair $f_n$, $g_n$ of linearly independent solutions. We are interested in the special case where there exists such a pair having the property

$$\lim_{n\to\infty} \frac{f_n}{g_n} = 0. \tag{0.2}$$

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Serious problems then arise if one attempts to compute the solution $f_n$ or any constant multiple of $f_n$.

To see this, we first note that (0.2) implies

$$\lim_{n\to\infty} \frac{f_n}{y_n} = 0 \tag{0.3}$$

for any solution $y_n$ not proportional to $f_n$. Such a solution, indeed, is representable in the form $y_n = af_n + bg_n$, with $b \neq 0$, and therefore

$$\lim_{n\to\infty} \frac{f_n}{y_n} = \lim_{n\to\infty} \frac{f_n/g_n}{b + a(f_n/g_n)} = 0.$$

If we now generate $f_n$ by (0.1), using only approximate initial values $y_0 \doteq f_0$, $y_1 \doteq f_1$ (due to rounding, for example), but recurring with infinite precision, we obtain a solution $y_n$ which, in general, is linearly independent of $f_n$. Therefore, by (0.3), we will have

$$\left|\frac{y_n - f_n}{f_n}\right| \to \infty \quad \text{as} \quad n \to \infty,$$

i.e., the relative error of $y_n$, the intended approximation to $f_n$, becomes arbitrarily large. Therefore, this straightforward method of computing $f_n$ is utterly ineffective.

Observe that the set of all solutions $f_n$ of (0.1) having the property indicated in (0.3) forms a one-dimensional subspace of the space of all solutions. (There can be no two linearly independent solutions $f_n, f_n'$ enjoying this property, since, otherwise, $f_n/f_n'$ and $f_n'/f_n$ would both have the limit zero, as $n \to \infty$, which is absurd.) We call the solutions of this subspace *minimal at infinity*, or briefly *minimal*.[1] A nonminimal solution will be referred to as *dominant*. Each dominant solution is asymptotically proportional to $g_n$. Note that, in contrast to dominant solutions, a minimal solution is uniquely determined by one initial value.

To illustrate the difficulty of calculating minimal solutions, consider the problem of generating Bessel functions of the first kind, $J_n(x)$, for fixed $x$, and $n = 0, 1, 2, \cdots$.[2] As is well-known, these functions (of $n$) obey the three-term recurrence relation

$$y_{n+1} - \frac{2n}{x} y_n + y_{n-1} = 0. \tag{0.4}$$

From tables of Bessel functions we find, e.g., that for $x = 1, J_0(1) = .7651976866$, $J_1(1) = .4400505857$, accurate to ten figures. Generating the next 99 values of $J_n(1)$ on a digital computer by straightforward recursion, we obtain the results

[1] The notion of a minimal solution appears to have first been introduced by Pincherle in connection with his generalization of continued fractions [44]. Pincherle called it "distinguished" solution (soluzione distinta). In the theory of linear differential equations the term "principal" solution is also in use [24]. The minimal solution can often be identified with a solution "of type II" in a terminology of Schäfke [51].

[2] This example is well known, and has received considerable attention in the literature. See the references in §5.

TABLE 1

| $n$ | "$J_n(1)$" | $n$ | "$J_n(1)$" |
|---|---|---|---|
| 0 | 7.651976866 (−1) | 9 | −4.645246881 (−4) |
| 1 | 4.400505857 (−1) | 10 | −8.332374506 (−3) |
| 2 | 1.149034848 (−1) | 11 | −1.661829654 (−1) |
| 3 | 1.956335358 (−2) | 12 | −3.647692865 (0) |
| 4 | 2.476636684 (−3) | 13 | −8.737844579 (1) |
| 5 | 2.497398891 (−4) | ... | ... |
| 6 | 2.076220699 (−5) | 20 | −2.818590869 (12) |
| 7 | −5.934052751 (−7) | ... | ... |
| 8 | −2.906988084 (−5) | 100 | −2.586550446 (175) |

shown in Table 1.[3] (The numbers in parentheses denote powers of 10 by which the preceding numbers have to be multiplied.) Obviously, there is little resemblance with the true values of $J_n(1)$, which are known to decrease steadily with increasing $n$, and to approach zero very rapidly as $n \to \infty$. In fact, since $J_7(1)$ came out to be negative, all digits shown, for $n \geqq 7$, including the sign and the exponent, must be illusory.

The disastrous build-up of errors, in this example, is due to the fact that with $f_n = J_n(x)$, also $g_n = Y_n(x)$, the Bessel function of the second kind, is a solution of (0.4) and, moreover,

$$\frac{f_n}{g_n} \sim -\frac{(x/2)^{2n}}{2(n!)^2} \quad \text{as} \quad n \to \infty.$$

Therefore, $J_n(x)$ is indeed highly minimal at infinity.

Methods of calculating minimal solutions of three-term recurrence relations, including applications, constitute the main theme of this paper. In §1 we begin with a brief survey of continued fractions, emphasizing computational methods. The relevance of continued fractions is contained in a result due to Pincherle which expresses ratios of a minimal solution in terms of continued fractions. In §2 we recall some classical results from the asymptotic theory of linear difference equations which will find repeated use in the later parts of the paper. §3 brings a first algorithm for calculating a minimal solution, based on the result of Pincherle. The problem considered is to calculate a minimal solution $f_n$ known to satisfy

$$\sum_{m=0}^{\infty} \lambda_m f_m = s, \qquad s \neq 0. \tag{0.5}$$

The special case $\lambda_0 = 1, \lambda_m = 0, m > 0$, amounts to prescribing $f_0$. Consideration of an infinite series (0.5) has the distinct advantage that the resulting algorithm does not require the computation of $f_n$ for any value of $n$. Our first algorithm is mathematically (though not computationally) equivalent to the

[3] Computation was performed on the CDC 3600 computer, which in floating point arithmetic allows precision of about 12 decimal digits.

backward recurrence algorithm of J. C. P. Miller. While this algorithm is widely regarded as just a "trick of the trade," our presentation will show that it derives naturally from rather elegant results of classical analysis. In §4 two alternate algorithms are described which are more flexible, but more elaborate, than the first algorithm. The remaining paragraphs discuss a number of applications, mostly to the computation of higher transcendental functions such as Bessel functions (§5), associated Legendre functions (§6), regular Coulomb wave functions (§7), and other miscellaneous functions (§§8–10). §11 contains an application to a Sturm-Liouville boundary value problem on an infinite interval.

The extent to which our algorithms are affected by rounding errors will not be discussed in detail. Our experience seems to indicate, however, that none of the algorithms is sensitive to rounding, unless the series (0.5) is subject to cancellation of terms. The rigorous analysis of error propagation is an interesting, though difficult, outstanding problem in this area. A significant contribution in this direction is due to Olver, who recently analyzed the error accumulation in Miller's algorithm [38].

In principle, there are other stable procedures that could be used to calculate minimal solutions of (0.1). For example, we could set up the boundary value problem of finding the solution $y_n$ of (0.1) which satisfies

$$y_0 = f_0\,, \qquad y_N = f_N$$

for some sufficiently large $N$.[4] Clearly, this amounts to solving the linear system of equations

$$\begin{pmatrix} a_1 & 1 & & & & & \\ b_2 & a_2 & 1 & & & 0 & \\ & b_3 & a_3 & 1 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & 0 & & & \cdot & a_{N-2} & 1 \\ & & & & & b_{N-1} & a_{N-1} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \cdot \\ \cdot \\ \cdot \\ y_{N-1} \end{pmatrix} = \begin{pmatrix} -b_1 f_0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ -f_N \end{pmatrix}, \tag{0.6}$$

whose matrix is tridiagonal. Any of the standard methods, such as triangular decomposition methods, may be used to solve (0.6). Unfortunately, the procedure requires two values, $f_0$ and $f_N$, of the desired solution to be known in advance. Either one may be difficult, or time-consuming, to obtain.

The problem of computing minimal solutions is clearly not peculiar to three-term recurrence relations. It may equally arise in connection with other functional equations, such as linear homogeneous difference and differential equations of arbitrary order, and systems of such equations. Whenever the space $S$ of all solutions is the direct sum $S = S_1 \oplus S_2$ of two subspaces $S_1$ and $S_2$, and every solution $s_1 \in S_1$ dominates, in some appropriate sense, over every solution $s_2 \in S_2$, we may consider $S_2$ as the set of minimal solutions with respect to

[4] The author is indebted to Dr. M. E. Rose for pointing this out.

the decomposition $S = S_1 \oplus S_2$. (There may be several such decompositions.) The problem of computing minimal solutions in this sense has not been thoroughly studied, though the work of Clenshaw [7] and Schäfke [51] suggests that effective computational methods may exist also in this more general context.

**1. Three-term recursion and continued fractions.** It is well-known that the concepts of three-term recursion and continued fraction are closely related. To every continued fraction we may in fact associate a three-term recurrence relation, namely the fundamental recurrence formula for the numerators and denominators. Vice versa, every three-term recurrence relation may be interpreted as the fundamental recurrence formula for some continued fraction. The first point of view is useful for computing continued fractions, the second for computing the minimal solution. We begin by considering several methods of calculating a continued fraction.

Suppose we are given the continued fraction

$$\frac{a_1}{b_1+}\,\frac{a_2}{b_2+}\,\frac{a_3}{b_3+}\cdots, \tag{1.1}$$

where the partial numerators $a_n$ and partial denominators $b_n$ are real or complex numbers. Denote its $n$th numerator and $n$th denominator by $A_n$ and $B_n$, respectively, so that

$$\frac{a_1}{b_1+}\,\frac{a_2}{b_2+}\cdots\frac{a_n}{b_n} = \frac{A_n}{B_n}. \tag{1.2}$$

The value of the continued fraction (1.1), if it exists, is defined as the limit $\lim_{n\to\infty} A_n/B_n$. The quantities $A_n$, $B_n$ satisfy the fundamental recurrence formulas (see, e.g., [59, p. 15])

$$\begin{aligned} A_n &= b_nA_{n-1} + a_nA_{n-2}, \\ B_n &= b_nB_{n-1} + a_nB_{n-2}, \end{aligned} \qquad n = 1, 2, 3, \cdots, \tag{1.3}$$

where

$$A_{-1} = 1, \quad A_0 = 0; \quad B_{-1} = 0, \quad B_0 = 1. \tag{1.4}$$

This shows that $\alpha_n = A_{n-1}$ and $\beta_n = B_{n-1}$ constitute a pair of linearly independent solutions of the three-term recurrence relation

$$y_{n+1} - b_ny_n - a_ny_{n-1} = 0, \qquad n = 1, 2, 3, \cdots. \tag{1.5}$$

A first method of computation flows directly from these fundamental recurrence relations. Thus, one generates the $A$'s and $B$'s recursively, by means of (1.3) and (1.4), and concurrently the ratios $A_n/B_n$, until the latter converge within the required tolerance. As $A_n$ and $B_n$ are likely to grow rapidly with $n$, some care must be exercised if this method is used on a digital computer. Initial scaling, and possibly repeated subsequent scaling, may be necessary to avoid overflow.

A second method, which avoids the necessity of scaling, consists in evaluating

the finite continued fraction in (1.2) "from tail to head." Thus, formally, we set

$$f_k^{(n)} = \frac{a_k}{b_k+}\,\frac{a_{k+1}}{b_{k+1}+}\,\cdots\,\frac{a_n}{b_n}, \qquad 1 \leqq k \leqq n, \tag{1.6}$$

and generate these quantities recursively by

$$f_k^{(n)} = \frac{a_k}{b_k + f_{k+1}^{(n)}}, \qquad k = n, n-1, \cdots, 1, \tag{1.7}$$

using as initial value

$$f_{n+1}^{(n)} = 0. \tag{1.8}$$

Then, $f_1^{(n)} = A_n/B_n$. To obtain the value of the continued fraction, the backward recursion (1.7) will have to be carried out repeatedly, with increasing values of $n$, until successive values of $f_1^{(n)}$ agree within the accuracy desired. While certainly an inconvenience, the repetitive nature of this process nevertheless provides some self-checking features not possessed by the previous method.

A third method of computation, finally, exploits the connection between continued fractions and infinite series, expressed by the relation

$$\frac{A_n}{B_n} = \sum_{k=1}^{n} \rho_1\rho_2\cdots\rho_k,$$

where

$$1 + \rho_{k+1} = \frac{1}{1 + (a_{k+1}/b_k b_{k+1})(1+\rho_k)}, \qquad k = 2, 3, \cdots, n-1,$$

$$\rho_1 = a_1/b_1, \qquad 1 + \rho_2 = \frac{1}{1 + (a_2/b_1 b_2)}.$$

(This result may be obtained from Theorem 2.1 and formula (2.6) in [59], by an appropriate equivalence transformation. See also [56]; the formula defining $\rho_k$ in this reference contains a typographical error.) Clearly, these relations can be modelled into a recursive algorithm to generate successive approximants of a continued fraction. Let, indeed,

$$u_1 = 1, \qquad u_k = 1 + \rho_k, \qquad k \geqq 2,$$

$$v_k = \rho_1\rho_2\cdots\rho_k, \qquad k \geqq 1,$$

$$w_k = \sum_{i=1}^{k} v_i, \qquad k \geqq 1,$$

so that $w_k = A_k/B_k$. Then

$$\begin{aligned} u_{k+1} &= \frac{1}{1 + \dfrac{a_{k+1}}{b_k b_{k+1}}\,u_k}, \\ v_{k+1} &= v_k(u_{k+1} - 1), \\ w_{k+1} &= w_k + v_{k+1}, \end{aligned} \qquad k = 1, 2, 3, \cdots, \tag{1.9}$$

the initial values being

$$u_1 = 1, \qquad v_1 = w_1 = \frac{a_1}{b_1}. \tag{1.10}$$

None of the disadvantages noted in the previous two methods are present here.

We have seen that the continued fraction (1.1) leads naturally to the three-term recursion (1.5). Suppose now, conversely, that we are given a three-term recurrence relation

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad b_n \neq 0,\ n = 1, 2, 3, \cdots. \tag{1.11}$$

Define $\alpha_n$, $\beta_n$ to be the special solutions of (1.11) with initial values

$$\alpha_0 = 1, \quad \alpha_1 = 0; \qquad \beta_0 = 0, \quad \beta_1 = 1. \tag{1.12}$$

Then, evidently, $A_n = \alpha_{n+1}$ and $B_n = \beta_{n+1}$ are the numerators and denominators, respectively, of the continued fraction

$$\frac{-b_1}{-a_1-}\ \frac{b_2}{-a_2-}\ \frac{b_3}{-a_3-}\ \cdots, \tag{1.13}$$

which is equivalent to the continued fraction

$$\frac{b_1}{a_1-}\ \frac{b_2}{a_2-}\ \frac{b_3}{a_3-}\ \cdots. \tag{1.14}$$

We may formally arrive at this continued fraction also in the following way. Let us introduce the ratios

$$r_n = \frac{y_{n+1}}{y_n}, \qquad n = 0, 1, 2, \cdots.$$

Dividing (1.11) by $y_n$ then gives

$$r_n + a_n + \frac{b_n}{r_{n-1}} = 0,$$

from which

$$r_{n-1} = \frac{-b_n}{a_n + r_n}.$$

Applying this formula repeatedly, with $n$ successively increasing, we get

$$r_{n-1} = \frac{y_n}{y_{n-1}} = \frac{-b_n}{a_n-}\ \frac{b_{n+1}}{a_{n+1}-}\ \frac{b_{n+2}}{a_{n+2}-}\ \cdots. \tag{1.15}$$

In particular, when $n = 1$,

$$\frac{y_1}{y_0} = \frac{-b_1}{a_1-}\ \frac{b_2}{a_2-}\ \frac{b_3}{a_3-}\ \cdots.$$

This derivation indicates that the continued fraction (1.14), and similarly

the continued fractions in (1.15), are related to ratios of consecutive values for some solution $y_n$. The argument, however, neither insures us of the convergence of these continued fractions, nor does it tell us for what particular solution the ratios are to be formed. These matters are clarified by the following theorem.

THEOREM 1.1 (Pincherle [45]). *The continued fraction* (1.14) *converges if and only if the recurrence relation* (1.11) *possesses a minimal solution* $f_n$, *with* $f_0 \neq 0$. *In case of convergence, moreover, one has*

$$\frac{f_n}{f_{n-1}} = \frac{-b_n}{a_n -} \frac{b_{n+1}}{a_{n+1} -} \frac{b_{n+2}}{a_{n+2} -} \cdots, \qquad n = 1, 2, 3, \cdots, \tag{1.16}$$

*provided* $f_n \neq 0$ *for* $n = 0, 1, 2, \cdots$.

*Proof.* (a) Assume the continued fraction in (1.14) converges. Then so does the equivalent continued fraction (1.13). Therefore

$$\lim_{n\to\infty} \frac{\alpha_n}{\beta_n} = c,$$

where $\alpha_n$, $\beta_n$ are the solutions of (1.11) defined by the initial values (1.12), and $c$ is some constant. Let

$$f_n = \alpha_n - c\beta_n . \tag{1.17}$$

Take any other solution of (1.11), say $y_n = a\alpha_n + b\beta_n$. Then $ac + b \neq 0$, and

$$\lim_{n\to\infty} \frac{f_n}{y_n} = \lim_{n\to\infty} \frac{\alpha_n - c\beta_n}{a\alpha_n + b\beta_n} = \lim_{n\to\infty} \frac{(\alpha_n/\beta_n) - c}{a(\alpha_n/\beta_n) + b} = 0.$$

This shows that the solution $f_n$ defined in (1.17) is a minimal solution of (1.11). Moreover, $f_0 = \alpha_0 \neq 0$.

(b) Assume now that (1.11) possesses a minimal solution, $f_n$ say, for which $f_0 \neq 0$. Then

$$f_n = f_0\alpha_n + f_1\beta_n , \qquad n \geqq 0.$$

We note that $\beta_n$ is not a constant multiple of $f_n$, since $f_0 \neq 0$. Therefore, $f_n$ being minimal,

$$\lim_{n\to\infty} \frac{f_n}{\beta_n} = f_0 \lim_{n\to\infty} \frac{\alpha_n}{\beta_n} + f_1 = 0,$$

and so

$$\lim_{n\to\infty} \frac{\alpha_n}{\beta_n} = -\frac{f_1}{f_0}.$$

This establishes convergence of the continued fraction (1.13), and thus of that in (1.14), and also proves (1.16) for $n = 1$.

To prove (1.16) for general $n > 1$, we need only observe that $z_m = f_{n+m-1}$, considered as a function of $m$, is a minimal solution of

$$z_{m+1} + a_{n+m-1}z_m + b_{n+m-1}z_{m-1} = 0, \qquad m = 1, 2, 3, \cdots .$$

Since by assumption, $z_0 = f_{n-1} \neq 0$, the portion of Theorem 1.1 already proved yields

$$\frac{z_1}{z_0} = \frac{f_n}{f_{n-1}} = \frac{-b_n}{a_n -} \frac{b_{n+1}}{a_{n+1} -} \frac{b_{n+2}}{a_{n+2} -} \cdots$$

as asserted. This completes the proof of Theorem1.1.

Consider again the three-term recurrence relation

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad b_n \neq 0, \tag{1.18}$$

but assume, for simplicity, that the coefficients $a_n$, $b_n$ are defined, and (1.18) holds, for all integers $n = 0, \pm 1, \pm 2, \cdots$. Let $\nu$ be an arbitrary integer, and let $\eta_n^{(\nu)}$ denote the solution of (1.18) having starting values

$$\eta_\nu^{(\nu)} = 1, \qquad \eta_{\nu+1}^{(\nu)} = 0 \tag{1.19}$$

at $n = \nu$ and $n = \nu + 1$, respectively. Then the following duality theorem holds.

