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# Computational Methods in Special Functions–A Survey

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## Introduction

Scientific computing often requires special functions. In the past, the need for numerical values was partly satisfied by extensive mathematical tables. Today, with powerful digital computers available, such values are obtained almost invariably by direct computation. We wish to review here the principal methods used in computing special functions.

We may group these methods into two large classes, namely those based on direct approximation, and those based on functional equations. Among the former, we consider only rational approximation methods (§1). We thus leave aside a multitude of possible expansions in terms of other special functions. These expansions, indeed, while often helpful, still leave us with the problem of evaluating the special functions involved. Among the functional equations most useful for computation are linear and nonlinear recurrence relations. These are discussed in §§2 and 3. We omit references to other functional equations, such as differential and integral equations, since we consider them of secondary importance in our context. In §4 we give a brief account of the current state of computer software development for special functions.

Due to limitations in time and space, a number of important topics are omitted in this survey. Nothing is said, e.g., about elementary functions and special computational techniques related to them. Good accounts of this can be found in Lyusternik, Chervonenkis and Yanpol'skii [1965] and Fike [1968]. Other topics not covered include methods based on numerical quadrature and on Euler-Maclaurin and Poisson summation formulas, the computation of zeros of special functions and of inverse functions, and the computation of special constants to very high precision.

Few references are given to computer algorithms for special functions, as they can be retrieved from the indices in the journal "Communications of the ACM" and in "Collected Algorithms from CACM" (a looseleaf collection issued by ACM of all algorithms published in Comm. ACM since 1960). Another topic dealt with only superficially are asymptotic methods, as these are discussed more fully elsewhere in this volume.

There are not many general references on computational methods for special functions. The only book devoted entirely to this subject is Hart et al. [1968]. The two volumes of Luke [1969] also contain much relevant material, and informative survey articles have been written by Bulirsch and Stoer [1968] and Thacher [1969].

As to notations for special functions, we try to be consistent with Abramowitz and Stegun [1964]. With regard to bibliographic references, we give special emphasis to the literature of the past twenty years or so. Little attempt has been made to trace all results back to the original sources.

## §1. Methods based on preliminary approximation

Our concern in this paragraph is with the approximation of a given function of a real or complex variable by means of "simpler" functions. Most attractive among these simpler functions are polynomials and rational functions, since they can be evaluated by a finite number of rational operations. Hence we restrict ourselves to polynomial and rational approximation. One should keep in mind, however, that other means of approximation, e.g., expansions in special functions like Bessel functions, can be equally effective if one takes advantage of appropriate recursive schemes of computation. (cf., e.g., 1.5.3, 2.2.2.)

The selection of a particular rational approximation depends on a number of circumstances. If the region of interest is an interval on the real line and our objective is to produce an approximation of high efficiency, and if we are prepared to expend the necessary effort, then we may seek to obtain a best rational approximation, i.e., one whose maximum error on the interval in question is as small as possible. This is often the preferred choice in computer subroutines. If, on the other hand, we are dealing with functions of a complex variable, or functions of several variables, we are led to use analytic approximation methods, the constructive theory of best approximation in the multivariate case still being in its infancy. (See, e.g., Collatz [1968], Williams [1972], Harris [1973], Fletcher, Grant and Hebden [1974], Watson [1975].) Even if we decide to construct a best approximation, in the process of doing so we still need to be able to calculate the function to high accuracy. Here again, analytic methods can be useful.

With regard to polynomial vs. rational approximation, folklore has it that "in some overall sense, rational approximation is essentially no better than polynomial approximation" (Newman [1964]). Precise theorems to this effect (Walsh [1968b], Feinerman and Newman [1974, p. 71 ff]) add further support to this contention. Experience, nevertheless, seems to show that for the special functions encountered in everyday practice, rational approximations are in fact somewhat superior.

In designing a rational approximation, certain preliminary decisions need to be made regarding the best form in which to approximate the function, the choice of auxiliary variables, and the best type of segmentation of the independent variable. As there is little theory to go by, such decisions are usually made by trial and error. Taylor series, or asymptotic expansions, usually suggest appropriate forms. For the problem of segmentation, see Lawson [1964], Collatz [1965], Meinardus [1966], [1964, §11 of English translation], Hawkins [1972].

### 1.1. Best rational approximation

Many computer subroutines for special functions employ rational approximations in appropriate segments of the real line. If the subroutine operates in an environment in which every value of the independent variable is equally likely to occur, it is natural to design the approximation in such a way that the error on each segment is "uniformly distributed", and about the same from segment to segment. In this way, no user is going to be punished if he happens to prefer one particular region over another. The logical conclusion of this philosophy is to employ the principle of best uniform approximation (Chebyshev approximation) on each segment and to arrange the maximum error to be about the same from segment to segment. The "uniform distribution" of the error is then guaranteed by the equi-oscillation property of the best approximation (cf. 1.1.1).

The theory of best uniform approximation is an important chapter of approximation theory, and is dealt with in a number of excellent books. We mention, e.g., Achieser [1956], Davis [1963], Meinardus [1964], Natanson [1964], Rice [1964b], [1969], Cheney [1966], Werner [1966], Rivlin [1969], Walsh [1969], Schönhage [1971], Feinerman and Newman [1974]. A treatise on numerical methods of Chebyshev approximation (not including, however, rational approximation) is Remez [1969]. Practical aspects of generating rational and polynomial approximations are reviewed by Cody [1970].

1.1.1. Best uniform rational approximation. We denote by $\mathbb{P}_n$ the class of polynomials of degree $\leq n$, and by $\mathbb{R}_{m,n}$ the family of rational functions

$$(1) \qquad r(x) = \frac{p(x)}{q(x)}, \quad p \in \mathbb{P}_n, \quad q \in \mathbb{P}_m, \quad q \not\equiv 0 .$$

Given a real-valued continuous function $f$ on the compact interval $[a, b]$, there exists a unique element $r^*_{m,n} \in \mathbb{R}_{m,n}$ such that

$$(2) \qquad \|r^*_{m,n} - f\|_\infty \leq \|r - f\|_\infty \quad \text{for all } r \in \mathbb{R}_{m,n} .$$

Here the norm is $\|u\|_\infty = \max\limits_{a\leq x\leq b} |u(x)|$ or, more generally, $\|u\|_\infty = \max\limits_{a\leq x\leq b} w(x)|u(x)|$, where $w$ is a positive weight function. One calls

$r^*_{m,n}$ the rational function of best uniform approximation to $f$ from $\mathbb{R}_{m,n}$ (or briefly the rational Chebyshev approximation of $f$ from $\mathbb{R}_{m,n}$). The associated error is denoted by

$$(3) \qquad E_{m,n}(f) = \|r^*_{m,n} - f\|_\infty .$$

In particular, there is a unique polynomial $p^*_n \in \mathbb{P}_n$ of best uniform approximation, with associated error $E_n(f) = E_{0,n}(f)$. The array of rational functions

$$\begin{array}{cccc} r^*_{0,0} & r^*_{0,1} & r^*_{0,2} & \cdots \\ r^*_{1,0} & r^*_{1,1} & r^*_{1,2} & \cdots \\ r^*_{2,0} & r^*_{2,1} & r^*_{2,2} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{array}$$

is referred to as the $L_\infty$ Walsh array of $f$ on $[a,b]$.