THEOREM 1.2. *The function $\eta_n^{(\nu)}$ satisfies, for fixed $\nu$ and variable $n$, the three-term recurrence relation*

$$\eta_{n+1}^{(\nu)} + a_n \eta_n^{(\nu)} + b_n \eta_{n-1}^{(\nu)} = 0, \qquad n = 0, \pm 1, \pm 2, \cdots, \tag{1.20}$$

*and for fixed $n$ and variable $\nu$, the three-term recurrence relation*

$$\eta_n^{(\nu)} + \frac{a_\nu}{b_\nu} \eta_n^{(\nu-1)} + \frac{1}{b_{\nu-1}} \eta_n^{(\nu-2)} = 0, \qquad \nu = 0, \pm 1, \pm 2, \cdots. \tag{1.21}$$

*Proof.* The first part of the theorem follows from the definition of $\eta_n^{(\nu)}$. To prove the second part, we first observe that (1.21) holds true for $\nu = n - 1$, $n$, $n + 1$. For example, when $\nu = n$, using (1.19) and (1.20), we have

$$\begin{aligned} \eta_n^{(n)} + \frac{a_n}{b_n} \eta_n^{(n-1)} + \frac{1}{b_{n-1}} \eta_n^{(n-2)} &= 1 + \frac{1}{b_{n-1}} \left( -a_{n-1} \eta_{n-1}^{(n-2)} - b_{n-1} \eta_{n-2}^{(n-2)} \right) \\ &= 1 + 0 - 1 = 0. \end{aligned}$$

The verification for $\nu = n \pm 1$ is analogous. Assume now (1.21) to be true for all integers $n$, $\nu$ satisfying $|n - \nu| \leqq k$, where $k \geqq 1$ is some integer. We show that (1.21) then also holds for $|n - \nu| = k + 1$. We consider the two cases $n - \nu = k + 1$, $n - \nu = -(k + 1)$ separately. In the first case, we use (1.20) in the form

$$\eta_n^{(\nu)} = -a_{n-1} \eta_{n-1}^{(\nu)} - b_{n-1} \eta_{n-2}^{(\nu)},$$

and observe that (1.21) can be applied to both terms on the right, since $|n - 1 - \nu| = k$, and $|n - 2 - \nu| = k - 1 < k$. We obtain

$$\begin{aligned} \eta_n^{(\nu)} &= -a_{n-1} \left( -\frac{a_\nu}{b_\nu} \eta_{n-1}^{(\nu-1)} - \frac{1}{b_{\nu-1}} \eta_{n-1}^{(\nu-2)} \right) - b_{n-1} \left( -\frac{a_\nu}{b_\nu} \eta_{n-2}^{(\nu-1)} - \frac{1}{b_{\nu-1}} \eta_{n-2}^{(\nu-2)} \right) \\ &= -\frac{a_\nu}{b_\nu} \left( -a_{n-1} \eta_{n-1}^{(\nu-1)} - b_{n-1} \eta_{n-2}^{(\nu-1)} \right) - \frac{1}{b_{\nu-1}} \left( -a_{n-1} \eta_{n-1}^{(\nu-2)} - b_{n-1} \eta_{n-2}^{(\nu-2)} \right) \\ &= -\frac{a_\nu}{b_\nu} \eta_n^{(\nu-1)} - \frac{1}{b_{\nu-1}} \eta_n^{(\nu-2)}, \end{aligned}$$

having again used (1.20). The second case is verified similarly, using (1.20) in the form

$$\eta_n^{(\nu)} = -\frac{1}{b_{n+1}}\,(a_{n+1}\eta_{n+1}^{(\nu)} + \eta_{n+2}^{(\nu)}).$$

Since we already established (1.21) for $|\, n - \nu \,| \leqq 1$, it now follows by induction that the result holds for $|\, n - \nu \,| = k$, $k = 0, 1, 2, 3, \cdots$, that is, for all integers $n$, $\nu$. Theorem 1.2 is proved.

We note that relation (1.21), for $\nu > n$, can also be obtained from the known fact (cf. [43, vol. I, p. 3]) that $\eta_{n-1}^{(\nu)}$ and $\eta_n^{(\nu)}$ are the numerators and denominators, respectively, of the continued fraction

$$b'_{n-1} + \frac{a_n'}{b_n'+}\,\frac{a'_{n+1}}{b'_{n+1}+}\,\cdots\,\frac{a'_{\nu-1}}{b'_{\nu-1}},$$

where

$$b'_{m-1} = -\frac{a_m}{b_m}, \qquad a_m' = -\frac{1}{b_m}.$$

Alternatively, Theorem 1.2 may be obtained, as a special case, from the known result that "multipliers" of a linear difference equation satisfy the adjoint difference equation (cf. [35, §12.6]).

**2. Some results from the asymptotic theory of linear second order difference equations.** In applications of Theorem 1.1, it is in general easier to recognize a given solution of a three-term recurrence relation to be minimal than to establish convergence of the corresponding continued fraction. One is aided in this by classical results from the asymptotic theory of difference equations, notably by a theorem of Poincaré, and by refinements and extensions thereof due to Perron and Kreuser. For convenience of the reader, we are recalling here these theorems for the special case of a second-order difference equation

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots. \tag{2.1}$$

We assume, throughout, that

$$b_n \neq 0, \qquad n = 1, 2, 3, \cdots. \tag{2.2}$$

We begin with the case where the coefficients $a_n$ and $b_n$ in (2.1) have finite limits

$$a_n \to a, \qquad b_n \to b, \qquad n \to \infty, \tag{2.3}$$

not excluding that $b = 0$. One then calls (2.1) a *Poincaré difference equation*, and calls

$$\Phi(t) = t^2 + at + b \tag{2.4}$$

the *characteristic polynomial* of (2.1). As may be expected, the solutions of (2.1) behave similarly, for large $n$, to the solutions of the difference equation (2.1) with *constant* coefficients $a_n = a$, $b_n = b$. This is borne out by the following two theorems.

THEOREM 2.1 (Poincaré [46]). *If the characteristic polynomial* (2.4) *of* (2.1) *has zeros* $t_1$, $t_2$ *of distinct moduli,*

$$|t_1| > |t_2|, \tag{2.5}$$

*then for every nontrivial solution* $y_n$ *of* (2.1) *we have*

$$\lim_{n\to\infty} \frac{y_{n+1}}{y_n} = t_r, \qquad r = 1, \text{ or } r = 2. \tag{2.6}$$

THEOREM 2.2 (Perron [41]). *Under the assumption of Theorem* 2.1 *there exist two linearly independent solutions* $y_{n,1}$ *and* $y_{n,2}$ *of* (2.1) *such that*

$$\lim_{n\to\infty} \frac{y_{n+1,r}}{y_{n,r}} = t_r, \qquad r = 1, 2. \tag{2.7}$$

Theorem 2.2 implies that

$$f_n = y_{n,2}$$

is a minimal solution of (2.1). To see this, choose $\tau_1$ and $\tau_2$ such that

$$|t_2| < \tau_2 < \tau_1 < |t_1|,$$

which under the assumption (2.5) is certainly possible. By (2.7) we then have, for $n$ sufficiently large,

$$\left|\frac{y_{n+1,1}}{y_{n,1}}\right| \geqq \tau_1, \qquad \left|\frac{y_{n+1,2}}{y_{n,2}}\right| \leqq \tau_2, \qquad n \geqq n_0.$$

Hence

$$|y_{n,1}| \geqq \tau_1^{n-n_0} |y_{n_0,1}|, \qquad |y_{n,2}| \leqq \tau_2^{n-n_0} |y_{n_0,2}|,$$

and

$$\left|\frac{y_{n,2}}{y_{n,1}}\right| \leqq \left(\frac{\tau_2}{\tau_1}\right)^{n-n_0} \left|\frac{y_{n_0,2}}{y_{n_0,1}}\right|, \qquad n \geqq n_0.$$

This shows that

$$\lim_{n\to\infty} \frac{y_{n,2}}{y_{n,1}} = 0,$$

from which the assertion follows.

We also note that in (2.6) one has $r = 2$ for the minimal solution, and $r = 1$ for any other solution.

We shall require a generalization of Theorem 2.2 relating to a difference equation (2.1) whose coefficients satisfy

$$a_n \sim an^\alpha, \qquad b_n \sim bn^\beta, \qquad ab \neq 0; \quad \alpha, \beta \text{ real}; \quad n \to \infty. \tag{2.8}$$

The asymptotic structure of the solutions now depends on the *Newton-Puiseux* diagram formed with the points $P_0(0, 0)$, $P_1(1, \alpha)$, $P_2(2, \beta)$. This is the broken line $\overline{P_0P_1P_2}$, if $P_1$ is above the straight line joining $P_0$ with $P_2$; otherwise it

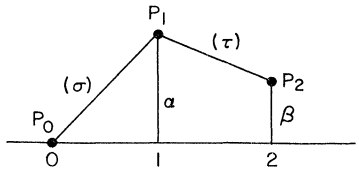


FIG. 1. *Newton-Puiseux diagram for difference equation* (2.1), (2.8)

is the line segment $\overline{P_0P_2}$. We denote by $\sigma$ the slope of $\overline{P_0P_1}$, and by $\tau$ the slope of $\overline{P_1P_2}$ (Fig. 1), so that $\sigma = \alpha$, $\tau = \beta - \alpha$.

THEOREM 2.3 (Perron [42], Kreuser [29]). (a) *If the point $P_1$ is above the line segment $\overline{P_0P_2}$ (i.e., $\sigma > \tau$), the difference equation* (2.1) *has two linearly independent solutions, $y_{n,1}$ and $y_{n,2}$, for which*

$$\frac{y_{n+1,1}}{y_{n,1}} \sim -an^{\sigma}, \qquad \frac{y_{n+1,2}}{y_{n,2}} \sim -\frac{b}{a}n^{\tau}, \qquad n \to \infty. \tag{2.9}$$

(b) *If the points $P_0$, $P_1$, $P_2$ are collinear (i.e., $\sigma = \tau = \alpha$), let $t_1$, $t_2$ be the roots of $t^2 + at + b = 0$, and $|t_1| \geqq |t_2|$. Then* (2.1) *has two linearly independent solutions, $y_{n,1}$ and $y_{n,2}$, such that*

$$\frac{y_{n+1,1}}{y_{n,1}} \sim t_1 n^{\alpha}, \qquad \frac{y_{n+1,2}}{y_{n,2}} \sim t_2 n^{\alpha}, \qquad n \to \infty, \tag{2.10}$$

*provided $|t_1| > |t_2|$. If $|t_1| = |t_2|$ (in particular, if $t_1$, $t_2$ are complex conjugates) then*

$$\limsup_{n\to\infty} \left[\frac{|y_n|}{(n!)^{\alpha}}\right]^{1/n} = |t_1| \tag{2.11}$$

*for all nontrivial solutions of* (2.1).

(c) *If the point $P_1$ lies below the line segment $\overline{P_0P_2}$ then*

$$\limsup_{n\to\infty} \left[\frac{|y_n|}{(n!)^{\beta/2}}\right]^{1/n} = \sqrt{|b|} \tag{2.12}$$

*for all nontrivial solutions of* (2.1).

An argument similar to the one following Theorem 2.2 will show that in both case (a) and the first part of case (b) the solution $f_n = y_{n,2}$ is a minimal solution of (2.1). Furthermore, in the first part of case (b),

$$\lim_{n\to\infty} \frac{y_{n+1}}{n^{\alpha}y_n} = t_r, \qquad r = 1, \text{ or } r = 2, \tag{2.13}$$

where $r = 2$ for the minimal solution, and $r = 1$ for any other solution.

The second part of (b), and part (c) of Theorem 2.3 are somewhat inconclusive for our purposes, as they do not permit distinguishing two solutions with distinct asymptotic properties. In this connection, the example given later in §9 is of interest.

Proofs of Poincaré's theorem may be found, e.g., in [21], [35], [37]. An elegant

proof of Perron's theorem is given in [14], and reproduced in [34]. Far-reaching generalizations, and simplified proofs, of all these theorems, including Kreuser's theorem, were recently obtained in [51].

**3. A first algorithm for computing the minimal solution.** We assume now that the recurrence relation

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots, \tag{3.1}$$

has a nonvanishing[5] minimal solution, $f_n$. We wish to calculate $f_n$ for $n = 0, 1, 2, \cdots, N$. In order to specify $f_n$ uniquely, we can impose *one* condition, for example prescribe the value of $f_0$. For later applications, we consider the more general normalization

$$\sum_{m=0}^{\infty} \lambda_m f_m = s, \qquad s \neq 0, \tag{3.2}$$

where $s$ and $\lambda_0, \lambda_1, \cdots$ are given quantities, and the series is known to converge. We do not exclude that $\lambda_m = 0$ for all $m > 0$, in which case (3.2) amounts to prescribing $f_0$.

In a sense, (3.2) represents the most general linear condition that may be imposed. A class of nonlinear conditions will also be considered briefly.

To introduce the algorithm, let

$$r_n = \frac{f_{n+1}}{f_n}, \qquad s_n = \frac{1}{f_n} \sum_{m=n+1}^{\infty} \lambda_m f_m. \tag{3.3}$$

Suppose first that $r_n$, $s_n$ are known for some value $n = \nu \geqq N$. The desired solution $f_n$, $n = 0(1)N$, can then be obtained as follows.

From Theorem 1.1 we know that

$$r_{n-1} = \frac{-b_n}{a_n -} \frac{b_{n+1}}{a_{n+1} -} \frac{b_{n+2}}{a_{n+2} -} \cdots, \qquad n = 1, 2, 3, \cdots. \tag{3.4}$$

Hence, we can generate the ratios $r_n$ for $0 \leqq n < \nu$ as in (1.6)–(1.8) by

$$r_{n-1} = \frac{-b_n}{a_n + r_n}, \qquad n = \nu, \nu - 1, \cdots, 1. \tag{3.5}$$

Similarly, we have

$$\begin{aligned} s_{n-1} &= \frac{1}{f_{n-1}} \sum_{m=n}^{\infty} \lambda_m f_m = \frac{1}{f_{n-1}} \left( \lambda_n f_n + \sum_{m=n+1}^{\infty} \lambda_m f_m \right) \\ &= \lambda_n r_{n-1} + r_{n-1} \left( \frac{1}{f_n} \sum_{m=n+1}^{\infty} \lambda_m f_m \right), \end{aligned}$$

so that

$$s_{n-1} = r_{n-1}(\lambda_n + s_n), \qquad n = \nu, \nu - 1, \cdots, 1. \tag{3.6}$$

Hence, also the quantities $s_n$ for $0 \leqq n < \nu$, and thus in particular $s_0$, can be ob-

[5] The assumption of $f_n$ to be nonvanishing is no serious restriction from the practical point of view. This is further discussed at the end of this paragraph.

tained recursively. Using (3.2) we now have

$$s_0 = \frac{1}{f_0}\sum_{m=1}^{\infty}\lambda_m f_m = \frac{1}{f_0}(s - \lambda_0 f_0),$$

and so

$$f_0 = \frac{s}{\lambda_0 + s_0}.$$

This gives us the initial value of the desired solution. The remaining values can now be obtained immediately from

$$f_n = r_{n-1}f_{n-1}, \qquad n = 1, 2, \cdots, N.$$

The actual algorithm follows this procedure very closely, except that for the infinite continued fraction, and the infinite series, representing $r_{n-1}$ and $s_n$, respectively, we now substitute truncated continued fractions, and truncated series. More precisely, we define

$$r_\nu^{(\nu)} = 0, \qquad r_{n-1}^{(\nu)} = \frac{-b_n}{a_n -}\,\frac{b_{n+1}}{a_{n+1} -}\,\cdots\,\frac{b_\nu}{a_\nu}, \qquad 1 \leqq n \leqq \nu, \tag{3.7}$$

and

$$s_\nu^{(\nu)} = 0, \qquad s_n^{(\nu)} = \sum_{m=n+1}^{\nu}\lambda_m r_n^{(\nu)} r_{n+1}^{(\nu)}\cdots r_{m-1}^{(\nu)}, \qquad 0 \leqq n < \nu. \tag{3.8}$$

One then verifies readily that the formulas (3.5), (3.6) continue to hold if $r_n$ is replaced by $r_n^{(\nu)}$, and $s_n$ by $s_n^{(\nu)}$ throughout. Hence the following set of recursions arises naturally,

$$\begin{aligned} &r_\nu^{(\nu)} = 0, \qquad r_{n-1}^{(\nu)} = \frac{-b_n}{a_n + r_n^{(\nu)}}, \\ &s_\nu^{(\nu)} = 0, \qquad s_{n-1}^{(\nu)} = r_{n-1}^{(\nu)}(\lambda_n + s_n^{(\nu)}), \end{aligned} \qquad n = \nu, \nu - 1, \cdots, 1, \tag{3.9}$$

$$f_0^{(\nu)} = \frac{s}{\lambda_0 + s_0^{(\nu)}}, \qquad f_n^{(\nu)} = r_{n-1}^{(\nu)} f_{n-1}^{(\nu)}, \qquad n = 1, 2, \cdots, N.$$

While our initial procedure gave us the exact values $f_n$ of the minimal solution, the quantities $f_n^{(\nu)}$ now derived are at best approximations to $f_n$. It remains to successively improve $f_n^{(\nu)}$ by repeating (3.9) for a sequence of increasing values of $\nu$. The complete algorithm for computing the minimal solution may thus be defined as follows:

Step 1: Select an integer $\nu \geqq N$, and let $\phi_n^{(\nu)} = 0$, $n = 0, 1, \cdots, N$.

Step 2: Calculate $f_n^{(\nu)}$, $n = 0, 1, \cdots, N$, according to the formulas in (3.9).

Step 3: If the $N + 1$ values of $f_n^{(\nu)}$ obtained in Step 2 do not agree with the current values of $\phi_n^{(\nu)}$ to within the desired accuracy, then redefine $\phi_n^{(\nu)}$ by $\phi_n^{(\nu)} = f_n^{(\nu)}$, $n = 0, 1, \cdots, N$, increase $\nu$ by some fixed integer, say 5, and repeat Step 2; otherwise accept $f_n^{(\nu)}$ as the final approximations to $f_n$, $n = 0, 1, \cdots, N$.

We note that in the special case $\lambda_0 = 1, \lambda_1 = \lambda_2 = \cdots = 0$, all $s_n^{(\nu)}$ vanish, so that the recursion for $s_{n-1}^{(\nu)}$ in (3.9) may be omitted. Moreover, $s = f_0$, and there-

fore $f_0^{(\nu)} = f_0$. In this case, the value of $f_0$ must be known before the algorithm (3.9) can be applied. The use of an infinite series (3.2), instead, has the remarkable advantage of not requiring any value of $f_n$ to be known in advance.

Our derivation of (3.9) also demonstrates that $f_n^{(\nu)} = f_n$ if instead of zero initial values in the first two recursions we select initial values $r_\nu^{(\nu)} = r_\nu$, $s_\nu^{(\nu)} = s_\nu$. While these quantities in general are not known beforehand, they may sometimes be approximated closely when $\nu$ is large. This suggests to modify (3.9) by defining

$$r_\nu^{(\nu)} = \rho_\nu, \qquad s_\nu^{(\nu)} = \sigma_\nu, \tag{3.10}$$

where $\rho_\nu$ and $\sigma_\nu$ are suitable approximations to $r_\nu$ and $s_\nu$, respectively. The better these approximations are, the faster we expect our algorithm to converge. We return to this point later.

We may give (3.9) a somewhat different interpretation as follows. Consider the solution $\eta_n^{(\nu)}$ of the difference equation (3.1), defined by "initial" values

$$\eta_\nu^{(\nu)} = 1, \qquad \eta_{\nu+1}^{(\nu)} = 0 \tag{3.11}$$

at $n = \nu$ and $n = \nu + 1$, respectively. The values of $\eta_n^{(\nu)}$ for $0 \leqq n \leqq \nu$ may be obtained by applying (3.1) in the backward direction, starting at $n = \nu$. Then we assert that

$$f_n^{(\nu)} = \frac{s}{\sum_{m=0}^{\nu} \lambda_m \eta_m^{(\nu)}} \eta_n^{(\nu)}, \qquad 0 \leqq n \leqq N. \tag{3.12}$$

To verify this, we observe, first of all, that the quantities $r_{n-1}^{(\nu)}$ defined in (3.7) are consecutive ratios of the solution $\eta_n^{(\nu)}$,

$$r_{n-1}^{(\nu)} = \frac{\eta_n^{(\nu)}}{\eta_{n-1}^{(\nu)}}, \qquad 1 \leqq n \leqq \nu + 1. \tag{3.13}$$

This is trivial for $n = \nu + 1$, and for $n \leqq \nu$ follows from the fact that the ratio $\eta_n^{(\nu)}/\eta_{n-1}^{(\nu)}$ satisfies the same nonlinear recursion (3.5) satisfied by $r_{n-1}^{(\nu)}$. Inserting (3.13) into (3.8), we find

$$s_n^{(\nu)} = \frac{1}{\eta_n^{(\nu)}} \sum_{m=n+1}^{\nu} \lambda_m \eta_m^{(\nu)},$$

and using this for $n = 0$, we obtain

$$f_0^{(\nu)} = \frac{s}{\lambda_0 + s_0^{(\nu)}} = \frac{s\eta_0^{(\nu)}}{\lambda_0 \eta_0^{(\nu)} + \eta_0^{(\nu)} s_0^{(\nu)}} = \frac{s}{\lambda_0 \eta_0^{(\nu)} + \sum_{m=1}^{\nu} \lambda_m \eta_m^{(\nu)}} \eta_0^{(\nu)}.$$

This proves our assertion (3.12) for $n = 0$. To prove it for $n > 0$, we need only observe that in view of (3.13), the quantities $f_n^{(\nu)}$ in (3.12) satisfy $f_n^{(\nu)}/f_{n-1}^{(\nu)} = r_{n-1}^{(\nu)}$, as required by (3.9).

The algorithm of generating the $\eta_n^{(\nu)}$ and using (3.12) is often referred to as *Miller's backward recurrence algorithm*. It was first proposed as a computational scheme by J. C. P. Miller in connection with the tabulation of Bessel functions (see [5, p. xvii]). An error analysis has recently been given by Olver [38].

While algorithm (3.9) and Miller's algorithm are mathematically equivalent, they have different computational characteristics. In many cases, e.g., the quantities $\eta_n^{(\nu)}$ grow rapidly as $\nu$ increases, and may cause "overflow" on a digital computer. In contrast to this, the quantity $r_n^{(\nu)}$ in (3.9) converges to a finite limit as $\nu \to \infty$, and so does $s_n^{(\nu)}$ if the algorithm converges at all.

We now use (3.12) to discuss convergence as $\nu \to \infty$ of the algorithm (3.9). Let $g_n$ denote any solution of the difference equation (3.1) other than $f_n$, so that

$$\lim_{n\to\infty} \frac{f_n}{g_n} = 0. \tag{3.14}$$

Clearly,

$$\eta_n^{(\nu)} = a^{(\nu)} f_n + b^{(\nu)} g_n ,$$

for some constants $a^{(\nu)}$, $b^{(\nu)}$. By (3.11), we must have

$$a^{(\nu)} f_{\nu+1} + b^{(\nu)} g_{\nu+1} = 0,$$
$$a^{(\nu)} f_\nu + b^{(\nu)} g_\nu = 1.$$

The first of these relations gives $b^{(\nu)} = -(f_{\nu+1}/g_{\nu+1})a^{(\nu)}$, so that

$$\eta_n^{(\nu)} = a^{(\nu)} \left( f_n - \frac{f_{\nu+1}}{g_{\nu+1}} g_n \right).$$

Substituting in (3.12), and simplifying, we obtain

$$f_n^{(\nu)} = \frac{f_n \left( 1 - \dfrac{f_{\nu+1}}{g_{\nu+1}} \dfrac{g_n}{f_n} \right)}{1 - \dfrac{1}{s} \displaystyle\sum_{m=\nu+1}^{\infty} \lambda_m f_m - \frac{f_{\nu+1}}{s g_{\nu+1}} \sum_{m=0}^{\nu} \lambda_m g_m} . \tag{3.15}$$

In view of (3.14) and the convergence of the infinite series in (3.2), it is clear that $\lim_{\nu\to\infty} f_n^{(\nu)} = f_n$ if and only if

$$\lim_{\nu\to\infty} \frac{f_{\nu+1}}{g_{\nu+1}} \sum_{m=0}^{\nu} \lambda_m g_m = 0. \tag{3.16}$$

We have proved the following theorem.

THEOREM 3.1. *Suppose the recurrence relation* (3.1) *has a nonvanishing minimal solution,* $f_n$, *for which* (3.2) *holds. Let* $g_n$ *be any other solution of* (3.1). *Then the algorithm* (3.9) *converges in the sense*

$$\lim_{\nu\to\infty} f_n^{(\nu)} = f_n$$

*if and only if* (3.16) *is satisfied.*

Condition (3.16) holds, e.g., if the $\lambda$'s are uniformly bounded, and

$$\frac{g_{\nu+1}}{g_\nu} \to t_1, \qquad \frac{f_{\nu+1}}{f_\nu} \to t_2, \qquad \nu \to \infty,$$
$$|t_1| > |t_2|, \qquad |t_2| < 1.$$

If all but a finite number of the $\lambda$'s are zero, then (3.16) is a consequence of (3.14). Theorem 3.1, in this case, has been noted previously in [16].

It is useful to observe that convergence of the algorithm (3.9), in the sense of Theorem 3.1, implies that

$$r_n^{(\nu)} \to r_n\,, \qquad s_n^{(\nu)} \to s_n\,, \qquad \nu \to \infty\,, \tag{3.17}$$

where $r_n$, $s_n$ are the quantities defined in (3.3). The first of these relations follows directly from (3.4) and (3.7). The second follows by induction on $n$. Indeed, if $n = 0$, we have from the third line in (3.9),

$$s_0^{(\nu)} = \frac{s - \lambda_0 f_0^{(\nu)}}{f_0^{(\nu)}} \to \frac{s - \lambda_0 f_0}{f_0} = s_0\,, \qquad \nu \to \infty.$$

Assuming now $s_{n-1}^{(\nu)} \to s_{n-1}$, we get from the second line in (3.9), and from (3.6), that

$$s_n^{(\nu)} = \frac{s_{n-1}^{(\nu)}}{r_{n-1}^{(\nu)}} - \lambda_n \to \frac{s_{n-1}}{r_{n-1}} - \lambda_n = s_n\,, \qquad \nu \to \infty.$$

In case of convergence of the algorithm (3.9), we may obtain from (3.15) the following approximate expression for the relative error, valid for $\nu$ sufficiently large,

$$\frac{f_n^{(\nu)} - f_n}{f_n} \doteq \frac{1}{s}\sum_{m=\nu+1}^{\infty} \lambda_m f_m + \frac{f_{\nu+1}}{s g_{\nu+1}} \sum_{m=0}^{\nu} \lambda_m g_m - \frac{f_{\nu+1}}{g_{\nu+1}} \frac{g_n}{f_n}. \tag{3.18}$$

It is interesting to examine what effect the modification (3.10) of algorithm (3.9) will have upon the relative error (3.18). We assume that

$$\rho_\nu = r_\nu(1 + \epsilon_\nu), \qquad \sigma_\nu = s_\nu(1 + \eta_\nu),$$

where $r_\nu$, $s_\nu$ are defined by (3.3), and $\epsilon_\nu$, $\eta_\nu$ are small numbers. Then a simple computation will show that in place of (3.15) we now have

$$f_n^{(\nu)} = f_n \frac{1 + \epsilon_\nu \dfrac{f_{\nu+1}}{g_{\nu+1}} \dfrac{g_n}{f_n} \left(1 - \rho_\nu \dfrac{g_\nu}{g_{\nu+1}}\right)^{-1}}{1 + \dfrac{\eta_\nu}{s} \displaystyle\sum_{m=\nu+1}^{\infty} \lambda_m f_m + \dfrac{\epsilon_\nu f_{\nu+1}}{s g_{\nu+1}} \left(1 - \rho_\nu \dfrac{g_\nu}{g_{\nu+1}}\right)^{-1} \sum_{m=0}^{\nu} \lambda_m g_m}\,.$$

Since $|\, \rho_\nu g_\nu / g_{\nu+1} \,|$ is usually substantially smaller than 1 (at least for large $\nu$) we see that the modification (3.10) reduces the relative error of $f_n^{(\nu)}$ effectively by a factor of $|\, \epsilon_\nu \,|$, or $|\, \eta_\nu \,|$, whichever is larger. Hence, our statement made earlier that the convergence of $f_n^{(\nu)}$ to $f_n$ is faster the better $\rho_\nu$ approximates $r_\nu$, and $\sigma_\nu$ approximates $s_\nu$, is clearly vindicated.

It is tempting to try a substitution of the type

$$F_n = c_n f_n\,, \qquad c_n \neq 0, \tag{3.19}$$

to exert influence upon the convergence criteria (3.14) and (3.16). We note, however, that *these criteria are invariant with respect to any linear substitution of the form* (3.19).

We now briefly consider the case in which condition (3.2) is replaced by a nonlinear condition of the form

$$\sum_{m=0}^{\infty} \lambda_m {f_m}^p = s, \qquad s \neq 0, \tag{3.2p}$$

where $p$ is some real number. It must be noted that this condition specifies the minimal solution only to within a constant factor $c$ satisfying $c^p = 1$.

Algorithm (3.9) extends readily to the case of general $p$, if we define $r_{n-1}^{(\nu)}$ as before, and let

$$s_\nu^{(\nu)} = 0, \qquad s_n^{(\nu)} = \sum_{m=n+1}^{\nu} \lambda_m [r_n^{(\nu)} r_{n+1}^{(\nu)} \cdots r_{m-1}^{(\nu)}]^p, \qquad 0 \leqq n < \nu.$$

We obtain

$$\begin{aligned} &r_\nu^{(\nu)} = 0, \qquad r_{n-1}^{(\nu)} = \frac{-b_n}{a_n + r_n^{(\nu)}}, && n = \nu, \nu - 1, \cdots, 1, \\ &s_\nu^{(\nu)} = 0, \qquad s_{n-1}^{(\nu)} = [r_{n-1}^{(\nu)}]^p (\lambda_n + s_n^{(\nu)}), && \\ &f_0^{(\nu)} = \left[\frac{s}{1 + s_0^{(\nu)}}\right]^{1/p}, \qquad f_n^{(\nu)} = r_{n-1}^{(\nu)} f_{n-1}^{(\nu)}, && n = 1, 2, \cdots, N. \end{aligned} \tag{3.9p}$$

The nonuniqueness of $f_n$ is reflected in the multivalued definition of $f_0^{(\nu)}$.

As in the proof of Theorem 3.1, one shows that (3.9$p$) converges as $\nu \to \infty$ if

$$\lim_{\nu \to \infty} h_\nu^{(i)} = 0, \qquad i = 1, 2, \cdots, p,$$

where

$$h_\nu^{(i)} = \left(\frac{f_{\nu+1}}{g_{\nu+1}}\right)^i \sum_{m=0}^{\nu} \lambda_m g_m {}^i {f_m}^{p-i}.$$

We conclude this paragraph with some practical remarks concerning the algorithm (3.9).

The effectiveness of the algorithm is clearly enhanced if good estimates of the initial value of $\nu$ are available. Such estimates can sometimes be obtained from (3.18), and from known asymptotic properties of the solutions $f_n$ and $g_n$. (See §§5, 7 for examples.)

It is worth noting that the storage requirements on a digital computer do not depend on $\nu$. It suffices to store permanently only those $N$ quantities $r_n^{(\nu)}$ which are needed to build up the final results $f_n^{(\nu)}$. All the other $r_n^{(\nu)}$, as well as the $s_n^{(\nu)}$, can be generated in temporary storage cells.

The assumption

$$f_{n-1} \neq 0, \qquad n = 1, 2, 3, \cdots,$$

in Theorem 3.1 is ordinarily fulfilled in practice, if for no other reason than rounding errors. Nevertheless, one might think, in view of $\lim_{\nu \to \infty} r_{n-1}^{(\nu)} = f_n / f_{n-1}$, that the case of $f_{n-1}$ nearly equal to zero for some $n \geqq 1$ might cause numerical diffi-

culties. By the following, admittedly superficial, considerations we wish to show that the presence, or proximity, of such zeros need be of no great concern.

Suppose, indeed, that $f_{n-1}$ is very small in modulus, compared to $f_n$. For definiteness, let $n > 1$. Then, by (3.3), $|\, r_{n-1} \,|$ is very large, and so is $|\, r_{n-1}^{(\nu)} \,|$, when $\nu$ is sufficiently large. From the first line in (3.9) it follows that $|\, a_n + r_n^{(\nu)} |$ must be very small compared to $|\, b_n \,|$. Since neither $a_n$ nor $r_n^{(\nu)}$ will normally be small, this means that many digits will cancel when the sum $a_n + r_n^{(\nu)}$ is formed, and so $r_{n-1}^{(\nu)}$ is not only very large, but also very inaccurate in terms of significant digits. Consequently, $r_{n-2}^{(\nu)}$ will be very small, and also inaccurate. However, $r_{n-3}^{(\nu)} = -b_{n-2}/(a_{n-2} + r_{n-2}^{(\nu)})$ (if $n > 2$) will again be accurate, since $a_{n-2}$ in the denominator picks up lost accuracy, $r_{n-2}^{(\nu)}$ being normally much smaller than $a_{n-2}$. Later on, in the formation of the final results, $f_{n-1}^{(\nu)} = r_{n-2}^{(\nu)} f_{n-2}^{(\nu)}$ will come out very small and inaccurate, as one must expect. The really questionable point is the computation of $f_n^{(\nu)} = r_{n-1}^{(\nu)} f_{n-1}^{(\nu)}$, since $r_{n-1}^{(\nu)}$ is large and $f_{n-1}^{(\nu)}$ is small, and both are inaccurate. We note, however, that

$$f_n^{(\nu)} = r_{n-1}^{(\nu)} r_{n-2}^{(\nu)} f_{n-2}^{(\nu)} = r_{n-1}^{(\nu)} \frac{-b_{n-1} f_{n-2}^{(\nu)}}{a_{n-1} + r_{n-1}^{(\nu)}} = \frac{-b_{n-1} f_{n-2}^{(\nu)}}{1 + (a_{n-1}/r_{n-1}^{(\nu)})},$$

which shows that the largeness of $r_{n-1}^{(\nu)}$ saves $f_n^{(\nu)}$ from becoming inaccurate, even though $r_{n-1}^{(\nu)}$ is. A similar reasoning applies to $s_{n-1}^{(\nu)}$, $s_{n-2}^{(\nu)}$.

More serious is a possible loss of accuracy in the calculation of $f_0^{(\nu)}$, as this would affect all subsequent $f_n^{(\nu)}$. It could indeed occur that $|\, \lambda_0 + s_0^{(\nu)} |$ is small in comparison with $|\, \lambda_0 \,|$, so that many digits cancel when $\lambda_0 + s_0^{(\nu)}$ is formed. The resulting value of $f_0^{(\nu)}$ would then be quite inaccurate. The same difficulty might arise if $\lambda_0 = 0$. Suppose, indeed, that $\lambda_p$ $(p > 0)$ is the first nonvanishing coefficient in the series (3.2),

$$\lambda_p \neq 0, \qquad \lambda_m = 0, \qquad 0 \leqq m < p,$$

and that $|\lambda_p + s_p^{(\nu)}|$ happens to be very small compared to $|\, \lambda_p \,|$. Then $s_{p-1}^{(\nu)}$ is necessarily inaccurate, and this inaccuracy will be transmitted to all subsequent $s_{n-1}^{(\nu)}$, and finally to $f_0^{(\nu)}$, in view of the relations $s_{n-1}^{(\nu)} = r_{n-1}^{(\nu)} s_n^{(\nu)}$, $n = p - 1$, $p - 2, \cdots, 1$, and $f_0^{(\nu)} = s/s_0^{(\nu)}$.

Now for large $\nu$, and $p \geqq 0$, we have

$$\lambda_p + s_p^{(\nu)} \doteq \lambda_p + \frac{1}{f_p} \sum_{m=p+1}^{\infty} \lambda_m f_m = \lambda_p + \frac{1}{f_p} (s - \lambda_p f_p) = \frac{s}{f_p},$$

so that $|(\lambda_p + s_p^{(\nu)})/\lambda_p \,|$ is small if $|\, s/(\lambda_p f_p) |$ is small. Hence, *dangerous cancellation occurs when s is small in absolute value compared to the first nonvanishing term* $\lambda_p f_p$ *in* (3.2), i.e., when cancellation occurs in the series (3.2) itself. For this reason, some care must be exercised in the selection of the identity (3.2).

**4. Second and third algorithm for computing the minimal solution.** The effectiveness of our first algorithm (3.9) is somewhat limited if no reasonable estimate of the starting value $\nu$ of $n$ is known a priori. The recursions in (3.9) must then be repeated with increasing values of $\nu$, until sufficient agreement is obtained between successive results $f_n^{(\nu)}$, for all $n = 0, 1, \cdots, N$. This disadvantage can

be removed, at the expense of a more complex algorithm, by making use of the duality theorem 1.2, or, alternatively, by evaluating a sequence of continued fractions (3.4). The corresponding algorithms will now be developed. The first of these, though not in the form given here, is due to Shintani [52].

As was noted in the previous paragraph, we can obtain $r_n$ , $s_n$ recursively, for $0 \leqq n < N$, and hence also $f_n$ for $0 \leqq n \leqq N$, once $r_N$ , $s_N$ are known. In the following we derive a method for calculating $r_N$ , $s_N$ recursively. If $f_0$ is known, the $s_n$ will not be required, and the algorithm then reduces to one suggested by G. Blanch ([4, p. 405 ff]) in connection with Bessel functions.

As for $r_N$ , we may simply evaluate the continued fraction

$$r_N = \frac{-b_{N+1}}{a_{N+1}-} \frac{b_{N+2}}{a_{N+2}-} \frac{b_{N+3}}{a_{N+3}-} \cdots, \tag{4.1}$$

by either the first, or third method described in §1. In the first case we have

$$r_N = \lim_{k\to\infty} \frac{A_k}{B_k}, \tag{4.2}$$

where

$$\begin{aligned} A_{-1} &= 1, \quad A_0 = 0; \quad B_{-1} = 0, \quad B_0 = 1; \\ A_k &= a_{N+k}A_{k-1} - b_{N+k}A_{k-2}, \\ B_k &= a_{N+k}B_{k-1} - b_{N+k}B_{k-2}, \end{aligned} \qquad k = 1, 2, 3, \cdots. \tag{4.3}$$

In the second case we have

$$r_N = \lim_{k\to\infty} w_k, \tag{4.4}$$

where the $w$'s are generated as follows:

$$\begin{aligned} u_1 &= 1, \quad v_1 = w_1 = -\frac{b_{N+1}}{a_{N+1}}, \\ u_{k+1} &= \frac{1}{1 - (b_{N+k+1}/a_{N+k}a_{N+k+1})u_k}, \\ v_{k+1} &= v_k(u_{k+1} - 1), \\ w_{k+1} &= w_k + v_{k+1}, \end{aligned} \qquad k = 1, 2, 3, \cdots. \tag{4.5}$$

For the computation of $s_N$ , we make use of the fact that

$$s_N = \lim_{\nu\to\infty} s_N^{(\nu)}, \tag{4.6}$$

where $s_N^{(\nu)}$ is defined by (3.8). The quantities $s_N^{(\nu)}$, $\nu \geqq N$, may be obtained recursively as follows. From the definition (3.8) of $s_n^{(\nu)}$, and from (3.13), we note that

$$\eta_N^{(\nu)} s_N^{(\nu)} = \sum_{m=N+1}^{\nu} \lambda_m \eta_m^{(\nu)}. \tag{4.7}$$

Hence, using (1.21), we can write

$$\eta_N^{(\nu)} s_N^{(\nu)} = \sum_{m=N+1}^{\nu} \lambda_m \left[ -\frac{a_\nu}{b_\nu} \eta_m^{(\nu-1)} - \frac{1}{b_{\nu-1}} \eta_m^{(\nu-2)} \right]$$

$$= -\frac{a_\nu}{b_\nu} (\eta_N^{(\nu-1)} s_N^{(\nu-1)} + \lambda_\nu \eta_\nu^{(\nu-1)})$$

$$- \frac{1}{b_{\nu-1}} (\eta_N^{(\nu-2)} s_N^{(\nu-2)} + \lambda_{\nu-1} \eta_{\nu-1}^{(\nu-2)} + \lambda \eta^{(\cdot\cdot)})$$

Since

$$\eta_\nu^{(\nu-1)} = \eta_{\nu-1}^{(\nu-2)} = 0,$$

$$\eta_\nu^{(\nu-2)} = -a_{\nu-1}\eta_{\nu-1}^{(\nu-2)} - b_{\nu-1}\eta_{\nu-2}^{(\nu-2)} = -b_{\nu-1},$$

we get

$$\eta_N^{(\nu)} s_N^{(\nu)} = -\frac{a_\nu}{b_\nu} \eta_N^{(\nu-1)} s_N^{(\nu-1)} - \frac{1}{b_{\nu-1}} \eta_N^{(\nu-2)} s_N^{(\nu-2)} + \lambda_\nu, \tag{4.8}$$

or, alternatively,

$$s_N^{(\nu)} = -\rho_N^{(\nu-1)} \left[ \frac{a_\nu}{b_\nu} s_N^{(\nu-1)} + \frac{1}{b_{\nu-1}} \rho_N^{(\nu-2)} s_N^{(\nu-2)} \right] + \frac{\lambda_\nu}{\eta_N^{(\nu)}},$$

where we have set $\rho_N^{(\nu)} = \eta_N^{(\nu)}/\eta_N^{(\nu+1)}$. Taking into account the recursive relations for $\rho_N^{(\nu)}$, $\eta_N^{(\nu)}$, which follow from (1.21), we arrive at the following algorithm for generating $s_N^{(\nu)}$:

$$\rho_N^{(N-1)} = 0, \qquad \eta_N^{(N)} = 1, \qquad \eta_N^{(N-1)} = 0,$$

$$s_N^{(N)} = s_N^{(N-1)} = 0,$$

$$\rho_N^{(\nu-1)} = -\frac{1}{\dfrac{a_\nu}{b_\nu} + \dfrac{1}{b_{\nu-1}} \rho_N^{(\nu-2)}}$$

$$\eta_N^{(\nu)} = -\frac{a_\nu}{b_\nu} \eta_N^{(\nu-1)} - \frac{1}{b_{\nu-1}} \eta_N^{(\nu-2)} \qquad \nu = N+1, N+2, \cdots. \tag{4.9}$$

$$s_N^{(\nu)} = -\rho_N^{(\nu-1)} \left[ \frac{a_\nu}{b_\nu} s_N^{(\nu-1)} + \frac{\rho_N^{(\nu-2)}}{b_{\nu-1}} s_N^{(\nu-2)} \right] + \frac{\lambda_\nu}{\eta_N^{(\nu)}}$$

This, together with (4.2) [or (4.4)] and the remarks at the beginning of this paragraph constitutes our second algorithm for computing the minimal solution of (3.1).