The best approximation $r^*_{m,n}$ is characterized by the equi-oscillation property, which states (excepting certain degenerate cases) that the error curve $w(r^*_{m,n} - f)$ assumes its extreme value (3) at $m+n+2$ consecutive points of $[a,b]$ with alternating signs (Achieser [1956, p. 55]). Moreover (barring again degeneracies), if $r \in \mathbb{R}_{m,n}$ is any rational function bounded on $[a,b]$ which has the oscillation property, i.e., an error curve $e = w(r-f)$ assuming values of alternating sign on $m+n+2$ consecutive points $x_i \in [a,b]$, say,

$$e(x_i) = (-1)^i \lambda_i, \quad \lambda_i > 0, \qquad i = 1,2,\ldots, m+n+2 ,$$

then (Achieser [1956, p. 52])

$$(4) \qquad \min_i \lambda_i \le E_{m,n}(f) \le \|e\|_\infty .$$

Concerning the behavior of $E_{m,n}(f)$ as m and n both tend to infinity, little is known. If m, or n, remains fixed, there are asymptotic results for meromorphic functions, due to Walsh [1964b], [1965], [1968a], while in the polynomial case $m = 0$ one has the classical results of Jackson and Bernstein. The former states that $E_n(f) = o(n^{-p})$ if $f \in C^p[a, b]$, the latter that $\limsup [E_n(f)]^{1/n} < 1$ precisely if f is analytic on [a, b], and $[E_n(f)]^{1/n} = o(1)$ precisely if f is entire (see, e.g., Natanson [1964, pp. 127, 183]).

1.1.2. <u>A list of available Chebyshev approximations</u>. Some entries of the Walsh array, often those along or near the diagonal $m = n$, have proven to yield remarkably efficient approximations for many of the special functions in current use. Table 1 lists those for which (numerically constructed) rational Chebyshev approximations are available. The first column shows the function being approximated, in the notation of Abramowitz and Stegun [1964]. The second column records the segmentation used, where $[a_0, a_1, \ldots, a_s]$ is written to indicate that the interval $[a_0, a_s]$ is broken up into segments $[a_{i-1}, a_i]$, $i = 1, 2, \ldots, s$. The exact form of the function which is being approximated, as well as the type (m, n) of rational function, usually changes from segment to segment in a manner not shown in the table. The third column tells whether the approximant is truly rational or polynomial. The fourth column indicates the approximate range of accuracy, where S is to be read as "significant decimal digits" and D as "decimal digits after the decimal point". The final column gives the source of the approximation. For an extensive bibliography of approximations see also Hart et al. [1968, pp. 161-179].

<u>Table 1</u>. Chebyshev approximations to special functions

| f(x) | segmentation | type | accuracy | reference |
|---|---|---|---|---|
| $E_1(x)$ | $[0, 1, 4, \infty]$ | rat. | 2-20S | Cody & Thacher [1968] |
| $Ei(x)$ | $[0, 6, 12, 24, \infty]$ | rat. | 3-20S | Cody & Thacher [1969] |

| f(x) | segmentation | type | accuracy | reference |
|---|---|---|---|---|
| $\Gamma(x)$ | [2, 3] | pol. | 7-18S | Werner & Collinge [1961] |
| $\ell n\,\Gamma(x)$ | [.5, 1.5, 4, 12] | rat. | 2-17S | Cody & Hillstrom [1967] |
| $\Gamma(x)$ | [2, 3]$^{(1)}$ | pol.&rat. | 1-24D | Hart et al. [1968] |
| $\ell n\,\Gamma(x)-(x-\frac{1}{2})\ell n x + x - \ell n\sqrt{2\pi}$ | [8, 1000] | " | 8-18D | " |
| " | [12, 1000] | " | 9-23D | " |
| $\arg\Gamma(1+ix)$ | [0, 2, 4, ∞] | rat. | 4-20S | Cody & Hillstrom [1970] |
| $\psi(x)$ | [1, 2] | pol. | 6-8D | Moody [1967] |
| $\psi(x)$ | [.5, 3, ∞] | rat. | 2-20S | Cody, Strecok & Thacher [1973] |
| erfc x | [0, 10] | rat. | 1-23D | Hart et al. [1968] |
| " | [0, 20] | " | 4-6D | " |
| " | [0, 4] | " | 1-9D | " |
| " | [0, 8] | " | 1-16S | " |
| " | [8, 100] | " | 3-17S | " |
| erf x | [0, .5] | rat. | 5-19S | Cody [1969] |
| erfc x | [.46875, 4, ∞] | rat. | 2-18S | " |
| $e^{-x^2}\int_0^x e^{t^2}dt$ | [0, 2.5, 3.5, 5, ∞] | rat. | 1-21S | Cody, Paciorek & Thacher [1970] |
| $C(x)$, $S(x)$ | [0, 1.2, 1.6, 1.9, 2, 4, ∞] | rat. | 2-18S | Cody [1968] |
| $J_n(x), I_n(x), Y_n(x), K_n(x)$ $n=0,1$ | [0, 8] | pol. | 2-7D | Werner [1958/59] |
| $J_\nu(x)$, $I_\nu(x)$ $\nu=-\frac{2}{3}, -\frac{1}{3}, \frac{1}{3}, \frac{2}{3}$ | [0, 4] | pol. | 10D | Bhagwandin [1962] |
| $K_\nu(x)$, $\nu=\frac{1}{3}, \frac{2}{3}$ | [4, ∞] | pol. | 10D | " |
| $H_\nu^{(1)}(x)$, $\nu=\frac{1}{3}, \frac{2}{3}$ | [4, ∞] | rat. | 10D | " |
| $I_0(x), I_1(x)$ | [0, 8, 70] | rat. | 8S | Gargantini [1966] |
| $K_0(x)$ | [0, .1, 8] | rat. | 8S | " |