As noted previously, the quantities $\eta_N^{(\nu)}$ may grow rapidly, as $\nu$ increases, and may cause overflow on a computer. However, if $\eta_N^{(\nu)}$ is large, just short of overflowing, it is normally permissible to replace the term $\lambda_\nu/\eta_N^{(\nu)}$ in the last relation of (4.9) by zero, and to continue the recursion for $s_N^{(\nu)}$ in the truncated form.

To develop the third algorithm, let

$$q_n = \frac{1}{f_0} \sum_{m=0}^{n} \lambda_m f_m = \sum_{m=0}^{n} \lambda_m r_0 r_1 \cdots r_{m-1}, \tag{4.12}$$

where as before $r_{n-1} = f_n/f_{n-1}$. Denoting the product of the first $n$ of the $r$'s by $p_n$, we obtain

$$\begin{aligned} p_0 &= 1, \qquad p_n = r_{n-1}p_{n-1}, \\ q_0 &= \lambda_0, \qquad q_n = q_{n-1} + \lambda_n p_n, \end{aligned} \qquad n = 1, 2, 3, \cdots. \tag{4.13}$$

Each $r_{n-1}$ in (4.13) will be computed from the continued fraction

$$r_{n-1} = \frac{-b_n}{a_n -} \frac{b_{n+1}}{a_{n+1} -} \frac{b_{n+2}}{a_{n+2} -} \cdots$$

by applying either (4.2), (4.3), or (4.4), (4.5), with $N$ replaced by $n - 1$. From (4.12), and the identity (3.2), it follows that

$$q = \lim_{n\to\infty} q_n = \frac{s}{f_0}.$$

Hence we continue generating the $q_n$ in (4.13) until they meet some specific criterion of convergence. Thereafter, we may obtain as many of the final answers as desired by means of

$$f_0 = s/q, \qquad f_n = p_n f_0, \qquad n = 1, 2, 3, \cdots. \tag{4.14}$$

If the $q_n$ converge too rapidly, it may occur, of course, that some of the later $p_n$ required in (4.14) are not yet available, and must be generated by continuing the first recursion in (4.13). It should also be noted that the $q$-recursion in (4.13) can be omitted if $f_0$ is known in advance.

An obvious disadvantage of the third algorithm is the fact that a rather large number of continued fractions have to be evaluated, in contrast to just one continued fraction in the first two algorithms. Even though some of these continued fractions (especially the later ones) may converge quite rapidly, the expenditure of computation in the third algorithm is in general higher than in the first and second algorithm.

In spite of these shortcomings, there might be situations in which the third algorithm is more convenient than the others. Suppose, e.g., that we are to evaluate an infinite series

$$\sum_{m=0}^{\infty} \alpha_m f_m .$$

Not knowing the number of terms required, for given accuracy, one normally accumulates terms until, say, for the first time

$$| \alpha_n f_n | \leqq \epsilon \left| \sum_{m=0}^{n-1} \alpha_m f_m \right| .$$

Since this is equivalent to

$$| \alpha_n p_n | \leqq \epsilon \left| \sum_{m=0}^{n-1} \alpha_m p_m \right| ,$$

we could make use of this condition to terminate (4.13) at the proper time.

We also observe that the third algorithm converges under the sole condition that $f_n$ be minimal; no additional condition, such as (3.16), is required.

**5. Bessel functions of the first kind.** Bessel functions $J_\alpha(z)$ of the first kind, and Bessel functions $Y_\alpha(z)$ of the second kind, obey the same recurrence relation

$$y_{\alpha+1} - \frac{2\alpha}{z} y_\alpha + y_{\alpha-1} = 0. \tag{5.1}$$

It was the computation of modified Bessel functions $I_n(x)$ that led J. C. P. Miller to invent his backward recurrence algorithm [5, p. xvii].[6] Various authors, since then, observed that this algorithm can be used effectively to generate other Bessel functions as well, including Bessel functions of the second kind ([15], [54], [47], [22], [26], [39 §9.12, Exps. 1 and 7], [2] [32], [33]). To our knowledge the use of ratios of Bessel functions, and thus of a procedure resembling closely our algorithm (3.9), was first suggested by C. W. Jones [27], and is further described in [9], [40], [10]. The ideas involved are extended here in a natural way to Bessel functions of a complex argument. Some new technical details are also included, such as the estimation of the initial value of $\nu$ in our first algorithm.

Consider

$$f_n = J_{a+n}(z), \qquad g_n = Y_{a+n}(z), \qquad n = 0, 1, 2, \cdots, \tag{5.2}$$

where $0 \leqq a < 1$, and $z = x + iy$ is a complex number not on the negative real axis. Since $J_{a+n}(\bar{z}) = \overline{J_{a+n}(z)}$, we may assume $y \geqq 0$. As follows directly from (5.1), both functions in (5.2) satisfy the three-term recurrence relation

$$y_{n+1} - \frac{2(a+n)}{z} y_n + y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots. \tag{5.3}$$

However, their asymptotic behavior for large $n$ is quite different. We have, in fact,

$$J_{a+n}(z) \sim \frac{e^{-a}}{\sqrt{2\pi n}} \left(\frac{ez}{2n}\right)^{a+n}, \quad Y_{a+n}(z) \sim -e^a \sqrt{\frac{2}{\pi n}} \left(\frac{2n}{ez}\right)^{a+n}, \quad n \to \infty. \tag{5.4}$$

Therefore, $f_n$ is the minimal solution of (5.3), and the dominance of every other solution over $f_n$ is extremely pronounced: $f_n/g_n$ tends to zero about as rapidly as $|z|^{2n}/(2n)!$, when $n \to \infty$.

It may be noted that this behavior also follows from the general asymptotic results of §2. In fact, the Newton-Puiseux diagram (see Fig. 2) for equation (5.3) has two sides with slopes $+1$ and $-1$, respectively. Hence, by Theorem 2.3(a), there are two solutions, $y_{n,1}$ and $y_{n,2}$, of (5.3) with different asymptotic behavior, viz.,

$$\frac{y_{n+1,1}}{y_{n,1}} \sim \frac{2n}{z}, \qquad \frac{y_{n+1,2}}{y_{n,2}} \sim \frac{z}{2n}, \qquad n \to \infty.$$

[6] As pointed out by Logan [30], the idea of reversing recurrence schemes to control the propagation of errors can be traced back to Lord Rayleigh, who already recommended that spherical Bessel functions be calculated in the direction of decreasing order [48, p. 38ff].

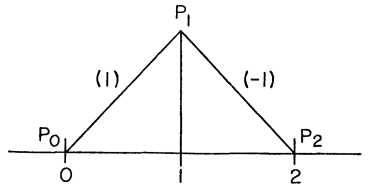


FIG. 2. *Newton-Puiseux diagram for* (5.3)

Since $\lim_{n\to\infty} J_{a+n}(z) = 0$ for any fixed $z$, we may readily identify $y_{n,2} = J_{a+n}(z)$ and $y_{n,1} = Y_{a+n}(z)$.

In view of the marked predominance of $Y_{a+n}$ over $J_{a+n}$, it is virtually impossible to generate $J_{a+n}$ directly by means of (5.3). Algorithm (3.9), however, appears to be very effective. In fact, various infinite series of the form (3.2) are available for bypassing the calculation of initial values. Moreover, rather close estimates can be derived for the initial value $\nu$ of the recursion index $n$, thus eliminating the need for many repetitions of the backward recurrence process, as well as the risk of doing too much unnecessary computing.

We first discuss the selection of a suitable infinite series (3.2). We may choose from a family of candidates furnished by Sonine's formula [13, p. 64], which may be written in the form

$$\sum_{m=0}^{\infty} i^m \frac{a+m}{a} C_m^a(\gamma) J_{a+m}(z) = \frac{(z/2)^a e^{i\gamma z}}{\Gamma(1+a)}. \tag{5.5}$$

The parameter $\gamma$ will presently be specified to suit our purpose; $C_m^a(\gamma)$ are the Gegenbauer polynomials, i.e., the coefficients in the expansion

$$(1 - 2\gamma t + t^2)^{-a} = \sum_{m=0}^{\infty} C_m^a(\gamma) t^m.$$

It is readily seen that

$$\begin{aligned} C_m^a(-\gamma) &= (-1)^m C_m^a(\gamma), \\ C_m^a(1) &= \frac{\Gamma(2a+m)}{m!\Gamma(2a)}, \qquad (5.6) \\ C_{2m-1}^a(0) &= 0, \qquad C_{2m}^a(0) = (-1)^m \frac{\Gamma(a+m)}{m!\Gamma(a)}, \qquad m > 0, \end{aligned}$$

while, of course, $C_0^a(\gamma) = 1$.

In accordance with our remark at the end of §3 we should try to select $\gamma$ in such a way that

$$\frac{s}{f_0} = \frac{(z/2)^a e^{i\gamma z}}{\Gamma(1+a) J_a(z)}$$

cannot become very small in absolute value. Now, if $|z|$ is small, then $J_a(z) \sim (z/2)^a/\Gamma(1+a)$, so that $|s/f_0| \sim 1$. For large $|z|$, we have $J_a(z) \sim (\pi z/2)^{-1/2} \cos(z - a\pi/2 - \pi/2)$, and again, $|s/f_0|$ cannot be small if $z$ is real.

However, if $z = x + iy$, and $y > 0$ is large, then $|\cos(z - a\pi/2 - \pi/2)| \sim e^y/2$, and so

$$\left|\frac{s}{f_0}\right| \sim \frac{2\sqrt{\pi}}{\Gamma(1+a)}\left(\frac{|z|}{2}\right)^{a+1/2} e^{-(1+\gamma)y}.$$

To prevent this from becoming exponentially small, we must require $\gamma \leqq -1$. For convenience, we choose $\gamma = -1$. In view of the first two relations in (5.6), identity (5.5) then becomes

$$\sum_{m=0}^{\infty} (-i)^m \frac{a+m}{a} \frac{\Gamma(2a+m)}{m!\Gamma(2a)} J_{a+m}(z) = \frac{(z/2)^a e^{-iz}}{\Gamma(1+a)},$$

or finally, noting that $a\Gamma(2a) = \Gamma(1+2a)/2$,

$$J_a(z) + 2\sum_{m=1}^{\infty} (-i)^m \frac{(a+m)\Gamma(2a+m)}{m!\Gamma(1+2a)} J_{a+m}(z) = \frac{(z/2)^a e^{-iz}}{\Gamma(1+a)}. \tag{5.7}$$

The coefficients

$$\lambda_m = 2(-i)^m \frac{(a+m)\Gamma(2a+m)}{m!\Gamma(1+2a)}, \qquad m = 1, 2, 3, \cdots, \tag{5.8}$$

are best obtained recursively as follows,

$$\begin{aligned} l_1 &= 1, \\ l_{m+1} &= \frac{m+2a}{m+1} l_m, \qquad m = 1, 2, 3, \cdots, \\ \lambda_m &= 2(-i)^m (a+m) l_m. \end{aligned}$$

In the special case $a = 0$, we simply have $\lambda_m = 2(-i)^m$.

If $z = x$ is real and positive we could choose the real or imaginary part of (5.7) as our normalization identity. We find it more convenient, however, to use (5.5) with $\gamma = 0$. By virtue of the last relations in (5.6), this identity can be written in the form

$$J_a(x) + \sum_{m=1}^{\infty} \frac{(a+2m)\Gamma(a+m)}{m!\Gamma(1+a)} J_{a+2m}(x) = \frac{(x/2)^a}{\Gamma(1+a)}. \tag{5.9}$$

The coefficients

$$\lambda_{2m} = (a+2m)\frac{\Gamma(a+m)}{m!\Gamma(1+a)}, \qquad m = 1, 2, 3, \cdots, \tag{5.10}$$

are obtained recursively by means of

$$\begin{aligned} l_1 &= 1, \\ l_{m+1} &= \frac{m+a}{m+1} l_m, \qquad m = 1, 2, 3, \cdots, \\ \lambda_{2m} &= (a+2m) l_m. \end{aligned}$$

Again, if $a = 0$, the expression for $\lambda_{2m}$ simplifies to $\lambda_{2m} = 2$. In this case, one could also use the second algorithm in its simplified form (without the $s$-recursions), if one computes $J_0(x)$ from an appropriate rational approximation. This would probably result in a more efficient algorithm to generate Bessel functions of integer order, than the use of (5.9).

We also note that in the special case of modified Bessel functions

$$I_{a+n}(x) = e^{-i(a+n)\pi/2} J_{a+n}(ix), \qquad x > 0,$$

the recurrence relation (5.3) assumes the form

$$y_{n+1} + \frac{2(a+n)}{x} y_n - y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots,$$

and relation (5.7) the form

$$I_a(x) + 2 \sum_{m=1}^{\infty} \frac{(a+m)\Gamma(2a+m)}{m!\Gamma(1+2a)} I_{a+m}(x) = \frac{(x/2)^a e^x}{\Gamma(1+a)}.$$

It is now an easy matter to verify that algorithm (3.9), whether the $\lambda_m$ be defined by (5.8), or by (5.10), converges as $\nu \to \infty$, provided $J_{a+n}(z) \neq 0$ for $n = 0, 1, 2, \cdots$. By Theorem 3.1 we need only show that

$$h_\nu = \frac{f_{\nu+1}}{g_{\nu+1}} \sum_{m=0}^{\nu} \lambda_m g_m$$

has the limit zero. Now in the case of (5.8), since $0 \leqq a < 1, \Gamma(1+2a) > .88$, we clearly have

$$|\lambda_m| = \frac{2}{\Gamma(1+2a)} \frac{a+m}{m} \frac{\Gamma(2a+m)}{\Gamma(m)}$$

$$< \frac{2}{\Gamma(1+2a)} \frac{m+1}{m} \frac{\Gamma(m+2)}{\Gamma(m)} < 2.3(m+1)^2.$$

Therefore, if $\nu$ is already so large that $|g_\nu| \geqq |g_m|$ for $0 \leqq m < \nu$, we shall have

$$|h_\nu| \leqq 2.3(\nu+1)^3 \left| \frac{f_{\nu+1} g_\nu}{g_{\nu+1}} \right| = O(\nu^2 f_{\nu+1}),$$

hence $\lim_{\nu \to \infty} h_\nu = 0$, by virtue of (5.4). A similar argument applies to (5.10).

We proceed now to estimate the initial value of $\nu$ to be used in algorithm (3.9), given the number of significant digits desired. Such an estimate may be found from the estimate (3.18) for the relative errors. For definiteness, we assume $z$ complex, and assume identity (5.7) in the role of (3.2).

If $\nu$ is large, the infinite series

$$\sum_{m=\nu+1}^{\infty} \lambda_m f_m$$

in (3.18) may roughly be approximated by its first term, $\lambda_{\nu+1} f_{\nu+1}$, and similarly

$$\sum_{m=0}^{\nu} \lambda_m g_m$$

may be approximated by the last term $\lambda_\nu g_\nu$. Then

$$\frac{f_n^{(\nu)} - f_n}{f_n} \doteq \frac{1}{s}\lambda_{\nu+1}f_{\nu+1}\left(1 + \frac{\lambda_\nu}{\lambda_{\nu+1}}\frac{g_\nu}{g_{\nu+1}}\right) - \frac{f_{\nu+1}}{g_{\nu+1}}\frac{g_n}{f_n} \tag{5.11}$$
$$\doteq \frac{1}{s}\lambda_{\nu+1}f_{\nu+1} - \frac{f_{\nu+1}}{g_{\nu+1}}\frac{g_n}{f_n}.$$

Our aim is to find an upper bound for the moduli of these expressions, valid for $n = 0, 1, 2, \cdots, N$. Since $|g_n/f_n|$ ultimately grows rapidly with $n$, it is plausible to expect that a bound which holds for $n = N$ will also be a valid bound when $n < N$, particularly if $N$ is large. We therefore consider the simplified problem of bounding the modulus of the last member in (5.11), when $n = N$. As a further simplification we assume $N$, and thus $\nu$, so large that the asymptotic expressions in (5.4) are reasonably accurate. In particular, then, $2N > e|z|$. Under these assumptions a short calculation gives

$$\left|\frac{f_n^{(\nu)} - f_n}{f_n}\right| \lesssim e^{-y}\left(\frac{e|z|}{2\nu}\right)^\nu + \left(\frac{e|z|}{2}\right)^{2(\nu-N)} N^{2N}\nu^{-2\nu}, \qquad y = \operatorname{Im} z,$$

where a few unimportant coefficients have been omitted. For $f_n^{(\nu)}$ to be an approximation of $f_n$ to $d$ significant digits, we are led to require, simultaneously,

$$e^{-y}\left(\frac{e|z|}{2\nu}\right)^\nu \leqq \frac{1}{4}\cdot 10^{-d}, \quad \left(\frac{e|z|}{2}\right)^{2(\nu-N)} N^{2N}\nu^{-2\nu} \leqq \frac{1}{4}\cdot 10^{-d}. \tag{5.12}$$

In the case of real arguments $z = x > 0$, and using relation (5.9) in place of (5.7), our reasoning must be slightly modified, but the conclusion is the same as in (5.12), with $y = 0$.

Now the first inequality in (5.12), after taking logarithms and multiplying by $-2/(e|z|)$, gives

$$\frac{2\nu}{e|z|}\ln\frac{2\nu}{e|z|} \geqq \frac{2(D-y)}{e|z|}, \tag{5.13}$$

where

$$D = d\ln 10 + \ln 4.$$

Similarly, the second inequality gives

$$\nu\ln\frac{2\nu}{e|z|} \geqq N\ln\left(\frac{2N}{e|z|}\right) + \frac{1}{2}D,$$

which may be rewritten in the form

$$\left(\frac{\nu}{N} - 1\right)\ln\left(\frac{2N}{e|z|}\right) + \frac{\nu}{N}\ln\frac{\nu}{N} \geqq \frac{D}{2N}.$$

Since $\nu > N$, and $2N > e|z|$, this is certainly satisfied if we require

$$\frac{\nu}{N}\ln\frac{\nu}{N} \geqq \frac{D}{2N}. \tag{5.14}$$

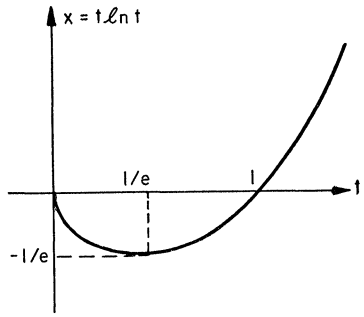


FIG. 3. *Graph of* $x = t \ln t$

Both conditions (5.13) and (5.14) have now the form $t \ln t \geqq c$. Since this is equivalent to $t \geqq t(c)$ with $t(x)$ the inverse function of $x = t \ln t$ in the region $t \geqq 1/e$ (see Fig. 3), our conditions may be given the final form

$$\nu \geqq \frac{e|z|}{2} t\left[\frac{2(D-y)}{e|z|}\right], \quad \text{if} \quad 0 \leqq y < D + \frac{|z|}{2}, \tag{5.15}$$

$$\nu \geqq Nt\left(\frac{D}{2N}\right). \tag{5.16}$$

Low-accuracy approximations to the function $t(x)$ are not hard to obtain. In the interval $1/e \leqq t \leqq 1$ we may first approximate the graph of $t \ln t$ by a quadratic parabola passing through the points $(1/e, -1/e)$, $(1, 0)$, and having zero slope at the first of these points:

$$t \ln t \doteq -\frac{1}{e} + \frac{e}{(e-1)^2}\left(t - \frac{1}{e}\right)^2.$$

Taking then the inverse function of the right-hand member to approximate $t(x)$, we obtain

$$t(x) \doteq \frac{1}{e} + \frac{e-1}{\sqrt{e}}\left(x + \frac{1}{e}\right)^{1/2} \doteq .36788 + 1.0422(x + .36788)^{1/2}, \quad -1/e \leqq x \leqq 0.$$

The accuracy of this approximation is about 4%, or better.

In the region $0 \leqq x \leqq 10$, we truncated the expansion of $t(x)$ in Chebyshev polynomials, having determined the first few expansion coefficients by numerical integration. We so obtained

$$t(x) \doteq 1.0125 + .8577x - .129013x^2 + .0208645x^3 - .00176148x^4 + .000057941x^5,$$

with a maximum percentage error of about 1%.

For larger values of $x$, we first observe that

$$t(x) \sim x/\ln x, \qquad x \to \infty.$$

In fact, $[t(x) \ln x]/x = (\ln x)/\ln t(x)$, and using the rule of Bernoulli-

L'Hospital, we find

$$\lim_{x\to\infty}\frac{\ln x}{\ln t(x)}=\lim_{x\to\infty}\frac{\dfrac{1}{x}}{\dfrac{1}{t(x)}\cdot\dfrac{1}{1+\ln t(x)}}=\lim_{x\to\infty}\frac{x+t(x)}{x}=1.$$

Unfortunately, the asymptotic expression so obtained does not give sufficient accuracy, unless $x$ is very large. Applying, however, one step of Newton's method to the equation $t \ln t = x$, with $x/\ln x$ as initial approximation, we get

$$t(x)\doteq\frac{x}{\ln x}\cdot\frac{1}{1-\dfrac{\ln\ln x}{1+\ln x}}.$$

This approximation now appears to be in error by less than 1% for $x \geqq 2$. As $x \to \infty$, the relative error clearly tends to zero.

An alternate method of selecting $\nu$ in the case $z = x > 0$, $a = 0$, was derived by W. Kahan [28], using Olver's error analysis [38]. Let $\epsilon$ be the largest relative error tolerated in the final results, $J_0(z), J_1(x), \cdots, J_N(x)$. Let $K$ be the integer

$$K = \max(N, [x]),$$

and, with $\beta > 0$ arbitrary (though small, in practice), define

$$y_K = 0, \qquad y_{K+1} = \beta,$$

$$y_{n+1} = \frac{2n}{x}y_n - y_{n-1}, \qquad n = K+1, K+2, \cdots.$$

Then $\nu$ may be taken to be the smallest $n$ for which $y_{n+1} \geqq \beta/\epsilon$.

We have seen that Bessel functions $J_{a+n}(z)$ of positive orders can be computed entirely from their recurrence relation. This remains true, to a certain extent, for Bessel functions

$$y_n = J_{a-n}(z), \qquad n = 1, 2, 3, \cdots; \quad 0 < a < 1, \tag{5.17}$$

of negative orders. They satisfy the recurrence relation

$$y_{n+1} + \frac{2(n-a)}{z}y_n + y_{n-1} = 0, \qquad n = 2, 3, 4, \cdots, \tag{5.18}$$

which has the same Newton-Puiseux diagram as (5.3). The solution (5.17), however, is now a dominant solution, the minimal solution being $f_n = (-1)^n J_{n-a}(z)$. It appears therefore safe to generate $J_{a-n}(z)$ by means of (5.18) in the ordinary fashion. Moreover, the recursion may be started with $n = 0$, and the initial values $y_{-1} = J_{a+1}(z)$, $y_0 = J_a(z)$ obtained by the methods previously discussed.

The assumption $a > 0$ is of course essential. If $a = 0$, the two solutions $y_n$ and $f_n$ above are the same (minimal) solution of (5.18), and forward recursion by (5.18) is doomed to fail. The same must be expected if $a$ is close to zero, and indeed if $a$ is close to one.

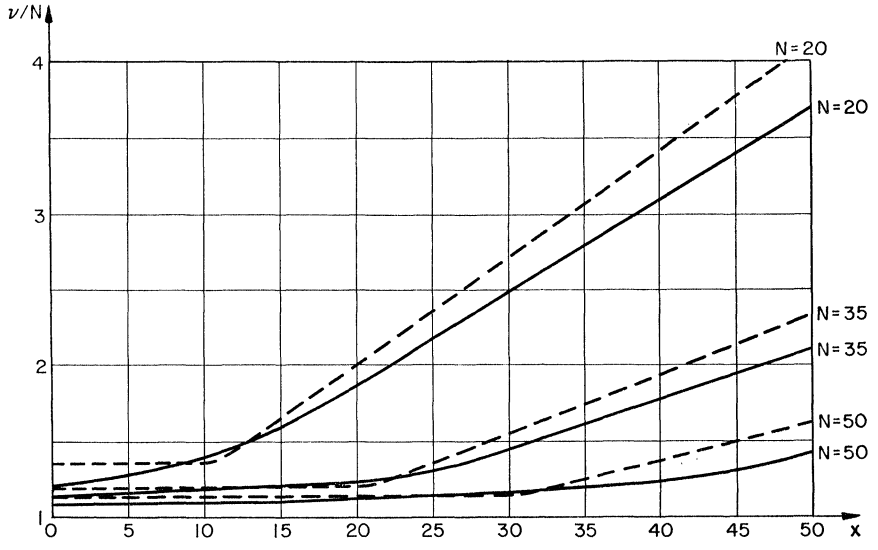


FIG. 4. ESTIMATED $\nu/N$ / EMPIRICAL $\nu/N$ FOR BESSEL FUNCTIONS $J_n(x)$, $n = 0(1)N$.

We present now a few numerical results concerning the first algorithm for computing $J_{a+n}(z)$. The performance of this algorithm was found to be quite insensitive to changes of $a$ in the interval $0 \leqq a < 1$, so that the results given for $a = 0$ may be considered as representative.

Our main concern was to determine the quality of the estimate of $\nu$ given above in (5.15), (5.16). We compared this estimate with the smallest value of $\nu$ empirically observed to yield $J_n(z)$, $n = 0(1)N$, to six significant digits.[7] For real $z = x$, the results are shown in Fig. 4, while for complex $z = re^{i\phi}$ they are depicted in Fig. 5. Both figures show that agreement between estimated and actual $\nu$ is rather satisfactory on the whole, even though for larger values of $|z|$ it is worsening. Remarkable is also the relative smallness of $\nu/N$ over an extended region of the complex plane.

ALGOL procedures based on the methods of this paragraph may be found in [18].

**6. Legendre functions.** A further class of special functions amenable to the methods of §§3 and 4 are the associated Legendre functions of the first and second kind, $P_\alpha^m(z)$ and $Q_\alpha^m(z)$. We assume that $m$ is a nonnegative[8] integer, $z$ a complex number outside the interval $(0, 1)$, with $\operatorname{Re} z > 0$, and $\alpha$ arbitrary real or

[7] More precisely, algorithm (3.9) was run with $\nu = N + 2, N + 4, N + 6, \cdots$ until for the first time the $N + 1$ values $f_n^{(\nu)}$, $n = 0, 1, \cdots, N$, agreed to six significant digits with the respective values of $f_n^{(\nu-2)}$.

[8] If $\alpha$ is an integer $\geqq m$, or nonintegral, then $P_\alpha^{-m}(z) = [\Gamma(\alpha - m + 1)/\Gamma(\alpha + m + 1)]P_\alpha^m(z)$, and the restriction to nonnegative integers $m$ is not essential. Similarly, $Q_\alpha^{-m}(z) = [\Gamma(\alpha - m + 1)/\Gamma(\alpha + m + 1)]Q_\alpha^m(z)$.

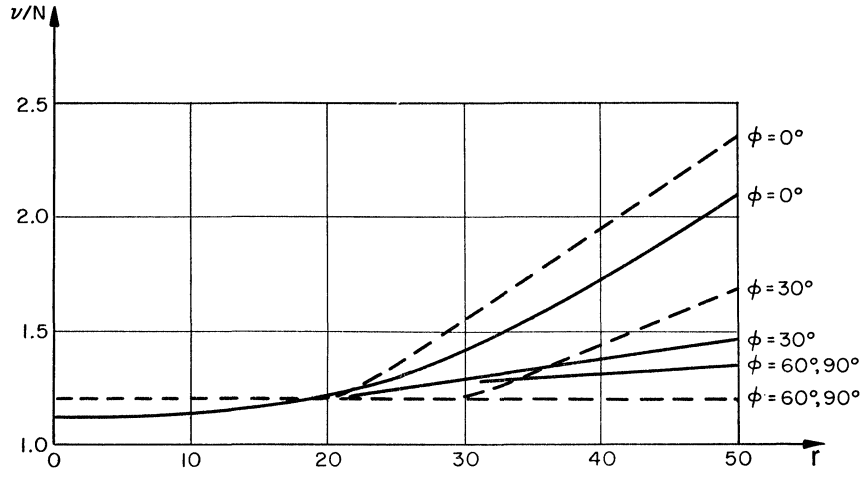


FIG. 5. — — — — ESTIMATED ν/N
———— EMPIRICAL ν/N
FOR BESSEL FUNCTIONS $J_n(re^{i\phi})$, n = 0(1)N, WHERE N = 35.

complex, but $\alpha \neq -1, -2, -3, \cdots$. The Legendre functions of the first kind are then representable by a definite integral,

$$P_\alpha^m(z) = \frac{\Gamma(\alpha + m + 1)}{\pi\Gamma(\alpha + 1)} \int_0^\pi [z + (z^2 - 1)^{1/2} \cos t]^\alpha \cos mt \, dt.$$

A similar representation holds for Legendre functions of the second kind,

$$Q_\alpha^m(z) = (-1)^m \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha - m + 1)} \int_0^\infty \frac{\cosh mt}{[z + (z^2 - 1)^{1/2} \cosh t]^{\alpha+1}} \, dt,$$

provided Re $(\alpha - m) > -1$. In both these formulas the meaning of the expressions $(z - 1)^{1/2}$, $(z + 1)^{1/2}$ is as usual obtained by continuity in the complex plane, cut along the interval $(-\infty, 1)$, assuming them real for $z > 1$. A similar remark applies to the other fractional powers.

It is well known that $P_\alpha^m$ and $Q_\alpha^m$ satisfy identical three-term recurrence relations, both with respect to order $m$ and degree $\alpha$. (See, e.g., [12, p. 160].) The fact that backward recursion techniques are applicable to obtain Legendre functions of integral order and argument greater than unity was already mentioned in [10]. The use of Miller's algorithm (cf. §3) for calculating toroidal functions of the second kind is described in [50]. No mention is made, in this reference, of the usefulness of infinite series for normalization purposes, which makes this algorithm even more attractive.

We begin with considering the recurrence with respect to order $m$. Both $P_\alpha^m(z)$ and $Q_\alpha^m(z)$, as functions of $m$, are solutions of

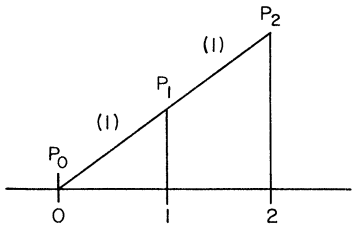


FIG. 6. *Newton-Puiseux diagram for* (6.1)

$$y_{m+1} + \frac{2mz}{(z^2 - 1)^{1/2}} y_m + (m + \alpha)(m - \alpha - 1)y_{m-1} = 0, \tag{6.1}$$

$$m = 1, 2, 3, \cdots.$$

We first assume that $\alpha$ is not an integer. The case of integral $\alpha$ will be dealt with later.

The Newton-Puiseux diagram (see Fig. 6) for the difference equation (6.1) is a straight line segment with slope 1, and thus case (b) of Theorem 2.3 applies. The characteristic equation is

$$t^2 + \frac{2z}{(z^2 - 1)^{1/2}} t + 1 = 0,$$

which has the roots

$$t_1 = -\left(\frac{z + 1}{z - 1}\right)^{1/2}, \qquad t_2 = t_1^{-1}.$$

Since $\operatorname{Re} z > 0$, it is readily seen that

$$|t_1| > 1 > |t_2|.$$

By Theorem 2.3, and the remarks following it, the difference equation (6.1) thus possesses a minimal solution, $y_{m,2}$, for which

$$\lim_{m\to\infty} \frac{y_{m+1,2}}{m y_{m,2}} = t_2;$$

for any other solution the corresponding limit is $t_1$. Let

$$f_m = \frac{P_\alpha^m(z)}{\Gamma(\alpha + m + 1)} = \frac{1}{\pi\Gamma(\alpha + 1)} \int_0^\pi [z + (z^2 - 1)^{1/2} \cos t]^\alpha \cos mt \, dt, \tag{6.2}$$

so that

$$\frac{f_{m+1}}{f_m} \sim \frac{P_\alpha^{m+1}(z)}{m P_\alpha^m(z)}, \qquad m \to \infty.$$

The second member of this relation, as was just observed, has a finite limit as

$m \to \infty$, which is either $t_1$ or $t_2$. Were it $t_1$, then $|f_m|$ would tend to $\infty$, since $|t_1| > 1$. This, however, is impossible, since $f_m$ by (6.2) are essentially the Fourier coefficients of a smooth function, and thus $\lim_{m\to\infty} f_m = 0$. Therefore, the limit is $t_2$, and $P_\alpha^m(z)$ is indeed the minimal solution of (6.1), while $Q_\alpha^m(z)$ belongs among the dominant solutions.

It follows that $P_\alpha^m(z)$, $m = 0, 1, 2, \cdots$, can be obtained by the algorithms of §§3 and 4. As will be seen shortly, an infinite series can be used for normalization, so that no values of $P_\alpha^m(z)$ need to be known in advance. The functions $Q_\alpha^m(z)$, $m = 0, 1, 2, \cdots$, on the other hand, can safely be generated by forward use of (6.1); this requires two initial values for $m = 0$ and $m = 1$ to be available. In the important special case $\alpha = -\frac{1}{2} + n$, where $n$ is an integer, these initial values may also be obtained by the aforementioned algorithms, applied to the recurrence with respect to degree (cf. below).

It is more convenient, computationally, to deal with $f_m$ defined in (6.2), rather than $P_\alpha^m$, since then we not only avoid excessively large numbers, but also obtain a very simple identity for normalization. It is well known, indeed, that (see [12, p. 166])[9]

$$P_\alpha(z) + 2\sum_{m=1}^{\infty} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha+m+1)} P_\alpha^m(z) = [z + (z^2-1)^{1/2}]^\alpha, \tag{6.3}$$

valid for $\operatorname{Re} z > 0$ and arbitrary $\alpha$. Hence,

$$f_0 + 2\sum_{m=1}^{\infty} f_m = \frac{[z + (z^2-1)^{1/2}]^\alpha}{\Gamma(\alpha+1)}, \tag{6.4}$$

which may serve in the capacity of condition (3.2), with

$$s = \frac{[z + (z^2-1)^{1/2}]^\alpha}{\Gamma(\alpha+1)}, \qquad \lambda_0 = 1, \lambda_m = 2, m > 0.$$

The convergence of the first algorithm then follows from the remark made after Theorem 3.1.

To insure numerical stability, the ratio

$$\frac{s}{f_0} = \frac{[z + (z^2-1)^{1/2}]^\alpha}{P_\alpha(z)} \tag{6.5}$$

should not be allowed to become excessively small (cf. §3). While it is difficult to check the magnitude of this function for the full range of $z$ and $\alpha$, we shall at least look into the behavior of this function near the singular points $z = -1$, $z = +1$, $z = \infty$.

As $z$ tends to $+1$, or $-1$, in the plane cut from $-\infty$ to 1, we have $P_\alpha(z) \to 1$, and so $|s/f_0| \to 1$.

To study the behavior at infinity, we make use of the following facts (see [49, §54]): If $\alpha \neq -\frac{1}{2} + n$, where $n$ is an integer, we have, as $z \to \infty$,

$$P_\alpha(z) \sim A_\alpha(2z)^{-(\alpha+1)} + B_\alpha(2z)^\alpha,$$

[9] As is customary, we write $P_\alpha(z)$ for $P_\alpha^0(z)$.

where

$$A_\alpha = \frac{\Gamma(-\alpha - \frac{1}{2})}{\sqrt{\pi}\Gamma(-\alpha)}, \qquad B_\alpha = \frac{\Gamma(\alpha + \frac{1}{2})}{\sqrt{\pi}\Gamma(\alpha + 1)}.$$

Otherwise, when $\alpha = -\frac{1}{2} + n$, then

$$P_{-(1/2)+n}(z) \sim \begin{cases} \dfrac{\sqrt{2}}{\pi} z^{-1/2} \ln z, & \text{if } n = 0, \\ \dfrac{1}{\sqrt{\pi}} \dfrac{\Gamma(|n|)}{\Gamma(|n| + \frac{1}{2})} (2z)^{|n|-1/2}, & \text{if } n \neq 0. \end{cases}$$

Hence, in the former case,

$$\frac{s}{f_0} \sim \frac{(2z)^\alpha}{A_\alpha(2z)^{-(\alpha+1)} + B_\alpha(2z)^\alpha} = \frac{1}{A_\alpha(2z)^{-(2\alpha+1)} + B_\alpha},$$

which becomes small in modulus only if $\operatorname{Re}(2\alpha + 1) < 0$, i.e., $\operatorname{Re}\alpha < -\frac{1}{2}$. In the case $\alpha = -\frac{1}{2} + n$, we have

$$\frac{s}{f_0} \sim \begin{cases} \dfrac{\pi}{2 \ln z}, & \text{if } n = 0, \\ \sqrt{\pi} \dfrac{\Gamma(n + \frac{1}{2})}{\Gamma(n)}, & \text{if } n > 0, \\ \sqrt{\pi} \dfrac{\Gamma(|n| + \frac{1}{2})}{\Gamma(|n|)} (2z)^{-2|n|}, & \text{if } n < 0. \end{cases}$$

Here, the third case ($n < 0$) is critical, and also the first, but to a much lesser degree.

For all practical purposes, then, (6.5) will be small in modulus only if $\operatorname{Re}\alpha < -\frac{1}{2}$. This can easily be avoided by employing the relation

$$P_\alpha{}^m(z) = P^m_{-\alpha-1}(z), \tag{6.6}$$

when necessary. If $\operatorname{Re}\alpha < -\frac{1}{2}$, then indeed $\operatorname{Re}(-\alpha - 1) > -\frac{1}{2}$.

Restricting $\alpha$ to have real part $-\frac{1}{2}$ one obtains *Mehler's conical functions* $P^m_{-(1/2)+i\tau}(z)$, where $\tau$ is real. Since $P^m_{-(1/2)+i\tau}(z) = P^m_{-(1/2)-i\tau}(z)$, by (6.6), these functions are real when $z$ is real. It suffices, moreover, to consider nonnegative values of $\tau$. We shall assume $z = x > 1$, which is a case of practical interest.

Since $\Gamma(\alpha + m + 1)$ is now complex, the scaled functions (6.2) used previously are not as convenient anymore. To maintain the computational advantages noted before, we consider

$$f_m = \frac{1}{m!} P^m_{-(1/2)+i\tau}(x). \tag{6.7}$$

As follows from (6.1) and our previous discussion, $f_m$ so defined is a minimal solution of

$$y_{m+1} + \frac{2mx}{(m+1)(x^2-1)^{1/2}} y_m + \frac{(m - \frac{1}{2})^2 + \tau^2}{m(m+1)} y_{m-1} = 0, \tag{6.8}$$

$$m = 1, 2, 3, \cdots.$$

To arrive at a normalizing identity for $f_m$, involving real quantities only, we write down (6.3) (with $z = x$) once for $\alpha = -\frac{1}{2} + i\tau$, and once for $\alpha = -\frac{1}{2} - i\tau$, and then form the arithmetic mean of the two identities. Noting (6.7), we then obtain

$$f_0 + \sum_{m=1}^{\infty} \lambda_m f_m = [x + (x^2 - 1)^{1/2}]^{-1/2} \cos(\tau \ln [x + (x^2 - 1)^{1/2}]),$$

where

$$\lambda_m = u_m + \bar{u}_m, \qquad u_m = \frac{m!\Gamma(\frac{1}{2} + i\tau)}{\Gamma(\frac{1}{2} + i\tau + m)}.$$

The $\lambda$'s are best obtained from a three-term recurrence relation. We clearly have

$$u_{m+1} = \frac{(m+1)u_m}{m + \frac{1}{2} + i\tau} = \frac{(m+1)(m + \frac{1}{2} - i\tau)}{(m + \frac{1}{2})^2 + \tau^2} u_m.$$

For notational simplicity, let

$$\alpha_m = m + \frac{1}{2}, \qquad \beta_m = \frac{(m + \frac{1}{2})^2 + \tau^2}{m + 1}. \tag{6.9}$$

Then

$$\beta_m u_{m+1} = (\alpha_m - i\tau)u_m,$$
$$\beta_m \bar{u}_{m+1} = (\alpha_m + i\tau)\bar{u}_m.$$

Adding, and subtracting, we get

$$\begin{aligned} \beta_m \lambda_{m+1} &= \alpha_m \lambda_m - \tau \mu_m, \\ \beta_m \mu_{m+1} &= \alpha_m \mu_m + \tau \lambda_m, \end{aligned} \tag{6.10}$$

where $\mu_m = i(u_m - \bar{u}_m)$. Eliminating the $\mu$'s, we find

$$\lambda_{m+1} - \frac{\alpha_{m-1} + \alpha_m}{\beta_m} \lambda_m + \frac{\alpha_{m-1}^2 + \tau^2}{\beta_{m-1}\beta_m} \lambda_{m-1} = 0,$$

or, with the values (6.9) inserted,

$$\lambda_{m+1} - \frac{2m(m+1)}{(m + \frac{1}{2})^2 + \tau^2} \lambda_m + \frac{m(m+1)}{(m + \frac{1}{2})^2 + \tau^2} \lambda_{m-1} = 0, \quad m = 2, 3, \cdots. \tag{6.11}$$

The initial values are

$$\lambda_1 = \frac{1}{\frac{1}{4} + \tau^2}, \qquad \lambda_2 = \frac{3 - 4\tau^2}{(\frac{1}{4} + \tau^2)(\frac{9}{4} + \tau^2)}. \tag{6.12}$$

We observe that the recursion (6.11) belongs to case (b) of Theorem 2.3, the characteristic equation being $(t-1)^2 = 0$. Because of the double root $t_1 = t_2 = 1$, Theorem 2.3 does not permit us to decide whether the recursion in (6.11), (6.12) is numerically stable. We observe, however, that another solution of (6.11) is $\mu_m$, as follows by eliminating the $\lambda$'s in (6.10). Therefore, Re $u_m$ and Im $u_m$ are a pair

of linearly independent solutions of (6.11). Using Stirling's formula, and disregarding constant factors, we find

$$u_m \sim m e^{-i r \ln m}, \qquad m \to \infty,$$

so that both solutions oscillate, for large $m$, with linearly increasing amplitudes. Therefore, numerical instability cannot arise.