| f(x) | segmentation | type | accuracy | reference |
|---|---|---|---|---|
| $K_1(x)$ | [0, 8] | rat. | 7S | Gargantini [1966] |
| $J_0(x), J_1(x), Y_0(x), Y_1(x)$ | $[0, 8, \infty]$ | rat. | 3-25D | Hart et al. [1968] |
| $I_0(x),\ I_1(x)$ | [0, 1] | rat. | 2-23S | Russon & Blair [1969] |
| $K_0(x),\ K_1(x)$ | $[0, 1, \infty]$ | rat. | 2-23S | " |
| $I_0(x),\ I_1(x)$ | $[0, 15, \infty]$ | rat. | 8-23S | Blair [1974] |
| $I_0(x),\ I_1(x)$ | $[0, 15, \infty]$ | rat. | 1-23S | Blair & Edwards [1974] |
| $Ki_r(x),\ r=1, 2, 3$ | $[0, \infty]$ | rat. | 2-7S | Gargantini & Pomentale [1964] |
| $\int_0^x I_0(t)dt$ | [0, 8, 30] | rat. | 8-9S | Gargantini [1966] |
| $\int_x^\infty K_0(t)dt$ | [0, .1, 8, 70] | rat. | 7S | " |
| $G_0(\eta, 2\eta), G_0'(\eta, 2\eta)$ | [1, 2, 3.5, 15] | rat. | 13-14S | Strecok & Gregory [1972] |
| $G_0(\eta, 1), G'_0(\eta, 1)$ | [0, 1] | rat. | 16S | " |
| $G_0(\eta, 30), G_0'(\eta, 30)$ | [15, 18.5, 22] | rat. | 13-14S | " |
| $\ell n(G_0(\eta, 30))$, $\ell n(-G_0'(\eta, 30))$ | [22, 30] | rat. | 13S | " |
| $\int_0^{\pi/2} (1-x^2 \sin^2 t)^{\pm\frac{1}{2}}dt$ | [0, 1] | pol. | 4-17D | Cody [1965] |
| $\zeta(x)$ | [.5, 5, 11, 25, 55] | rat. | 8-22S | Cody, Hillstrom & Thacher [1971] |
| $x^{-1} \int_0^x t^k(e^t-1)^{-1}dt$, $k = 1, 2, 3, 4$ | [0, 10] | rat. | 2-5D | Thacher [1960] |
| $\int_0^\infty t^{\frac{1}{2}}(e^{t-x}+1)^{-1}dt$ | $[-\infty, 1, \infty]$ | pol. | 3S | Werner & Raymann [1963] |
| $\int_0^\infty t^\nu(e^{t-x}+1)^{-1}dt$, $\nu = -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$ | $[-\infty, 1, 4, \infty]$ | rat. | 2-10S | Cody & Thacher [1967] |

(1) range incorrectly stated in Hart et al. [1968].

1.1.3. Computation of Chebyshev approximations. Most, if not all, of the approximations in Table 1 were generated by some version of Remez' second algorithm. This is a procedure, originally devised for polynomials (Remes [1934]) and later extended to rational functions, which attempts to achieve the equi-oscillation property in an iterative fashion. The object of the iteration, basically, is to move the two bounds in (4) ever closer together. There are many variants of the procedure, differing somewhat in the technical execution of each iteration step. Detailed descriptions of these can be found in some books on approximation theory, e.g., Meinardus [1964], Rice [1964b], Cheney [1966], Werner [1966], Remez [1969], Rivlin [1969], as well as in survey articles by Cheney and Southard [1963], Stiefel [1959], [1964], Fraser [1965], Ralston [1967], Krabs [1969], Cody [1970]. Computer algorithms are given in Stoer [1964], Werner [1966], Cody and Stoer [1966/67], Werner, Stoer and Bommas [1967], Cody, Fraser and Hart [1968], Huddleston [1972], Johnson and Blair [1973]. The construction of rational Chebyshev approximants, in spite of the many aids available, is still a tricky business due to the possibility of near-degeneracies. For a discussion of this, the reader is referred to Rice [1964a], Cody [1970], Huddleston [1972], Ralston [1973].

There are other methods of obtaining best rational approximations which rely more heavily on mathematical programming. Some of these are referenced in Lee and Roberts [1973] and compared there with Remez' algorithm. Others, more recently, are proposed by Har-El and Kaniel [1973] and Kaufman and Taylor [1974].

## 1.2. Truncated Chebyshev expansion

There is some effort involved in generating a best rational, or even polynomial, approximation to a given function $f$. Polynomials which approximate $f$ "nearly best" can be obtained more easily by truncating the Chebyshev expansion of $f$.

Assuming that the interval of interest has been transformed to $[-1, 1]$, we can formally expand $f$ into a series of Chebyshev polynomials,

$$\text{(1)} \qquad f(x) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} a_k T_k(x), \qquad -1 \le x \le 1 ,$$

where

$$\text{(2)} \qquad a_k = \frac{2}{\pi} \int_0^{\pi} f(\cos\theta) \cos k\theta \, d\theta, \qquad k = 0, 1, 2, \ldots .$$

In effect, (1) is the Fourier cosine expansion of $f(\cos\theta)$ . It converges uniformly and absolutely on $[-1,1]$ if $f \in C[-1,1]$ and $f' \in L_p[-1,1]$, $p > 1$ (Zygmund [1959, p. 242]). The polynomials referred to above are the partial sums of (1),

$$\text{(3)} \qquad s_n(f;x) = \frac{1}{2}a_0 + \sum_{k=1}^{n} a_k T_k(x), \qquad n = 0, 1, 2, \ldots .$$

The classical source on Chebyshev polynomials and their applications is Lanczos' introduction in National Bureau of Standards [1952]. More recent accounts can be found in the books of Fox and Parker [1968] and Rivlin [1974].

1.2.1. Convergence. The functions f encountered in practice are usually quite smooth, typically real-valued analytic on $[-1,1]$ and holomorphic in a domain of the complex plane enclosing the segment $[-1,1]$ . If $\epsilon$ is the eccentricity of the largest ellipse, with foci at $\pm 1$, in which f is holomorphic, then (1) converges like a geometric series with ratio $\epsilon/(1+\sqrt{1-\epsilon^2})$ (see, e.g., Werner [1966, §20], Rivlin [1974, p. 143]). For entire functions one has $\epsilon = 0$, and the convergence is supergeometric.

Scraton [1970] observes that convergence can be enhanced if one uses a suitable bilinear, rather than linear, transformation of variables to obtain the canonical interval $[-1,1]$ . Experimental evidence of this has previously been presented by Thacher [1966].

Compared with expansions of f in other orthogonal polynomials, particularly ultraspherical polynomials $P_k^{(\alpha,\alpha)}$, Lanczos early recognized

(National Bureau of Standards [1952]) that convergence is most rapid when $\alpha = -1/2$, i.e., when the expansion is indeed in Chebyshev polynomials. Some firm results in this direction, for restricted classes of functions, are due to Rivlin and Wilson [1969] and Handscomb [1973].