A further interesting special case is obtained by assuming $\alpha$ a nonnegative integer, $\alpha = p$. Then, in fact,

$$P_p^m(z) = \frac{(z^2 - 1)^{m/2}}{2^p p!} \frac{d^{p+m}}{dz^{p+m}} (z^2 - 1)^p.$$

This shows that

$$P_p^m(z) \equiv 0 \quad \text{if} \quad m > p.$$

We note that Theorem 1.1 with $f_m = P_p^m(z)$ is no longer applicable, since the assumption $f_m \neq 0$ (all $m$) does not hold. Neither apply the asymptotic results of §2, the assumption (2.2) now being violated.

Nevertheless, $f_m$ still satisfies the recurrence relation (6.1) (with $\alpha = p$) for *all* values of $m$, thus in particular for $m = p, p - 1, \cdots, 1$, whereby $f_{p+1} = 0$. The algorithm described at the beginning of §3 becomes applicable, and it follows that the $r$-recursion in our algorithm (3.9), if started with $\nu = p$, furnishes the *exact* ratios $r_{m-1} = f_m/f_{m-1}$, apart from rounding errors. The same is true for the $s$-recursion, which yields exact values of

$$s_{m-1} = \sum_{r=m}^{p} \lambda_r f_r / f_{m-1},$$

the infinite series in (6.3) reducing to a finite sum, when $\alpha = p$. In short, (3.9) *with $\nu = p$ now represents the complete algorithm for computing $f_m = P_p^m(z)$, $m = 0, 1, 2, \cdots, p$, and no iteration on $\nu$ is required.*

We now proceed to the recurrence relation with respect to degree. Let $a$, $m$, and $z$ be fixed, and consider $P_{a+n}^m(z)$, $Q_{a+n}^m(z)$ as functions of $n$. They both obey the relation

$$(n + a - m + 1)y_{n+1} - (2n + 2a + 1)zy_n + (n + a + m)y_{n-1} = 0, \quad n = 0, 1, 2, \cdots. \tag{6.13}$$

This is a Poincaré difference equation whose characteristic equation is

$$t^2 - 2zt + 1 = 0.$$

The roots are

$$t_1 = z + (z^2 - 1)^{1/2}, \qquad t_2 = t_1^{-1} = z - (z^2 - 1)^{1/2},$$

and it is readily verified that for $\operatorname{Re} z > 0$,

$$|t_1| > 1 > |t_2|.$$

From Theorem 2.3(b), and the remarks following this theorem, we conclude that (6.13) has a minimal solution $f_n$ for which $\lim_{n\to\infty} f_{n+1}/f_n = t_2$, while the limit is $t_1$ for every other solution. Now it is known (see, e.g., [12, p. 162]) that

$$Q_{a+n}^m(z) \sim (-1)^m \sqrt{\frac{\pi}{2}}\, n^{m-1/2}(z^2-1)^{-1/4} t_2^{a+n+1/2}, \qquad n \to \infty,$$

for $z$ outside the cut from $-\infty$ to 1, thus in particular for those $z$ which we are considering here. It follows immediately, therefore, that the minimal solution is $f_n = Q_{a+n}^m(z)$, and that $g_n = P_{a+n}^m(z)$ is now a dominant solution.

The computation of $P_{a+n}^m(z)$ for $n = 0, 1, 2, \cdots$ can proceed using (6.13) in the normal fashion. The required initial values $P_a{}^m(z)$, $P_{a+1}^m(z)$ may be obtained by the methods discussed above. These functions are thus again computable entirely from their recurrence relations. On the other hand, $Q_{a+n}^m(z)$, as the minimal solution of (6.13), is amenable to the algorithms of §§3 and 4.

Unfortunately, no simple infinite series involving the $f_n = Q_{a+n}^m(z)$ for arbitrary $a$ exists, which would be convergent in the region considered here. Normalization of $f_n$, therefore, has to be accomplished by computing the initial value $Q_a{}^m(z)$. In the special case of *toroidal functions* $Q_{-(1/2)+n}^m(z)$, however, we have the following relation [12, p. 166]:

$$Q_{-1/2}^m(z) + 2\sum_{n=1}^{\infty} Q_{-(1/2)+n}^m(z) = (-1)^m \sqrt{\frac{\pi}{2}}\,\Gamma\left(m+\frac{1}{2}\right)(z-1)^{-1/2}\left(\frac{z+1}{z-1}\right)^{m/2},$$

which lends itself well for normalization, unless $z$ is complex and near the singular point $-1$.

We wish now to give some additional numerical information concerning the algorithms described in this paragraph.

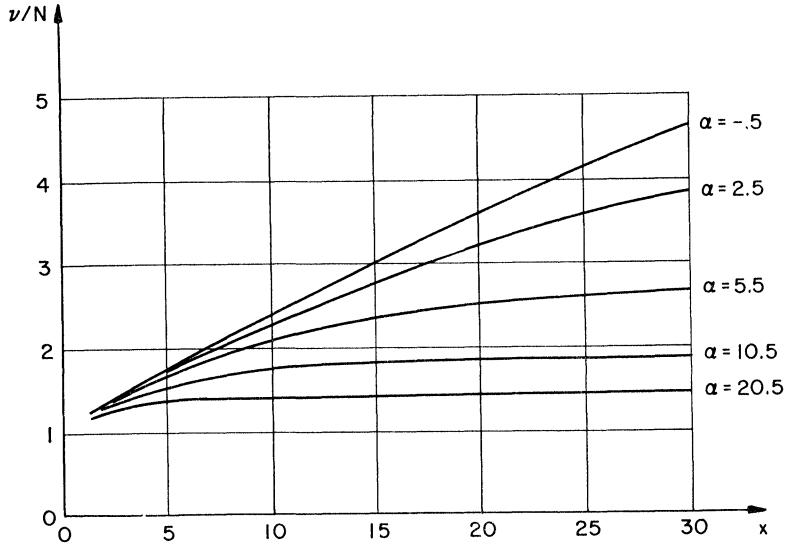


FIG. 7. *Empirical ν/N for Legendre functions* $P_\alpha{}^n(x)$, $n = 0(1)N$, *where* $N = 50$

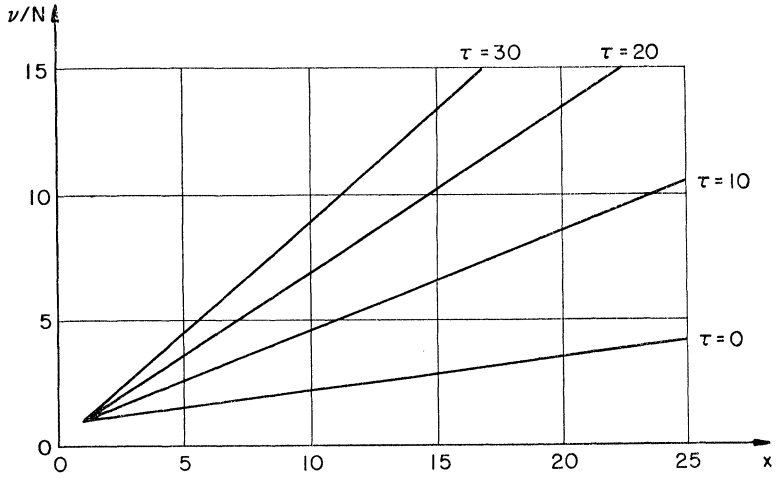


FIG. 8. *Empirical $\nu/N$ for conical functions $P^n_{-(1/2)+i\tau}(x)$, $n = 0(1)N$, where $N = 50$*

Of foremost interest is again the determination of $\nu/N$ in our first algorithm. A derivation of an estimate by analytical means appears to be out of question. We tried, therefore, to determine the behavior of $\nu/N$ empirically, as a function of the various parameters involved. To simplify the task, we assumed a fixed accuracy requirement of six significant digits. Moreover, we decided to consider a fixed value of $N$. Since $\nu/N$ was found to decrease with $N$, we deemed it desirable to select a relatively large value of $N$ as representative, namely, $N = 50$. If we would not do so, we would considerably overestimate $\nu/N$, and pay heavily for this in cases where $N$ is actually large. To compensate for a possible underestimation in cases where $N$ is small, we suggest that a relatively large increment of $\nu$, say 10, or even 20, be used in the iteration process of the first algorithm. Having thus disposed of two parameters, we are still left with two in each case.

In the case of Legendre functions $f_n = P_\alpha{}^n(x)/\Gamma(\alpha + n + 1)$, where $x > 1$, $\alpha \geqq -\frac{1}{2}$, the value of $\nu/N$ found empirically for $N = 50$ is depicted in Fig. 7 as a function of $x$ and $\alpha$. A reasonably good approximation to these curves was obtained in the form

$$\frac{\nu}{N} \doteq \frac{37.26 + .1283(\alpha + 38.26)x}{37.26 + .1283(\alpha + 1)x}.$$

For the conical functions $P^n_{-(1/2)+i\tau}(x)/n!$, where $x > 1$, $\tau \geqq 0$, the empirical value of $\nu/N$ as a function of $x$ and $\tau$ is shown in Fig. 8. The curves were fitted by a function which is linear in both $x$ and $\tau$, viz.,

$$\frac{\nu}{N} \doteq 1 + (.140 + .0246\tau)(x - 1).$$

As the graphs in Fig. 8 show, the conical functions are by far the hardest to compute. As $\nu/N$ becomes large, considerable accumulation of rounding errors must be expected.

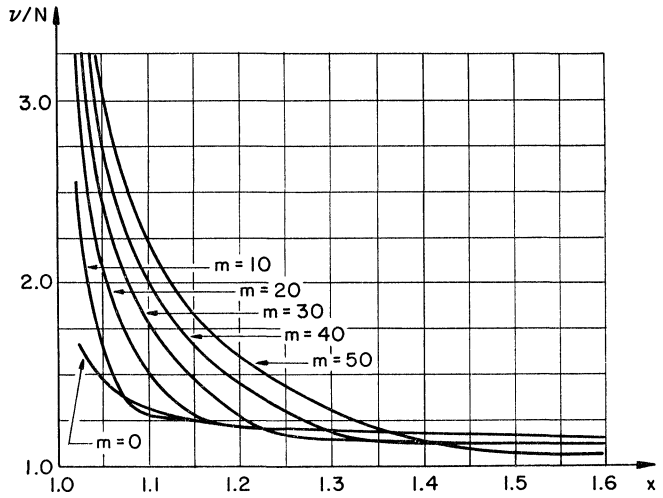


FIG. 9. *Empirical $\nu/N$ for toroidal functions $Q^m_{-(1/2)+n}(x)$, $n = 0(1)N$, where $N = 50$*

Finally, in the case of toroidal functions $Q^m_{-(1/2)+n}(x)$, where $x > 1$, $m \geqq 0$, the behavior of $\nu/N$ as a function of $x$ and $m$ is shown in Fig. 9, and is roughly approximated by

$$\frac{\nu}{N} \doteq 1.15 + \frac{.0146 + .00122m}{x - 1}.$$

ALGOL procedures based on the methods of this paragraph are available in [19].

**7. Coulomb wave functions.** Coulomb wave functions are of importance in the study of nuclear interactions. They arise when Schrödinger's equation for a charged particle in the Coulomb field of a fixed charge is separated in polar coordinates. The radial component then satisfies the differential equation

$$\frac{d^2y}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{L(L+1)}{\rho^2}\right] y = 0, \tag{7.1}$$

where $\eta$ is a real parameter, $L$ a nonnegative integer, and $\rho > 0$. Physically, $\eta$ depends on the relative charges. If both are of equal sign, then $\eta > 0$, otherwise, $\eta < 0$. The variable $\rho$ is a radial distance, suitably scaled, while $L$ is the orbital angular-momentum quantum number of the particle.

The origin $\rho = 0$ is a regular singular point of (7.1), with indicial equation

$$\lambda(\lambda - 1) = L(L + 1).$$

Since the roots of this equation are $\lambda_1 = L + 1$, $\lambda_2 = -L$, the differential equation (7.1) has a solution corresponding to $\lambda_1$ which is regular at $\rho = 0$, admitting an expansion of the form

$$y_1(\rho) = \rho^{L+1} \sum_{n=0}^{\infty} c_n \rho^n.$$

In quantum mechanics it is customary to normalize this solution to have sinusoidal behavior as $\rho \to \infty$, with amplitude equal to 1. So normalized, the solution is called the *regular Coulomb wave function*, and denoted by $F_L(\eta, \rho)$. The solution corresponding to $\lambda_2$, on the other hand, will contain a logarithmic term, since $\lambda_1$ differs from $\lambda_2$ by a positive integer. If normalized similarly as $F_L$, it is called the *irregular Coulomb wave function*, and denoted by $G_L(\eta, \rho)$.

The line

$$\rho = 2\eta, \qquad \eta > 0,$$

which separates regions of different asymptotic behavior of the solutions of (7.1) as $\rho \to \infty$ and $\eta \to \infty$, is called the *transition line*.

In terms of Whittaker's function $M_{\kappa,\mu}(z)$ (see [12] for notation), we have

$$F_L(\eta, \rho) = (2i)^{-(L+1)} C_L(\eta) M_{i\eta, L+1/2}(2i\rho), \tag{7.2}$$

where

$$C_L(\eta) = \frac{2^L e^{-\pi\eta/2} \, |\, \Gamma(L + 1 + i\eta)|}{(2L + 1)!}. \tag{7.3}$$

We note for later use,

$$C_0(\eta) = \left(\frac{2\pi\eta}{e^{2\pi\eta} - 1}\right)^{1/2}, \qquad C_L(\eta) = \frac{(L^2 + \eta^2)^{1/2}}{L(2L + 1)} C_{L-1}(\eta), \tag{7.4}$$

$$L = 1, 2, 3, \cdots.$$

As functions of $L$, both the regular and irregular Coulomb wave function satisfy the three-term recurrence relation

$$L[(L + 1)^2 + \eta^2]^{1/2} y_{L+1} - (2L + 1)\left[\eta + \frac{L(L + 1)}{\rho}\right] y_L + (L + 1)[L^2 + \eta^2]^{1/2} y_{L-1} = 0, \qquad L = 1, 2, 3, \cdots. \tag{7.5}$$

This difference equation has the same Newton-Puiseux diagram as the recurrence relation for the Bessel functions (see Fig. 2). Hence, there are two solutions of (7.5) with markedly distinct asymptotic properties as $L \to \infty$. These, in fact, are precisely the regular and irregular Coulomb wave functions, since for fixed $\eta$ and $\rho$, it is known that

$$F_L(\eta, \rho) \sim C_L(\eta) \rho^{L+1}, \qquad G_L(\eta, \rho) \sim \frac{1}{2LC_L(\eta)\rho^L}, \qquad L \to \infty, \tag{7.6}$$

and furthermore,

$$C_L(\eta) \sim \frac{1}{e\sqrt{2}} e^{-\pi\eta/2} \left(\frac{e}{2L}\right)^{L+1}, \qquad L \to \infty. \tag{7.7}$$

In particular, $F_L$ is the minimal solution of (7.5). Therefore, $F_L$ may be obtained by the algorithm in (3.9), provided a suitable infinite series can be found for normalization. The proper selection of this series is a rather crucial matter, and will be discussed next.

For computational convenience we first let

$$f_L = \frac{2^L L!}{(2L)!C_L(\eta)} F_L(\eta, \rho). \tag{7.8}$$

Among other things (relatively slow rate of growth of the coefficients $\lambda_L$ in (7.11) below), this effectively removes square roots in (7.5). In fact, using (7.4), one finds that $f_L$ is the minimal solution of

$$\frac{L[(L+1)^2+\eta^2]}{(L+1)(2L+3)} y_{L+1} - \left[\eta + \frac{L(L+1)}{\rho}\right] y_L + \frac{L(L+1)}{2L-1} y_{L-1} = 0. \tag{7.9}$$

The following expansion is known (see, e.g., [6, p. 131, formula (16$\beta$)]),

$$z^{(1+\mu)/2} e^{\alpha z/2} = \sum_{n=0}^{\infty} \frac{\Gamma(\mu+n)}{\Gamma(\mu+2n)} P_n^{((\mu-1)/2+\kappa,(\mu-1)/2-\kappa)}(\alpha) M_{\kappa,\mu/2+n}(z), \tag{7.10}$$

where $P_n^{(\alpha,\beta)}(z)$ is the Jacobi polynomial of degree $n$. (For notation, see [55].) Letting $\mu = 1$, $\kappa = i\eta$, $z = 2i\rho$, $\alpha = -i\omega$, and writing $L$ for $n$, this becomes in view of (7.2), (7.8),

$$\rho e^{\omega\rho} = \sum_{L=0}^{\infty} \lambda_L f_L, \qquad \lambda_L = i^L P_L^{(i\eta,-i\eta)}(-i\omega). \tag{7.11}$$

If $\omega = i$, then one easily shows that (7.11) reduces to a result attributed in [53] to P. Henrici. As one of several alternatives, it was suggested in this reference to apply Miller's backward recurrence algorithm to (7.9), using Henrici's series for normalization. Unfortunately, the process suffers from severe loss of accuracy when $\eta$ and $\rho$ are positive and large. We show that by selecting $\omega$ judiciously, the loss of accuracy can be kept under control.

We recall (cf. the end of §3) that loss of accuracy due to cancellation occurs if

$$\frac{s}{\lambda_0 f_0} = \frac{\rho e^{\omega\rho}}{f_0} \tag{7.12}$$

is very small in absolute value. Let

$$\tau = \frac{\rho}{2\eta},$$

so that the point $(\eta, \rho)$ is above or below the transition line, depending on whether $\tau > 1$ or $0 < \tau < 1$, respectively, and $\eta < 0$ if $-\infty < \tau < 0$. In each of these three cases, $f_0$ will behave differently as $|\eta| \to \infty$ and $\tau$ is held fixed. In fact, using general asymptotic results for Whittaker functions due to Buchholz (see [6, p. 101 ff, formulae (7), (11), (16a)]), one obtains from (7.2), after some computation,[10]

$$f_0 \sim \frac{1}{\sqrt{2\pi\eta}} \left(\frac{\tau}{\tau-1}\right)^{1/4} e^{\pi\eta} \cos\left\{2\eta[\sqrt{\tau(\tau-1)} - \ln(\sqrt{\tau} + \sqrt{\tau-1})] - \frac{\pi}{4}\right\},$$

$$\tau > 1, \eta \to \infty,$$

[10] In the cited formula (7) of [6], the factor $\exp(\mp\kappa i(\kappa - (1+\mu)/2))$ should read $\exp(\mp\pi i(\kappa - (1+\mu)/2))$.

$$f_0 \sim \frac{1}{2\sqrt{2\pi\eta}}\left(\frac{\tau}{1-\tau}\right)^{1/4} \exp\{\eta[\pi - 2\arccos\sqrt{\tau} + 2\sqrt{\tau(1-\tau)}]\},$$

$$0 < \tau < 1, \eta \to \infty,$$

$$f_0 \sim \frac{1}{\sqrt{2\pi|\eta|}}\left(\frac{|\tau|}{|\tau|+1}\right)^{1/4} \sin\left\{2|\eta|[\sqrt{|\tau|(|\tau|+1)} + \ln(\sqrt{|\tau|} + \sqrt{|\tau|+1})] - \frac{\pi}{4}\right\}, \qquad -\infty < \tau < 0, \eta \to -\infty.$$

To prevent the quantity in (7.12) from becoming exponentially small, as $\eta \to \infty$, we are led to choose

$$\omega \geqq \begin{cases} \dfrac{\pi}{2\tau}, & \tau \geqq 1, \\ \dfrac{1}{2\tau}[\pi - 2\arccos\sqrt{\tau} + 2\sqrt{\tau(1-\tau)}], & 0 < \tau < 1, \\ 0, & \tau < 0. \end{cases} \tag{7.13}$$

Since for reasons which become clear later, small values of $\omega$ are to be preferred, equality in (7.13) is suggested. The parameter $\omega$ so defined then depends continuously on $\tau$ in the interval $(0, \infty)$, and decreases monotonically from $\infty$ to 0. Clearly, as long as $\eta$ is small, say $<1$, the choice $\omega = 0$ is entirely satisfactory.

Other series expansions obtained by letting $\mu = 2L_0 + 1$, $\alpha = 0$ in (7.10) have also been suggested for normalization [57], whereby the integer $L_0$ is adjusted empirically to control the loss of accuracy.

The normalization identity now completely determined by (7.11) and (7.13) (with equality sign), we proceed with a discussion of the resulting algorithm (3.9).

We first observe that the coefficients $\lambda_L$ in (7.11) satisfy

$$\lambda_{L+1} = \frac{2L+1}{L+1}\omega\lambda_L + \frac{L^2+\eta^2}{L(L+1)}\lambda_{L-1}, \qquad L = 1, 2, 3, \cdots, \tag{7.14}$$

$$\lambda_0 = 1, \qquad \lambda_1 = \omega - \eta, \tag{7.15}$$

as follows readily from the well-known recurrence relation for Jacobi polynomials. In particular, they are all real. Using (7.14), (7.15) to generate the $\lambda_L$, algorithm (3.9) becomes

$$\begin{aligned} r_\nu^{(\nu)} &= 0, \qquad r_{L-1}^{(\nu)} = \frac{1}{(2L-1)}\left\{\eta/(L(L+1)) + 1/\rho \right. \\ &\quad \left. - \left[1 + \left(\frac{\eta}{L+1}\right)^2\right] r_L^{(\nu)}/(2L+3)\right\}^{-1}, \\ s_\nu^{(\nu)} &= 0, \qquad s_{L-1}^{(\nu)} = r_{L-1}^{(\nu)}(s_L^{(\nu)} + \lambda_L), \end{aligned} \qquad L = \nu, \nu-1, \cdots, 1, \tag{7.16}$$

$$f_0^{(\nu)} = \frac{\rho e^{\omega\rho}}{1 + s_0^{(\nu)}}, \qquad f_L^{(\nu)} = r_{L-1}^{(\nu)} f_{L-1}^{(\nu)}, \qquad L = 1, 2, \cdots, L_{\max}.$$

The final results $F_L$ are readily obtained from (7.8), with the help of (7.4).

It is worthwhile to examine more closely the three-term recurrence relation (7.14). We note that it is a difference equation of the Poincaré type, with characteristic equation

$$t^2 - 2\omega t - 1 = 0.$$

Since the roots are

$$t_1 = \omega + \sqrt{\omega^2 + 1}, \qquad t_2 = \omega - \sqrt{\omega^2 + 1},$$

it follows from Theorem 2.2 that (7.14) for $\omega \neq 0$ has a minimal solution $\lambda_L'$ for which

$$\frac{\lambda_{L+1}'}{\lambda_L'} \sim \omega - \sqrt{\omega^2 + 1}, \qquad L \to \infty, \tag{7.17}$$

while all other solutions behave according to

$$\frac{\lambda_{L+1}}{\lambda_L} \sim \omega + \sqrt{\omega^2 + 1}, \qquad L \to \infty. \tag{7.18}$$

To convince ourselves that the solution $\lambda_L$ defined by (7.15) is *not* a minimal solution, we make use of the asymptotic formula[11]

$$P_n^{(\alpha,\beta)}(z) \sim (z-1)^{-\alpha/2}(z+1)^{-\beta/2}[(z+1)^{1/2} + (z-1)^{1/2}]^{\alpha+\beta} \times (2\pi n)^{-1/2}(z^2-1)^{-1/4}[z + (z^2-1)^{1/2}]^{n+1/2}, \qquad n \to \infty,$$

where $z$ is outside the segment $[-1, 1]$. It follows, by a simple computation, that

$$\lambda_L = i^L P_L^{(i\eta,-i\eta)}(-i\omega) \sim e^{-\eta\phi}(2\pi L)^{-1/2}(1+\omega^2)^{-1/4}[\omega + \sqrt{\omega^2+1}]^{L+1/2}, \tag{7.19}$$
$$\omega \neq 0, \qquad L \to \infty,$$

where

$$\phi = \arctan\frac{1}{\omega}, \tag{7.20}$$

so that indeed (7.18) holds, rather than (7.17).

It may appear, therefore, that the use of (7.14) in forward direction is numerically "safe." Unfortunately, and surprisingly, it was observed by computation [applying algorithm (3.9) to (7.14)] that $\lambda_L$ *defined by* (7.14), (7.15) *approaches a minimal solution*, in the sense

$$\lambda_1 \to \lambda_1',$$

$\{\lambda_L'\}$ being normalized by $\lambda_0' = 1$, as either $\eta$, or $\rho$, or both, become large.

[11] See [55, p. 194], where the result is stated for real $\alpha$, $\beta$. The derivation by the method of steepest descent, however, is valid for arbitrary complex values of $\alpha$, $\beta$.

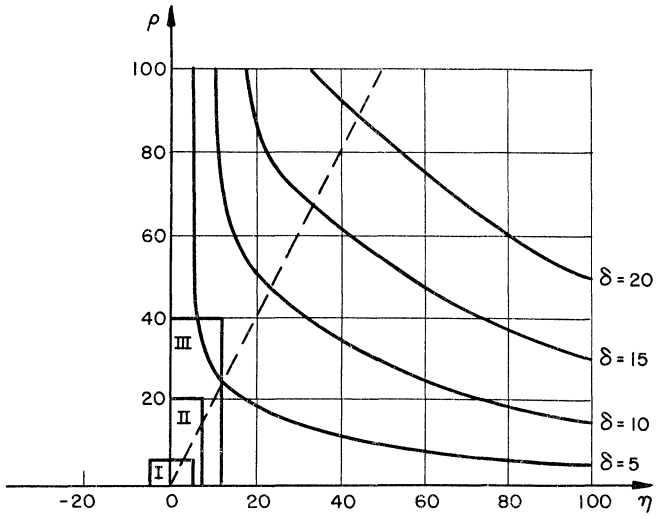


FIG. 10. *Degree of minimality of* $\{\lambda_L\}$. *The regions I, II, III indicate coverage of the tables* [36], [31], [58], *respectively, for* $F_L(\eta, \rho)$.

(Recall that $\omega$ is equal to the right-hand expressions in (7.13), and is thus a function of $\rho$ and $\eta$.) To describe this phenomenon more precisely, let

$$\delta = -\log | \lambda_1 - \lambda_1' |,$$

which may be considered a measure of the "degree of minimality" of the solution $\lambda_L$. (We expect, roughly speaking, that the generation of $\lambda_L$ by (7.14), (7.15) involves a loss of about $\delta$ decimal digits due to cancellation.) Fig. 10 shows the behavior of $\delta$ as a function of $\eta$ and $\rho$. In particular, it can be seen that no serious cancellation problems arise in the regions (marked, I II, III) which are commonly of interest in applications. However, in special applications which involve large values of $\eta$ and $\rho$, the loss of accuracy may indeed be quite substantial.

An obvious way to counteract this phenomenon is to generate the $\lambda_L$ in double precision arithmetic. However, this may not be very efficient, considering that $L$, in the region in question, may assume values as large as 100, or more. We suggest the following alternative.

Let

$$\epsilon = \lambda_1 - \lambda_1' = \omega - \eta - \lambda_1', \tag{7.21}$$

a quantity that can be calculated to any degree of accuracy (in double precision, if necessary) without too much effort, using algorithm (3.9) for $\lambda_1'$. Let furthermore $\lambda_L''$ be the solution of (7.14) defined by

$$\lambda_0'' = -\lambda_1', \qquad \lambda_1'' = 1. \tag{7.22}$$

Then, using elementary facts from the theory of linear difference equations, one finds that

$$\lambda_L = \lambda_L' + \frac{\epsilon}{1 + \lambda_1'^2}(\lambda_L'' + \lambda_1'\lambda_L'). \tag{7.23}$$

Having determined $\epsilon$ accurately, we may now use (7.23) to calculate $\lambda_L$. This requires the computation of the minimal solution $\lambda_L'$ by algorithm (3.9), and the computation of $\lambda_L''$ by (7.14), (7.22), but all of this can safely be done in single precision. Thus, double precision arithmetic will only be required in the computation of $\epsilon$ from (7.21).

For later use, we note the analogue of (7.19) for $\omega = 0$. In this case we use (cf. [55, p. 194] and footnote[11])

$$P_n^{(\alpha,\beta)}(0) \sim \frac{1}{\sqrt{\pi n}} 2^{(\alpha+\beta+1)/2} \cos\left([n + (\alpha + \beta + 1)/2]\frac{\pi}{2} - \left(\alpha + \frac{1}{2}\right)\frac{\pi}{2}\right), \qquad n \to \infty,$$

and find that

$$\lambda_L = i^L P_L^{(i\eta,-i\eta)}(0) \sim \frac{1}{\sqrt{2\pi L}}[(-1)^L e^{\pi\eta/2} + e^{-\pi\eta/2}], \qquad L \to \infty. \tag{7.24}$$

The starting value $\nu$ in (7.16) may be estimated similarly as for Bessel functions. Using (5.11), we may approximate the relative error of $f_L^{(\nu)}$ by

$$\frac{1}{\rho} e^{-\omega\rho}\lambda_{\nu+1} f_{\nu+1} - \frac{f_{\nu+1}}{g_{\nu+1}}\frac{g_L}{f_L}, \tag{7.25}$$

where $g_L = 2^L L!G_L(\eta, \rho)/((2L)!C_L(\eta))$. We wish to bound this for $L = L_{\max}$, assuming $L_{\max}$ and $\nu > L_{\max}$ large. By (7.6), (7.7), we have for large $L$,

$$\frac{f_L}{g_L} \sim \frac{e^{-\pi\eta}}{2e}\left(\frac{e\rho}{2L}\right)^{2L+1}.$$

Hence, the second term in (7.25), for large $\nu$ and $L$, may be estimated by

$$\frac{f_{\nu+1}}{g_{\nu+1}}\frac{g_L}{f_L} \sim \frac{\rho^2 L}{4\nu^3}\left(\frac{e\rho}{2}\right)^{2(\nu-L)} L^{2L}\nu^{-2\nu}. \tag{7.26}$$

To estimate the first term in (7.25) we observe from (7.19), (7.24), (7.6), and (7.8), that for $L$ large, and $\omega \geqq 0$,

$$|\lambda_L f_L| \lesssim \frac{\rho A(\eta)(1 + \omega^2)^{-1/4}[B(\omega)]^{1/2}}{\sqrt{4\pi L}}\left(\frac{e\rho B(\omega)}{2L}\right)^L,$$

where

$$A(\eta) = \begin{cases} 2\cosh(\pi\eta/2), & \omega = 0, \\ e^{-\eta\phi}, & \omega > 0, \end{cases}$$

$$B(\omega) = \omega + \sqrt{\omega^2 + 1},$$

$\phi$ being defined in (7.20) The total relative error (7.25) will thus be $\leqq \frac{1}{2}\cdot 10^{-d}$, if we require that

$$e^{-\omega\rho}A(\eta)(1+\omega^2)^{-1/4}[B(\omega)]^{1/2}\left(\frac{e\rho B(\omega)}{2(\nu+1)}\right)^{\nu+1} \leqq \frac{1}{4}\cdot 10^{-d},$$

$$\left(\frac{e\rho}{2}\right)^{2(\nu-L)} L^{2L}\nu^{-2\nu} \leqq \frac{1}{4}\cdot 10^{-d},\quad L = L_{\max}.$$

From here on, the analysis proceeds as for Bessel functions. Assuming (without loss of generality) that $L_{\max} > e\rho/2$, the result is that $\nu$ must satisfy both of the following conditions:

$$\begin{aligned}\nu &\geqq \frac{e\rho B(\omega)}{2}\, t\left(\frac{2}{e\rho B(\omega)}\,[D - \omega\rho + \ln\,(A(\eta)\sqrt{B(\omega)}(1+\omega^2)^{-1/4})]\right),\\ \nu &\geqq L_{\max}\, t\left(\frac{D}{2L_{\max}}\right),\end{aligned} \tag{7.27}$$

where we recall that $D = d \ln 10 + \ln 4$, and $t(x)$ is the inverse function of $x = t \ln t$.

An ALGOL procedure for the computation of $F_L(\eta, \rho)$, using the methods described in this paragraph, may be found in [20].

**8. Incomplete beta and gamma function.** The incomplete beta function is defined by the integral

$$B_x(p, q) = \int_0^x t^{p-1}(1-t)^{q-1}\,dt, \qquad p > 0, q > 0, 0 \leqq x \leqq 1. \tag{8.1}$$

The complete beta function is obtained when $x = 1$, and can be expressed in terms of gamma functions,

$$B_1(p, q) = \int_0^1 t^{p-1}(1-t)^{q-1}\,dt = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}. \tag{8.2}$$

For large $p$ or large $q$ Laplace's method (see [11, p. 37]) yields the asymptotic formulae,

$$B_x(p, q) \sim (1-x)^{q-1}\frac{x^p}{p}, \qquad p \to \infty, q \text{ fixed}, \tag{8.3}$$

$$B_x(p, q) \sim \Gamma(p)q^{-p}, \qquad q \to \infty, p \text{ fixed}. \tag{8.4}$$

In probability distribution theory the following ratio of beta functions is important,

$$I_x(p, q) = \frac{B_x(p, q)}{B_1(p, q)}. \tag{8.5}$$

Recurrence relations hold in both variables $p$ and $q$ (see [3]):[12]

$$\begin{aligned}pI_x(p+1, q) - [(p+q-1)x + p]I_x(p, q)\\ + (p+q-1)xI_x(p-1, q) = 0,\end{aligned} \tag{8.6}$$

[12] Formula (14) in [3] contains a misprint: the last term on the left should have the factor $q$, not $p$.

$$qI_x(p, q+1) - [(p+q-1)(1-x)+q]I_x(p, q) + (p+q-1)(1-x)I_x(p, q-1) = 0. \tag{8.7}$$

It also follows from (8.5) that

$$I_x(q, p) = 1 - I_{1-x}(p, q). \tag{8.8}$$

The calculation of $I_x(p, q)$ presents no difficulty when both $p$ and $q$ are small or moderately large. Expansion of $(1-t)^{q-1}$ into the binomial series then leads to a rapidly convergent series for $B_x(p, q)$, especially since by (8.8) we can always arrange to have $x$ in the interval $0 \leqq x \leqq \frac{1}{2}$. Moreover, the gamma functions in (8.2) are rapidly calculated by reducing the arguments to some standard interval for which rational approximations are available [60]. When $p$ or $q$ is large, however, it may be more efficient to make use of the recursions (8.6) or (8.7).

Consider then, first,

$$f_n = I_x(p+n, q), \qquad n = 0, 1, 2, \cdots; \quad 0 < p \leqq 1, \quad q > 0.$$

By (8.6) this is a solution of

$$y_{n+1} - \left(1 + \frac{n+p+q-1}{n+p}x\right)y_n + \frac{n+p+q-1}{n+p}xy_{n-1} = 0, \tag{8.9}$$

again a Poincaré difference equation. The characteristic equation $t^2 - (1+x)t + x = 0$ has the roots

$$t_1 = 1, \qquad t_2 = x.$$

By inspection (8.9) has the solution $y_n \equiv 1$, which clearly corresponds to the root $t_1$. On the other hand, from (8.3) and (8.5), we find

$$f_{n+1}/f_n \sim x, \qquad n \to \infty,$$

so that $f_n$ corresponds to the root $t_2$. Therefore, $f_n$ is the minimal solution of (8.9).

While our methods of §§3 and 4 again apply, it must be noted that in contrast to the previous examples the dominant solution is now bounded. Forward recursion by means of (8.9) should therefore cause no difficulties if the $f_n$ are to be obtained to a fixed number of decimals after the decimal point. If a given number of *significant* digits is required, however, it is more appropriate to employ the algorithms in §§3 and 4. The initial value $f_0 = I_x(p, q)$ needed in these algorithms may be obtained by first reducing $q$ modulo 1 to $q_0$, where $0 < q_0 \leqq 1$, then calculating $I_x(p, q_0)$, $I_x(p, q_0+1)$ by series expansion, and finally applying the second recursion (8.7) to connect with $I_x(p, q)$.

Consider next

$$g_n = I_x(p, q+n), \qquad n = 0, 1, 2, \cdots; \quad p > 0, \quad 0 < q \leqq 1.$$

From (8.7) we now get the difference equation

$$y_{n+1} - \left[1 + \frac{n+p+q-1}{n+q}(1-x)\right] y_n + \frac{n+p+q-1}{n+q}(1-x) y_{n-1} = 0, \tag{8.10}$$

which may also be obtained from (8.9) by interchanging $p$ with $q$ and, simultaneously, $x$ with $1 - x$. Therefore (8.10) has the solutions $g_n$ and $I_{1-x}(q+n, p)$, of which the latter is again the minimal solution. We see that $g_n$ is among the dominant solutions, and no problem of numerical instability arises.

For a detailed description of these algorithms we refer to [17].

The incomplete gamma function is defined by

$$P(a, x) = \frac{1}{\Gamma(a)} \int_0^x e^{-t} t^{a-1}\, dt, \qquad a > 0, x > 0. \tag{8.11}$$

It satisfies the well-known recurrence relation

$$P(a, x) = P(a-1, x) - \frac{x^{a-1} e^{-x}}{\Gamma(a)},$$

which, by elimination of the inhomogeneous term, can be brought into the form

$$aP(a+1, x) - (x+a)P(a, x) + xP(a-1, x) = 0.$$

Letting $f_n = P(a+n, x)$, we therefore find that $f_n$ is a solution of

$$(a+n)y_{n+1} - (x+a+n)y_n + xy_{n-1} = 0, \quad n = 1, 2, 3, \cdots. \tag{8.12}$$

This again is a Poincaré difference equation, whose characteristic equation $t^2 - t = 0$ has the roots $t_1 = 1$, $t_2 = 0$. The solution of (8.12) corresponding to $t_1$ is clearly $y_n \equiv 1$. The solution corresponding to $t_2$ is $f_n$, since

$$\frac{f_{n+1}}{f_n} \sim \frac{x}{n}, \qquad n \to \infty,$$

as follows from the well-known asymptotic formula

$$P(a, x) \sim x^a e^{-x}/\Gamma(a+1), \qquad a \to \infty.$$

(See, e.g., [13, p. 140].) Consequently, $f_n$ is a minimal solution of (8.12).

To obtain an infinite series in $f_n$, we multiply $f_m$ by

$$\lambda_m = \frac{\Gamma(a+m)}{m!\Gamma(a)}, \tag{8.13}$$

and sum over $m$. We get

$$\sum_{m=0}^{\infty} \lambda_m f_m = \frac{1}{\Gamma(a)} \sum_{m=0}^{\infty} \frac{1}{m!} \int_0^x e^{-t} t^{a+m-1}\, dt$$

$$= \frac{1}{\Gamma(a)} \int_0^x e^{-t} t^{a-1} \sum_{m=0}^{\infty} \frac{t^m}{m!}\, dt$$

$$= \frac{1}{\Gamma(a)} \int_0^x t^{a-1}\, dt = \frac{x^a}{a\Gamma(a)},$$

and therefore,

$$\sum_{m=0}^{\infty} \lambda_m f_m = \frac{x^a}{\Gamma(a+1)}. \tag{8.14}$$

The coefficients $\lambda_m$ can easily be obtained from the recursion

$$\lambda_0 = 1, \qquad \lambda_m = \frac{a+m-1}{m}\lambda_{m-1}, \qquad m = 1, 2, 3, \cdots. \tag{8.15}$$

Our algorithms may now be applied to (8.12), (8.14) to compute $P(a+n, x)$ for $n = 0, 1, 2, \cdots, N$.