Closely related to convergence is the asymptotic behavior of the expansion coefficients $a_k$ as $k \to \infty$. This is studied in detail by Elliott [1964] for meromorphic functions, and also for functions with a branchpoint at an endpoint of the basic interval, and by Elliott and Szekeres [1965] for entire functions. The case of logarithmic and branch-point singularities on the real line, and combinations of such, is treated by Chawla [1966/67] and Piessens and Criegers [1974]. It is not uncommon to also find essential singularities at an endpoint or midpoint of $[-1,1]$. This occurs, e.g., if the original interval is infinite and $f$ has an essential singularity at infinity. Mapping the interval onto $[-1,1]$ by a reciprocal transformation carries the singularity into a point of $[-1,1]$. The extent to which this slows down the convergence of (1) is studied by Miller [1966]. Asymptotic results for the expansion coefficients in the case of generalized hypergeometric functions are given by Németh [1974].

1.2.2. Relation to best uniform approximation. Letting

$$S_n(f) = \max_{-1 \le x \le 1} |s_n(f;x) - f(x)| , \tag{4}$$

we clearly have $E_n(f) \le S_n(f)$, where $E_n(f)$ is the error of best uniform approximation of $f$ by polynomials of degree $n$. The difference between $S_n(f)$ and $E_n(f)$ can be remarkably small if $f$ is smooth. This can be seen from de La Vallée Poussin's inequality [1919, p. 107]

$$\left| \sum_{r=0}^{\infty} a_{(2r+1)(n+1)} \right| \le E_n(f) \le S_n(f) \le \sum_{k=n+1}^{\infty} |a_k| , \tag{5}$$

and from other similar results (Hornecker [1958], [1960], Hewers and Zeller [1960/61], Blum and Curtis [1961], Cheney [1966, p. 131], Rivlin

[1974, p. 139ff]). If $a_{k+1} = o(a_k)$, for example, it follows from (5) that $S_n(f) \sim E_n(f)$ as $n \to \infty$. Even for larger classes of functions, e.g., the class $C^{n+1}_{M_n}$ of functions $f \in C^{n+1}[-1,1]$ with $\max\limits_{-1\leq x\leq 1} |f^{(n+1)}(x)| \leq M_n$, the spread is still infinitesimal in the sense (Remez and Gavriljuk [1963])

$$\sup_{f\in C^{n+1}_{M_n}} S_n(f) = [1 + O(\tfrac{1}{n})] \sup_{f\in C^{n+1}_{M_n}} E_n(f), \qquad n \to \infty . \tag{6}$$

Widening the class further to include all continuous functions $f \in C[-1,1]$ we have from the theory of orthogonal series (Alexits [1961, Theorem 4.5.1]) that

$$1 \leq \frac{S_n(f)}{E_n(f)} \leq 1 + \lambda_n , \tag{7}$$

where $\lambda_n$ is the Lebesgue constant for Fourier series (Zygmund [1959, p. 67]). Although these constants eventually grow logarithmically with $n$ (Fejér [1910]), they are fairly small in the domain of common interest. It is known that $\lambda_n$ is monotonically increasing, in fact totally monotone (Szegö [1921]), and $\lambda_1 = 1.436$, $\lambda_{1000} = 4.07$ (Powell [1967]). The error of the truncated Chebyshev expansion, in the range $1 \leq n \leq 1000$, is therefore never worse than five times the error of the corresponding best uniform approximation.

When $f$ is a polynomial of degree $n+1$, then in fact $S_n(f) = E_n(f)$. For polynomials of degree $> n+1$ the ratios in (7) are investigated by Clenshaw [1964], Lam and Elliott [1972] and Elliott and Lam [1973]. Some of this work, however, is based on conjectures. For related work, see also Riess and Johnson [1972].

It is possible to modify the truncated Chebyshev expansion so as to bring it closer to the best uniform approximation (Hornecker [1958], [1960], Korneĭčuk and Širikova [1968], Širikova [1970]). Other modifications can be made to fit interpolatory conditions at the end points (Cohen

[1971]). This may be useful in segmented approximation when continuity at the joints is desirable.

Using a method reminiscent of Lanczos' $\tau$-method, Stolyarčuk [1974a, b] obtains explicit polynomial approximations to the sine integral, error function, and Bessel functions of integer order, which are valid on an arbitrary interval and are infinitesimally close to the best polynomial approximations on that interval as the degree tends to infinity.

1.2.3. Calculation of expansion coefficients. There are a number of methods available to calculate (or approximate) the expansion coefficients $a_k$. Some will now be considered.

(i) Fourier analysis. Since we are dealing with Fourier coefficients, we can enlist the techniques of harmonic analysis, and thus, for example, approximate $a_k$, $k \le n$, by

$$\alpha_k^{(n)} = \frac{2}{n} \sum_{j=0}^{n}{}'' f(x_j)\, T_k(x_j), \qquad x_j = \cos(j\pi/n) \quad . \tag{8}$$

(The primes on the summation sign indicate that the first and last term is to be halved.) Since $T_k(x_j) = T_j(x_k)$, the sum in (8) can be evaluated effectively by Clenshaw's algorithm (cf. 1.5.1(ii)).

It is a relatively simple matter to increase the accuracy of (8), by doubling $n$, if one observes that about half of the terms in (8) can be reused, and only half of the $\alpha_k^{(n)}$ need to be computed, by virtue of

$$\alpha_k^{(n)} = \alpha_k^{(2n)} + \alpha_{2n-k}^{(2n)}$$

(Clenshaw [1964], Torii and Makinouchi [1968]).

(ii) Rearrangement of power series. The coefficients $a_k$ of the Chebyshev expansion (1) are related to the coefficients $c_k$ of the Maclaurin series, $f(x) = \sum_{k=0}^{\infty} c_k x^k$, by the linear transformation

$$(9)\qquad \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} u_{00} & u_{01} & u_{02} & \cdots \\ 0 & u_{11} & u_{12} & \cdots \\ 0 & 0 & u_{22} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \end{bmatrix},$$

where

$$u_{ij} = \begin{cases} 2^{1-j}\dbinom{j}{\frac{j-i}{2}} & \text{if } i+j \text{ is even}, \quad j \geq i \geq 0, \\[2ex] 0 & \text{otherwise} \end{cases}$$

(Minnick [1957], De Vogelaere [1959]). As some of the coefficients $c_k$ may be quite large, and of different signs, the application of (9) is likely to require high-precision work. Another complication occurs if the power series converges very slowly (Clenshaw [1962]). The infinite series implied in (9) then also converge very slowly, although, sometimes, they respond well to nonlinear acceleration techniques (Thacher [1964]).

(iii) Recurrence relations. In many cases of practical interest it is possible to derive recurrence relations for the coefficients $a_k$, either directly from the integral representation (2), or indirectly via differential equations. In using these recursions, a certain amount of skill is required to maintain numerical stability (Clenshaw [1962], Luke and Wimp [1963], Németh [1965], [1974], Clenshaw and Picken [1966], Hangelbroek [1967], Wood [1967], Luke [1969 , Vol. II, §12.5], [1971b, c], [1972a]).

(iv) Numerical quadrature. The integral in (2) can be approximated directly by numerical quadrature. Eq. (8), in fact, is an example. For others, see Rivlin [1974, p. 153ff] and Bjalkova [1963].

(v) Explicit formulas. Explicit formulas for $a_k$ in terms of easily computed functions are known for a number of important special functions, e.g., Bessel functions $J_\nu$, $I_\nu$, $Y_\nu$, $K_\nu$ (Wimp [1962], Cylkowski [1966/68]), Dawson's integral (Hummer [1964]), $\psi(a+x)$, $\ln \Gamma(a+x)$, $\mathrm{Ci}(x)$, $\mathrm{Si}(x)$ (Wimp [1961]). Luke and Wimp [1963] express the expansion coefficients for confluent hypergeometric functions in terms of Meijer's G-function.

1.2.4. Tables of Chebyshev expansions and computer programs. The most extensive tables are those of Clenshaw [1962], Clenshaw and Picken [1966], and Luke [1969, Vol. II, Ch. XVII]. References to additional tables are given in Luke [1969, Vol. II, pp. 287-291]. Among the more recent specialized tables are those of Németh [1967] for Stirling's series, Strecok [1968] for the inverse error function, Wood [1968] for Clausen's integral, Ng, Devine and Tooper [1969] for Bose-Einstein functions, Wimp and Luke [1969] for modified Bessel functions and their incomplete Laplace transform, Kölbig, Mignaco and Remiddi [1970] for generalized polylogarithms, Németh [1971] for Airy functions, Németh [1972] for zeros of Bessel functions $J_\nu$ (considered as functions of $\nu$), Németh [1974] for the integrals $\int_0^\infty t^{-\frac{1}{2}} \exp(-t-t^2/x^2)dt$, $\int_0^\infty (x+t)^{-1} \exp(-t^2)dt$, and Sheorey [1974] for Coulomb wave functions.

An interesting and potentially useful idea, advanced by Clenshaw and Picken [1966] and pursued further by Luke [1971b, c], [1972a], is to provide "miniaturized" tables for functions of several variables. These are tables of coefficients in multiple Chebyshev series. The idea is carried out for Bessel functions of real argument and real order.

A set of ALGOL procedures facilitating the use of Chebyshev expansions is given in Clenshaw, Miller and Woodger [1962/63]. FORTRAN programs for generating Chebyshev expansion coefficients can be found in Håvie [1968] and Amos and Daniel [1972].

1.3. Taylor series and asymptotic expansion

A special function $f$ is often naturally represented in the form

$$f(z) = \alpha(z)\, g(z), \qquad g(z) \sim \sum_{k=0}^{\infty} c_k (z - z_0)^k, \qquad c_0 = 1 \,, \tag{1}$$

where the factor $\alpha(z)$ may vanish at $z_0$, be singular there, or represent some other peculiar behavior. The expansion for $g$ is a Taylor series if it converges to $g(z)$ at some $z \neq z_0$, hence in some circle $|z-z_0| < \rho$, $\rho > 0$. It is called an asymptotic expansion if it possibly diverges for every $z \neq z_0$, but for each $n$ $(n = 1, 2, 3, \ldots)$ obeys the law

$$g(z) - \sum_{k=0}^{n-1} c_k (z-z_0)^k = O((z-z_0)^n) \quad \text{as} \quad z \to z_0 . \tag{2}$$

It is customary, then, to write (2) in terms of descending powers of $\zeta$, where $\zeta = (z-z_0)^{-1}$.

We will not give here a systematic account of Taylor's series and of asymptotic expansions, but limit ourselves to a few remarks on the computational uses of these expansions, and to an example. We refer to Olver [1974] for a thorough treatment of asymptotic expansions and their application to special functions.

1.3.1. Computational uses. As a computational tool, Taylor series are most useful near the point of expansion, $z_0$, and then indeed may be quite effective. Further away from $z_0$ one runs into several problems, notably slow convergence, or absence of it, and severe cancellation of terms, with the attendant loss of significant digits. Asymptotic expansions, likewise, may be quite useful sufficiently close to $z_0$. The accuracy obtainable from a divergent asymptotic expansion, however, is limited at any fixed $z \neq z_0$, in contrast to convergent expansions. Also, error bounds are not always available, and the evaluation of higher order terms may be laborious.

Both expansions may serve purposes other than direct evaluation of functions. For one, they suggest an appropriate form in which to seek best rational approximations. For another, they may be used as input to some of the methods of 1.2, 1.4 for generating polynomial or rational approximations (cf., in particular, 1.2.3(ii), 1.4.1, 1.4.2, 1.4.5).

Nontrivial problems arise in the expansion of functions of several complex variables. Expanding in one variable leaves the coefficients to be functions of the remaining variables. This creates challenging problems of effective computation, satisfactory rate of convergence, etc. An example in point is the Taylor expansion of the Bessel function $K_\nu(z)$ of complex order and complex argument, which is treated by Temme [1973]. Another example will be discussed below.

A further important problem is the computation of the Taylor expansion coefficients $c_k$, when $z_0$ is an arbitrary point in the complex plane. (In particular, this yields $g(z_0) = c_0$ .) There are various approaches one can take: numerical quadrature on Cauchy's integral (Lyness and Sande [1971]), recursive computation of higher derivatives (as, e.g., in Gautschi [1966] and Gautschi and Klein [1970]), or more general backward recurrence techniques in cases where $g$ satisfies a linear differential equation with polynomial coefficients (Thacher [1972], and work of Thacher in progress). The more obvious process of analytic continuation (Henrici [1966]), unfortunately, is inherently unstable.

1.3.2. An example (Van de Vel [1969]). Consider the incomplete elliptic integral of the first kind (cf. 3.1.1),

$$F(\varphi, k) = \int_0^{\varphi} (1 - k^2 \sin^2 \theta)^{-\frac{1}{2}} d\theta, \quad 0 \le k \le 1, \quad 0 \le \varphi < \pi/2 \ , \tag{3}$$

where $\varphi$ is the amplitude and $k$ the modulus of $F$ . The developments to be made for (3) apply similarly to the integral of the second kind. The complementary modulus $k'$ is defined by

$$k' = \sqrt{1-k^2} \ , \tag{4}$$

and the complete integral by

$$\mathbb{K}(k) = F(\tfrac{\pi}{2}, k) = \int_0^{\pi/2} (1 - k^2 \sin^2 \theta)^{-\frac{1}{2}} d\theta, \quad 0 \le k < 1 \ . \tag{5}$$

We are interested in Taylor's expansion of $F$ with respect to the modulus $k$.