**9. Repeated integrals of the error function.** In problems of heat conduction the complementary error function

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-t^2}\, dt$$

and its repeated integrals frequently occur. Following Hartree [25] we denote

$$\mathrm{i}^0 \operatorname{erfc} z = \operatorname{erfc} z,$$

$$\mathrm{i}^n \operatorname{erfc} z = \int_z^{\infty} \mathrm{i}^{n-1} \operatorname{erfc} t\, dt, \qquad n = 1, 2, 3, \cdots.$$

It is also convenient to define

$$\mathrm{i}^{-1} \operatorname{erfc} z = \frac{2}{\sqrt{\pi}} e^{-z^2}.$$

Expressed as a single integral, we have

$$\mathrm{i}^n \operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^{\infty} \frac{(t-z)^n}{n!} e^{-t^2}\, dt.$$

Writing

$$\mathrm{i}^{n+1} \operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \left( \frac{1}{n+1} \int_z^{\infty} \frac{(t-z)^n}{n!} te^{-t^2}\, dt - \frac{z}{n+1} \int_z^{\infty} \frac{(t-z)^n}{n!} e^{-t^2}\, dt \right),$$

and evaluating the first integral by parts, one finds

$$\mathrm{i}^{n+1} \operatorname{erfc} z + \frac{z}{n+1} \mathrm{i}^n \operatorname{erfc} z - \frac{1}{2(n+1)} \mathrm{i}^{n-1} \operatorname{erfc} z = 0, \quad n = 0, 1, 2, \cdots.$$

Consider now

$$f_n = e^{z^2} \mathrm{i}^n \operatorname{erfc} z, \qquad n = -1, 0, 1, 2, \cdots,$$

which clearly is a solution of

$$y_{n+1} + \frac{z}{n+1} y_n - \frac{1}{2(n+1)} y_{n-1} = 0, \qquad n = 0, 1, 2, \cdots. \tag{9.1}$$

To this difference equation case (c) of Theorem 2.3 could be applied with the result that all solutions behave "similarly" as $n \to \infty$, viz.,

$$\limsup_{n\to\infty} (|\, y_n \,| \sqrt{n!})^{1/n} = \frac{1}{\sqrt{2}}.$$

This conclusion is somewhat deceiving, as in fact $f_n$ is the minimal solution of (9.1).

To see this, we make use of the result that for any fixed $z$, as $n \to \infty$,

$$\mathrm{i}^n \operatorname{erfc} z \sim \frac{e^{-(1/2)z^2}}{2^n \Gamma\left(\frac{n}{2} + 1\right)} \exp\left(-\sqrt{2n}\, z\right). \tag{9.2}$$

[See [13, p. 123] and also recall that the repeated integrals of the error function are related to parabolic cylinder functions $D_\nu(z)$ by

$$\mathrm{i}^n \operatorname{erfc} z = (e^{-z^2}/2^{n-1}\pi)^{1/2} D_{-n-1}(z\sqrt{2}).]$$

By inspection, moreover, one sees that

$$g_n = (-1)^n e^{z^2} \mathrm{i}^n \operatorname{erfc}(-z)$$

also satisfies the recurrence relation (9.1). Applying (9.2) to both $f_n$ and $g_n$, we find

$$(-1)^n \frac{f_n}{g_n} \sim e^{-2\sqrt{2n}z}, \qquad n \to \infty. \tag{9.3}$$

This shows that $f_n$ is indeed the minimal solution of (9.1) whenever $\operatorname{Re} z > 0$. Otherwise, when $\operatorname{Re} z < 0$, $g_n$ is the minimal solution.

Our algorithms of §§3 and 4 for computing $f_n$ are particularly simple, in this case, since the initial value is known to be

$$f_{-1} = 2/\sqrt{\pi}.$$

From (9.3) it is evident that convergence of the first algorithm is better the further away $z$ is from the imaginary axis.

The application of Miller's backward recurrence algorithm in this connection was first suggested by M. Abramowitz [1], and is further analyzed in [16].

We note, incidentally, that Theorem 1.1 gives us the identity

$$\frac{f_n}{f_{n-1}} = \cfrac{\cfrac{1}{2(n+1)}}{\cfrac{z}{n+1} + \cfrac{\cfrac{1}{2(n+2)}}{\cfrac{z}{n+2} + \cfrac{\cfrac{1}{2(n+3)}}{\cfrac{z}{n+3} + \cdots}}},$$

which by an equivalence transformation can be brought into the form

$$\frac{\mathrm{i}^n \operatorname{erfc} z}{\mathrm{i}^{n-1} \operatorname{erfc} z} = \cfrac{1/2}{z + \cfrac{(n+1)/2}{z + \cfrac{(n+2)/2}{z + \cdots}}}, \qquad \operatorname{Re} z > 0.$$

For $n = 0$, this reduces to the well-known result

$$2e^{z^2}\int_z^\infty e^{-t^2}\,dt = \frac{1}{z+}\,\frac{1/2}{z+}\,\frac{1}{z+}\,\frac{3/2}{z+}\cdots.$$

**10. An example arising in the numerical computation of Fourier coefficients.** Let $f(t)$ be a function defined and continuous on the closed interval $[0, 2\pi]$, and let

$$(10.1)\qquad a_p = \int_0^{2\pi} f(t)\cos pt\,dt, \qquad b_p = \int_0^{2\pi} f(t)\sin pt\,dt, \quad p = 0, 1, 2, \cdots,$$

denote its Fourier coefficients. The computation of Fourier coefficients of high order ($p$ large) is notoriously difficult because of two reasons. Firstly, if one attempts to apply standard integration techniques, such as the trapezoidal rule, one is forced into a rather fine subdivision of the interval $[0, 2\pi]$ in order to cover adequately the many oscillations of the trigonometric factors in (10.1). Secondly, even if one adopts a sufficiently fine subdivision, substantial cancellation of digits will occur in the summation associated with the integration formula. Indeed, by Riemann's lemma, both $a_p$ and $b_p$ tend to zero when $p \to \infty$, whereas the individual terms of the integration formula need not be small at all. In matter of fact, cancellation will be more prominent the smoother the function $f$ is!

In order to circumvent these difficulties, it has been suggested to use Gauss type integration methods, treating the troublesome trigonometric factors as weight functions [61], [62]. As the general theory of Gaussian quadrature requires nonnegative weight functions, one first writes

$$(10.2)\qquad a_p = \int_0^{2\pi} f(t)\cos pt\,dt = \int_0^{2\pi} f(t)\,dt - \int_0^{2\pi} f(t)(1-\cos pt)\,dt,$$

and similarly for $b_p$. Then Gaussian integration is applied to the second integral, while the first integral is evaluated by some standard technique. Both integrals may have to be evaluated to high accuracy, since for large $p$, they are nearly equal. Thus, our cancellation problem is not entirely eliminated, but appears to be under better control.

Gaussian quadrature formulae of possibly various orders have to be obtained for each value of $p$. While this is a formidable task in itself, it appears feasible on current high-speed computers. One would presumably start from the moments

$$(10.3)\qquad c_n = \int_0^{2\pi} t^n(1-\cos pt)\,dt, \qquad s_n = \int_0^{2\pi} t^n(1-\sin pt)\,dt, \qquad n = 0, 1, 2, \cdots,$$

and use these to construct either the associated orthogonal polynomials, or the continued fractions associated with the formal power series

$$\sum_{n=0}^{\infty} c_n z^{-n-1}, \qquad \sum_{n=0}^{\infty} s_n z^{-n-1}.$$

The abscissae and weights of the desired quadrature formula then follow readily. Because of the inherent sensitivity of these quantities with respect to perturbations of the moments, it is rather important that the moments (10.3) be obtained as accurately as possible. Our concern here will be with a stable generation of these moments.

We assume $p$ a positive integer. Integrating by parts, we have[13]

$$c_{n+1} = \int_0^{2\pi} t^{n+1}(1 - \cos pt)\, dt = \left[t^{n+1}\left(t - \frac{\sin pt}{p}\right)\right]_0^{2\pi} - \int_0^{2\pi} (n+1)t^n \left(t - \frac{\sin pt}{p}\right) dt$$

$$= (2\pi)^{n+2} - (n+1)\int_0^{2\pi} t^{n+1}\, dt + \frac{n+1}{p}\int_0^{2\pi} t^n \sin pt\, dt$$

$$= (2\pi)^{n+2} - \frac{n+1}{n+2}(2\pi)^{n+2} - \frac{n+1}{p}\int_0^{2\pi} t^n(1 - \sin pt)\, dt + \frac{n+1}{p}\int_0^{2\pi} t^n\, dt$$

$$= (2\pi)^{n+2} - \frac{n+1}{n+2}(2\pi)^{n+2} + \frac{1}{p}(2\pi)^{n+1} - \frac{n+1}{p}s_n,$$

hence,

$$c_{n+1} = -\frac{n+1}{p}s_n + (2\pi)^{n+1}\left(\frac{1}{p} + \frac{2\pi}{n+2}\right), \quad n = 0, 1, 2, \cdots. \tag{10.4}$$

Similarly, one obtains

$$s_{n+1} = \frac{n+1}{p}c_n + \frac{(2\pi)^{n+2}}{n+2}, \quad n = 0, 1, 2, \cdots. \tag{10.5}$$

Replacing $n$ by $n - 1$ in (10.5), and inserting the result in (10.4), one gets

$$c_{n+1} = -\frac{n(n+1)}{p^2}c_{n-1} + \frac{(2\pi)^{n+2}}{n+2}, \quad n = 1, 2, 3, \cdots. \tag{10.6}$$

Eliminating similarly the $c$'s from (10.4) and (10.5), one gets

$$s_{n+1} = -\frac{n(n+1)}{p^2}s_{n-1} + (2\pi)^n\left(\frac{n+1}{p^2} + \frac{2\pi}{p} + \frac{4\pi^2}{n+2}\right), \quad n = 1, 2, 3, \cdots. \tag{10.7}$$

Writing down (10.6) once with $n$ increased by unity, and once with $n$ decreased

[13] In principle, $c_n$ and $s_n$ could be evaluated in closed form. However recursive generation of these quantities is more effective. Alternatively, we could integrate the additive term $t^n$ in closed form, and compute $\int_0^{2\pi} t^n \cos pt\, dt$ and $\int_0^{2\pi} t^n \sin pt\, dt$ recursively. No substantial simplification would result, however.

by unity, and eliminating the inhomogeneous terms, one finally obtains

$$c_{n+2} + \left[\frac{(n+1)(n+2)}{p^2} - \frac{4\pi^2(n+1)}{n+3}\right] c_n - 4\pi^2 \frac{(n-1)n(n+1)}{p^2(n+3)} c_{n-2} = 0. \tag{10.8}$$

Similarly,

$$s_{n+2} + \left[\frac{(n+1)(n+2)}{p^2} - \sigma_n\right] s_n - \sigma_n \frac{(n-1)n}{p^2} s_{n-2} = 0, \tag{10.9}$$

where

$$\sigma_n = 4\pi^2 \frac{n + 2 + 2\pi p + \dfrac{4\pi^2 p^2}{n+3}}{n + 2\pi p + \dfrac{4\pi^2 p^2}{n+1}}.$$

The recurrence relations (10.8), (10.9) are valid for $n \geqq 2$.

It is clear that (10.8), (10.9) permit, in principle, all moments of even order to be obtained from those of order 0 and 2,

$$\begin{aligned} c_0 &= 2\pi, \qquad c_2 = 4\pi\left(\frac{2\pi^2}{3} - \frac{1}{p^2}\right), \\ s_0 &= 2\pi, \qquad s_2 = 4\pi^2\left(\frac{2\pi}{3} + \frac{1}{p}\right), \end{aligned} \tag{10.10}$$

and all moments of odd order from those of order 1 and 3,

$$\begin{aligned} c_1 &= 2\pi^2, \qquad c_3 = 4\pi^2\left(\pi^2 - \frac{3}{p^2}\right), \\ s_1 &= 2\pi\left(\pi + \frac{1}{p}\right), \qquad s_3 = 4\pi\left(\pi^3 + \frac{2\pi^2}{p} - \frac{3}{p^3}\right). \end{aligned} \tag{10.11}$$

As it happens, however, the moments are minimal solutions of (10.8) and (10.9), respectively. Therefore, straightforward recursion, as indicated, is highly unstable. We expect the algorithms of §§3 and 4 to be rather more effective, especially since the first relations in (10.10), (10.11) can be used for normalization.

To establish the minimal character of the moments, let us first write

$$c_{2n+h} = C_n, \qquad s_{2n+h} = S_n,$$

where $h$ is either zero or one. Then $C_n$ and $S_n$ are both solutions of three-term recurrence relations of the standard form

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots, \tag{10.12}$$

the Newton-Puiseux diagram in both cases having the form shown in Fig. 11.

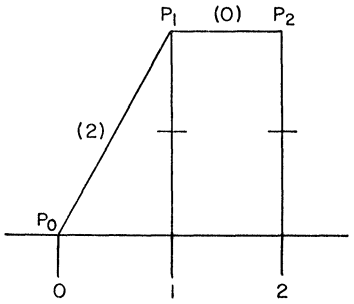


FIG. 11. *Newton-Puiseux diagram for* (10.8), (10.9)

Moreover,

$$a_n \sim \frac{4}{p^2} n^2, \qquad b_n \sim -\frac{16\pi^2}{p^2} n^2, \qquad n \to \infty.$$

It follows from part (a) of Theorem 2.3 that (10.12) has a pair of fundamental solutions, $y_{n,1}$ and $y_{n,2}$, for which

$$\frac{y_{n+1,1}}{y_{n,1}} \sim -\frac{4}{p^2} n^2, \qquad \frac{y_{n+1,2}}{y_{n,2}} \sim 4\pi^2, \qquad n \to \infty. \tag{10.13}$$

Both solutions thus tend with $n$ to infinity, but the first one much more rapidly than the second.

On the other hand, applying Laplace's method [11, p. 37] to the integrals in (10.3), one finds readily that for $n \to \infty$,

$$C_n \sim p^2(\pi/n)^3(2\pi)^{2n+h}, \qquad S_n \sim \frac{\pi}{n}(2\pi)^{2n+h}, \qquad h = 1, 2.$$

The $C$'s and $S$'s, therefore, exhibit the same asymptotic behavior as $y_{n,2}$ in (10.13). Consequently, they are both minimal solutions of the respective equation (10.12).

**11. A Sturm-Liouville boundary value problem.** Consider the Sturm-Liouville boundary value problem with one boundary condition at infinity,

$$(p(t)y')' + q(t)y = 0, \qquad y(0) = 1, \qquad y(\infty) = 0. \tag{11.1}$$

We assume that $p$ and $q$ are real-valued continuous functions in $[0, \infty)$, with $p(t) > 0$, $q(t) \leqq 0$, and in addition that

$$\int^{\infty} \frac{dt}{p(t)} = \infty, \qquad -\int^{\infty} q(t)\left(\int^{t} \frac{ds}{p(s)}\right) dt = \infty. \tag{11.2}$$

Then the boundary value problem (11.1) has an unique solution which is minimal in the continuous sense [24, p. 357 ff]. When solving the problem numerically, by a method of finite differences, we expect the approximate solution to be minimal in the discrete sense. We wish to illustrate this in the case of a simple finite difference scheme.

Consider mesh points $t_n = nh$, $n = 0, 1, 2, \cdots$, where $h > 0$ is small, but fixed, and let $y_n$ designate approximations at $t_n$ to the solution $y(t)$ of (11.1),

$$y_n \doteq y(t_n), \qquad n = 0, 1, 2, \cdots.$$

Such approximations may be obtained by first rewriting (11.1) as a system of two first-order differential equations, letting $z = p(t)y'$,

$$z' + q(t)y = 0,$$

$$y' - \frac{1}{p(t)} z = 0,$$

and then replacing derivatives by central difference quotients. We get

$$\frac{z_{n+1/2} - z_{n-1/2}}{h} + q_n y_n = 0,$$

$$\frac{y_{n+1/2} - y_{n-1/2}}{h} - \frac{1}{p_n} z_n = 0,$$

where $p_n = p(t_n)$, $q_n = q(t_n)$. Eliminating the $z$'s, we obtain the following discrete analogue of (11.1),

$$y_{n+1} - \frac{p_{n+1/2} + p_{n-1/2} - h^2 q_n}{p_{n+1/2}} y_n + \frac{p_{n-1/2}}{p_{n+1/2}} y_{n-1} = 0, \quad n = 1, 2, 3, \cdots, \tag{11.3}$$

$$y_0 = 1, \qquad \lim_{n\to\infty} y_n = 0. \tag{11.4}$$

It appears to be an open question whether under the assumptions (11.2), or some discrete analogue thereof, the difference equation (11.3) possesses a minimal solution satisfying (11.4), if $h$ is suitably restricted. The answer, however, is in the affirmative, if we make the stronger assumptions

$$\lim_{t\to\infty} p(t) = p > 0, \qquad \lim_{t\to\infty} q(t) = q < 0. \tag{11.5}$$

Then, indeed, (11.3) is a Poincaré difference equation having the characteristic equation

$$t^2 - \left(2 - h^2 \frac{q}{p}\right) t + 1 = 0.$$

Since $p > 0$, $q < 0$, the roots $t_1$, $t_2$ of this equation are real and distinct for all $h > 0$. In fact,

$$t_1 = 1 - h^2 \frac{q}{2p} + h \sqrt{\frac{-q}{p}\left(1 - h^2 \frac{q}{4p}\right)}, \qquad t_2 = t_1^{-1},$$

so that $t_1 > 1$, $0 < t_2 < 1$. The solution of (11.3) corresponding to $t_2$ therefore is a minimal solution, for arbitrary $h$, and can be normalized to satisfy the first condition in (11.4). The second condition (at infinity) is insured, since by Theorem 2.2,

$$\frac{y_{n+1}}{y_n} \sim t_2, \qquad n \to \infty,$$

for any minimal solution of (11.3).

Clearly, algorithm (3.9) applies in its simplified form (without the $s$-recursion), since $y_0$ is given to be 1.

By way of an example, consider

$$y'' = \frac{1+t}{2+t}\, y, \qquad y(0) = 1, \qquad y(\infty) = 0. \tag{11.6}$$

(This may be interpreted as a heat conduction problem for an infinite rod; cf. [8, p. 150]). Here,

$$p(t) \equiv 1, \qquad q(t) = -\frac{1+t}{2+t},$$

and (11.5) is satisfied with $p = 1$, $q = -1$. The discrete analogue of (11.6) takes the form

$$y_{n+1} - \left(2 + h^2 \frac{1+nh}{2+nh}\right) y_n + y_{n-1} = 0,$$

$$y_0 = 1, \qquad \lim_{n\to\infty} y_n = 0.$$

Applying algorithm (3.9), we obtain approximations $y_n^{(\nu)}$ to $y_n$ from

$$r_\nu^{(\nu)} = 0, \qquad r_{n-1}^{(\nu)} = \frac{1}{2 + h^2 \dfrac{1+nh}{2+nh} - r_n^{(\nu)}}, \qquad n = \nu, \nu-1, \cdots, 1,$$

$$y_0^{(\nu)} = 1, \qquad y_n^{(\nu)} = r_{n-1}^{(\nu)}\, y_{n-1}^{(\nu)}, \qquad n = 1, 2, \cdots, N. \tag{11.7}$$

Here, $N$ is determined by the length of the interval in which the solution $y(t)$ is sought.

Table 2 displays selected numerical results for integrating (11.6) by (11.7) on the interval [0, 5]. The first column shows the number $N$ of subintervals, the second column the corresponding value of $h$ ($= 5/N$), the third column the

TABLE 2

*Approximate solution $y_n^{(\nu)}$ of the boundary value problem* (11.6) *by means of* (11.7), *for* $n = kN/5$, $k = 0(1)5$

| $N$ | $h$ | $\nu$ | $t$ | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | 0 | 1 | 2 | 3 | 4 | 5 |
| 5 | 1 | 13 | 1.0 | .446887 | .191699 | .080285 | .033098 | .013494 |
| 10 | .5 | 25 | 1.0 | .443648 | .187645 | .077222 | .031219 | .012465 |
| 50 | .1 | 116 | 1.0 | .442753 | .186395 | .076251 | .030620 | .012137 |
| 250 | .02 | 511 | 1.0 | .442729 | .186352 | .076217 | .030598 | .012124 |

smallest integer $\nu$ for which six significant digits are achieved. The remaining columns contain the approximations $y_n^{(\nu)}$ corresponding to $t = 1(1)5$.

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