The most obvious attack is to expand the integrand in a binomial series and to integrate term by term. The result is

$$(6) \qquad F(\varphi, k) = \sum_{r=0}^{\infty} (-1)^r \binom{-\frac{1}{2}}{r} \sigma_r(\varphi) k^{2r}, \qquad \sigma_r(\varphi) = \int_0^{\varphi} \sin^{2r}\theta \, d\theta .$$

For the $\sigma_r$ one can find a simple recurrence formula. The series (6) converges geometrically, with an asymptotic quotient $k^2 \sin^2\varphi$. We have rapid convergence, therefore, if $k$ is small, but slow convergence, if $k$ is near 1 and $\varphi$ near $\pi/2$.

When $k$ is near 1, then (4) suggests finding an expansion in $k'$. This can be achieved by writing (3) as

$$F(\varphi, k) = \int_0^{\varphi} \frac{d\theta}{\cos\theta[1 + k'^2 \tan^2\theta]^{\frac{1}{2}}} ,$$

and again using the binomial expansion,

$$(7) \qquad F(\varphi, k) = \sum_{r=0}^{\infty} \binom{-\frac{1}{2}}{r} \tau_r(\varphi) k'^{2r}, \qquad \tau_r(\varphi) = \int_0^{\varphi} \frac{\sin^{2r}\theta}{\cos^{2r+1}\theta} d\theta .$$

As before, the $\tau_r$ can be generated by a simple recursion. The asymptotic convergence quotient of the series (7) is now $k'^2 \tan^2\varphi$, and thus satisfactory if $k'$ is small and $\varphi$ not too close to $\pi/2$.

It remains to deal with the last contingency, viz., $\varphi$ near $\pi/2$. Here we write

$$\mathbb{K}(k) - F(\varphi, k) = \int_0^{\frac{\pi}{2} - \varphi} \frac{d\theta}{\cos\theta[k'^2 + \tan^2\theta]^{\frac{1}{2}}} ,$$

and make the change of variables $\tan\theta = k' \tan\psi$. The result is

$$\mathbb{K}(k) - F(\varphi, k) = \int_0^u \frac{\cos\theta}{\cos\psi}\, d\psi = \int_0^u \frac{d\psi}{\cos\psi[1 + k'^2 \tan^2\psi]^{\frac{1}{2}}} ,$$

where

$$u = \cot^{-1}(k' \tan\varphi) .$$

Therefore, if $k'^2 \tan^2 u < 1$, i.e., $\varphi > \pi/4$, we can expand in a binomial series and find

$$\mathbb{K}(k) - F(\varphi, k) = \sum_{r=0}^{\infty} \binom{-\frac{1}{2}}{r} \tau_r(u) k'^{2r} . \tag{8}$$

We now have a series whose convergence quotient is $k'^2 \tan^2 u = \cot^2\varphi$, thus independent of $k$, and which converges more rapidly, the closer $\varphi$ is to $\pi/2$. Note, however, that (8) requires the computation of the complete elliptic integral. (For this, see 3.4.)

It is easily verified that for any $k$ and $\varphi$ in the region $0 \leq k \leq 1$, $0 \leq \varphi < \pi/2$, at least one of the series (6), (7), (8) converges geometrically with an asymptotic quotient $\leq 1/2$.

Other methods of computation, based on Gauss and Landen transformations, will be considered in 3.3. These are sometimes (but not always) more efficient than the expansions considered here.

## 1.4. Padé and continued fraction approximations

Given a formal power series about some point $z_0$ in the complex plane, one can associate with it certain rational functions having highest order contact with the power series at $z_0$. The rational functions in turn can be interpreted as convergents of continued fractions. These often converge faster, or in larger domains, than the original series, and may even converge when the series diverges. It is this property which makes them useful as a tool of approximation. Without loss of generality we shall assume the point of contact at the origin, $z_0 = 0$.

The basic references are Wall [1948], Perron [1957] and Khovanskii [1963]. On Padé approximation there are survey articles by Gragg [1972] and Chisholm [1973b], as well as a forthcoming book by Baker [1975]. Informative surveys on the use and application of Padé approximants and continued fractions can be found in the collection of articles edited by Baker and Gammel [1970], and in recent conference proceedings, e.g., Graves-Morris [1973a, b] and Jones and Thron [1974b]. We single out the extensive survey of Wynn [1974], containing many references, both to original sources and to newer developments. A good introduction into the numerical evaluation of continued fractions is Blanch [1964]. For a collection of computer algorithms see Wynn [1966b].

1.4.1. Padé table. Let

$$f(z) \sim c_0 + c_1 z + c_2 z^2 + \dots, \qquad c_0 \neq 0 \quad, \tag{1}$$

be a formal power series, and $\nu, \mu$ two nonnegative integers. It is possible to determine polynomials $\hat{p}_{\nu,\mu} \in \mathbb{P}_\mu$, $\hat{q}_{\nu,\mu} \in \mathbb{P}_\nu$, with $\hat{q}_{\nu,\mu} \not\equiv 0$, such that

$$\hat{q}_{\nu,\mu}(z)\, f(z) - \hat{p}_{\nu,\mu}(z) = (z^{\nu+\mu+1}) \quad, \tag{2}$$

where the symbol on the right stands for a formal power series beginning with a power $z^k$, $k \geq \nu + \mu + 1$. Although the polynomials $\hat{p}_{\nu,\mu}$ and $\hat{q}_{\nu,\mu}$ are not unique, they determine a unique rational function $\hat{p}_{\nu,\mu}(z)/\hat{q}_{\nu,\mu}(z)$, which may be expressed, in irreducible form, as

$$[\nu,\mu]_f(z) = \frac{p_{\nu,\mu}(z)}{q_{\nu,\mu}(z)}, \quad p_{\nu,\mu} \in \mathbb{P}_\mu, \quad q_{\nu,\mu} \in \mathbb{P}_\nu, \quad q_{\nu,\mu}(0) = 1 \quad. \tag{3}$$

One calls $[\nu,\mu]_f$ the Padé approximant of order $\nu, \mu$ generated by $f(z)$ (Wall [1948, p. 377ff], Perron [1957, p. 235ff]). We note from (2) and (3) that

(4)
$$[\nu,\mu]_f = \frac{1}{[\mu,\nu]_{\frac{1}{f}}}, \quad \nu \geq 0, \quad \mu \geq 0 \ .$$

The array of rational functions

(5)
$$\begin{matrix} [0,0]_f & [0,1]_f & [0,2]_f & \cdots \\ [1,0]_f & [1,1]_f & [1,2]_f & \cdots \\ [2,0]_f & [2,1]_f & [2,2]_f & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{matrix}$$

is called the <u>Padé table</u> of $f$ .

If $f(z) - [\nu,\mu]_f(z) = (z^{r+1})$, and $(z^{r+1})$ cannot be replaced by $(z^{s+1})$ with $s > r$, we say that $[\nu,\mu]_f$ has <u>contact of order</u> $r$ with $f$ . A Padé table in which each approximant $[\nu,\mu]_f$ has contact of order $\nu + \mu$ ,

(6)
$$f(z) - [\nu,\mu]_f(z) = (z^{\nu+\mu+1}) \ ,$$

is called <u>normal</u>. A necessary and sufficient condition for this is (Wall [1948, p. 398])

(7)
$$\Delta_{m,n} = \det \begin{bmatrix} c_{n-m} & c_{n-m+1} & \cdots & c_n \\ c_{n-m+1} & c_{n-m+2} & \cdots & c_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ c_n & c_{n+1} & \cdots & c_{n+m} \end{bmatrix} \neq 0, \quad n, m = 0, 1, 2, \ldots \ .$$

(The convention $c_k = 0$ for $k < 0$ is used here.) If this condition holds, $p_{\nu,\mu}$ and $q_{\nu,\mu}$ in (3) are of exact degrees $\mu$ and $\nu$, respectively. In the abnormal case, identical approximants lie in square blocks of the Padé table of the form $[i+r, j+s]_f$ $(r, s = 0, 1, \ldots, k)$, each approximant of this block having contact of order $i + j + k$ .

The question of convergence, $[\nu,\mu]_f \to F$ as $\nu,\mu$, or both, tend to infinity, where $F$ is a function associated in some way with $f$, is a difficult one, depending, as it does, on the behavior of the poles of $[\nu,\mu]_f$. We refer to Baker [1965], [1970], and Chisholm [1973c], for summaries of results and conjectures, and to Wynn [1972], Jones and Thron [1975], for more recent results.

1.4.2 Corresponding continued fractions. If the series in (1) is such that

(8) $$\Delta_{m,m} \neq 0 \quad \text{for} \quad m = 0,1,2,\dots ,$$

we can associate with it an infinite J-fraction,

(9) $$\sum_{k=0}^{\infty} c_k z^k \sim \frac{b_0}{1-a_0z-}\,\frac{b_1z^2}{1-a_1z-}\,\frac{b_2z^2}{1-a_2z-}\cdots, \quad b_k \neq 0, \quad b_0 = c_0 .$$

If the series is such that

(10) $$\Delta_{m,m} \neq 0, \quad \Delta_{m,m+1} \neq 0 \quad \text{for} \quad m = 0,1,2,\dots ,$$

we can also associate an infinite S-fraction,

(11) $$\sum_{k=0}^{\infty} c_k z^k \sim \frac{s_0}{1-}\,\frac{s_1z}{1-}\,\frac{s_2z}{1-}\,\frac{s_3z}{1-}\cdots, \qquad s_k \neq 0, \quad s_0 = c_0 .$$

Both continued fractions are completely characterized by their contact properties: the p-th convergent of the J-fraction $(p = 1,2,3,\dots)$ has contact of order $2p$, that of the S-fraction contact of order $p$, with the series (1). The J-fraction, in fact, is a contraction of the S-fraction.

The correspondences (9) and (11) are often written for series in descending powers of $z$ (usually asymptotic series), in which case they assume the form (Wall [1948, pp. 197, 202])

(9') $$\sum_{k=0}^{\infty} \frac{c_k}{z^{k+1}} \sim \frac{b_0}{z-a_0-}\,\frac{b_1}{z-a_1-}\,\frac{b_2}{z-a_2-}\cdots ,$$

(11')
$$\sum_{k=0}^{\infty} \frac{c_k}{z^{k+1}} \sim \frac{s_0}{z-} \frac{s_1}{1-} \frac{s_2}{z-} \frac{s_3}{1-} \cdots .$$

An important special case of (8), namely $\Delta_{m,m} > 0$, occurs precisely when $\{c_k\}$ is a moment sequence (Wall [1948, p. 325]),

(12)
$$c_k = \int_{-\infty}^{\infty} t^k d\phi(t), \qquad k = 0, 1, 2, \ldots ,$$

with $\phi$ a bounded nondecreasing function having infinitely many points of increase. The series (1), called Stieltjes series, is then the formal expansion of a Stieltjes transform,

(13)
$$\int_{-\infty}^{\infty} \frac{d\phi(t)}{1-tz} \sim c_0 + c_1 z + c_2 z^2 + \ldots .$$

The continued fraction (9) associated with (13) has all $a_k$ real, and all $b_k > 0$ (Perron [1957, p. 193]). Its convergents, as well as the convergents of (9'), are expressible in terms of the orthogonal polynomials $\{\pi_k(t)\}$ belonging to $d\phi(t)$, or in terms of Gaussian quadrature. For example, in the case of (9'),

(14)
$$\int_{-\infty}^{\infty} \frac{d\phi(t)}{z-t} \sim \frac{c_0}{z} + \frac{c_1}{z^2} + \ldots \sim \frac{b_0}{z-a_0-} \frac{b_1}{z-a_1-} \cdots ,$$

we have

(15)
$$\frac{b_0}{z-a_0-} \frac{b_1}{z-a_1-} \cdots \frac{b_{p-1}}{z-a_{p-1}} = \frac{1}{\pi_p(z)} \int_{-\infty}^{\infty} \frac{\pi_p(z) - \pi_p(t)}{z-t} d\phi(t)$$

(16)
$$= \sum_{k=1}^{p} \frac{\omega_k^{(p)}}{z-\tau_k^{(p)}} ,$$

where $\tau_k^{(p)}$ are the zeros of $\pi_p(t)$ and $\omega_k^{(p)}$ the associated Christoffel numbers. The polynomials $\pi_k(z)$ are thus the denominators of the continued fraction in (14), the associated orthogonal polynomials

$$\sigma_k(z) = \int_{-\infty}^{\infty} \frac{\pi_k(z)-\pi_k(t)}{z-t}\, d\phi(t)$$

the numerators. Both satisfy the same recurrence formula,

$$y_{r+1} = (z-a_r)y_r - b_r y_{r-1}, \qquad r = 0,1,2,\ldots, \tag{17}$$

where $y_0 = 1$, $y_{-1} = 0$ for $\{\pi_k\}$, and $y_0 = 0$, $y_{-1} = -1$ for $\{\sigma_k\}$. This is meaningful not only for Stieltjes series, but for any series which has an associated J-fraction, provided orthogonality is defined algebraically (Wall [1948, p. 192]). We also note that in terms of the continued fraction (11), we have

$$\begin{aligned} &a_0 = s_1, \quad b_0 = s_0, \\ &\left.\begin{aligned} a_r &= s_{2r} + s_{2r+1} \\ b_r &= s_{2r-1}s_{2r} \end{aligned}\right\} \quad r = 1,2,3,\ldots . \end{aligned} \tag{18}$$

A special case of (10), similarly, is $\Delta_{m,m} > 0$, $\Delta_{m,m+1} > 0$, and obtains precisely when (12) holds for some measure $d\phi(t)$ vanishing for $t < 0$ (Wall [1948, p. 327]). In this case, $s_k > 0$ for all $k \geq 0$ in (11), a source of useful inequalities when $z$ is real and negative.

With regard to convergence of the continued fractions in (9) and (11), and their limits, we refer to Perron [1957, p. 145ff].

1.4.3. Relation between Padé table and continued fractions. Assume that the series (1) is normal. The conditions (8) and (10) are then valid not only for the given series, but also for all delayed series

$$f_m(z) \sim c_m + c_{m+1}z + c_{m+2}z^2 + \ldots, \qquad m = 0,1,2,\ldots . \tag{$1_m$}$$

Each of these, therefore, has an associated J-fraction

$$(9_m) \qquad f_m(z) \sim \frac{b_0^{(m)}}{1-a_0^{(m)}z-}\,\frac{b_1^{(m)}z^2}{1-a_1^{(m)}z-}\,\frac{b_2^{(m)}z^2}{1-a_2^{(m)}z-}\cdots, \quad b_k^{(m)} \neq 0,\; b_0^{(m)} = c_m\,,$$

and an associated S-fraction,

$$(11_m) \qquad f_m(z) \sim \frac{s_0^{(m)}}{1-}\,\frac{s_1^{(m)}z}{1-}\,\frac{s_2^{(m)}z}{1-}\,\frac{s_3^{(m)}z}{1-}\cdots, \qquad s_k^{(m)} \neq 0, \quad s_0^{(m)} = c_m\,.$$

It turns out (Wall [1948, p. 380]) that the entries of the Padé table for $f = f_0$ in the stairlike sequence

$$\begin{array}{cccccc} [0,m-1] & [0,m] & & & & \\ & [1,m] & [1,m+1] & & & \\ & & [2,m+1] & [2,m+2] & & \\ & & & & \ddots & \end{array}$$

are identical with the successive convergents of the continued fraction

$$(19) \qquad c_0 + c_1 z + \ldots + c_{m-1}z^{m-1} + \frac{s_0^{(m)}z^m}{1-}\,\frac{s_1^{(m)}z}{1-}\,\frac{s_2^{(m)}z}{1-}\cdots\,,$$

while those along the para-diagonal

$$\begin{array}{cccc} [0,m-1] & & & \\ & [1,m] & & \\ & & [2,m+1] & \\ & & & \ddots \end{array}$$

are the successive convergents of

$$(20) \qquad c_0 + c_1 z + \ldots + c_{m-1}z^{m-1} + \frac{b_0^{(m)}z^m}{1-a_0^{(m)}z-}\,\frac{b_1^{(m)}z^2}{1-a_1^{(m)}z-}\,\frac{b_2^{(m)}z^2}{1-a_2^{(m)}z-}\cdots\,.$$

As in (15), the latter are expressible in terms of the orthogonal polynomials $\{\pi_k^{(m)}\}$ belonging to the measure $t^m\, d\phi(t)$. (See, in this connection, Allen, Chui, Madych, Narcowich and Smith [1974]). Similar statements can be obtained for the entries in the lower half of the Padé table by using (4).

We remark that in the case of convergence, the continued fraction

$$\frac{1}{1-}\;\frac{s_1^{(m)}z}{1-}\;\frac{s_2^{(m)}z}{1-}\cdots$$

in (19), and the analogous continued fraction in (20), serve as "converging factor", being the factor by which the last term $c_m z^m$ is to be multiplied in order to obtain the correct limit of the series (1).

1.4.4. Algorithms. The entries of the Padé table may be generated either in explicit form, as ratios of polynomials, or in their continued fraction form (19). For the former, there are a number of recursive schemes for generating the polynomials in question (Wynn [1960], Baker [1970], [1973], Longman [1971], Watson [1973]). For the latter, one has the quotient-difference (qd-) algorithm (Rutishauser [1954a, b], [1957], Henrici [1958], [1963], [1967]), which consists in generating the qd-array

$$\begin{array}{ccccccc}
e_0^{(0)} & & & & & & \\
 & q_1^{(0)} & & & & & \\
e_0^{(1)} & & e_1^{(0)} & & & & \\
 & q_1^{(1)} & & q_2^{(0)} & & & \\
e_0^{(2)} & & e_1^{(1)} & & e_2^{(0)} & \cdot & \\
 & q_1^{(2)} & & q_2^{(1)} & & & \cdot \\
e_0^{(3)} & & e_1^{(2)} & & e_2^{(1)} & \cdot & \\
 & q_1^{(3)} & & q_2^{(2)} & & & \cdot \\
\vdots & & e_1^{(3)} & & e_2^{(2)} & \cdot & \\
 & & & q_2^{(3)} & & & \cdot \\
 & \vdots & \vdots & & e_2^{(3)} & \cdot & \\
 & & & & & & \cdot \\
 & & & \vdots & \vdots & &
\end{array}$$

from left to right by means of

$$e_0^{(n)} = 0, \quad q_1^{(n)} = \frac{c_{n+1}}{c_n}, \qquad n = 0, 1, 2, \ldots ,$$

$$\left.\begin{aligned} e_k^{(n)} &= q_k^{(n+1)} - q_k^{(n)} + e_{k-1}^{(n+1)} \\ q_{k+1}^{(n)} &= \frac{e_k^{(n+1)}}{e_k^{(n)}} q_k^{(n+1)} \end{aligned}\right\} k = 1, 2, 3, \ldots, \quad n = 0, 1, 2, \ldots .$$

The coefficients in the continued fraction (19) are then given by

$$s_0^{(m)} = c_m, \quad s_{2k-1}^{(m)} = q_k^{(m)}, \quad s_{2k}^{(m)} = e_k^{(m)}, \quad k = 1, 2, 3, \ldots, \quad m = 0, 1, 2, \ldots .$$

Unfortunately, the generation of the qd-array, as described, is unstable, and should be carried out in high precision, or with some other precautions (Gargantini and Henrici [1967]). Thacher [1971] notes, however, that inaccuracies in the higher order coefficients $s_k^{(m)}$ need not necessarily imply an inaccurate value of the continued fraction (19).

In some instances one has explicit expressions for the $e_k^{(n)}$, $q_k^{(n)}$, for example, in the case of the complex error function (Thacher [1967]), or for certain special hypergeometric and confluent hypergeometric functions (Wynn [1960], Henrici [1963]). For series (1), with $c_m = \prod_{\mu=0}^{m-1} \{(a - q^{\alpha+\mu})(b - q^{\beta+\mu})^{-1}\}$, Wynn [1967] gives closed expressions for the numbers $e_k^{(n)}$, $q_k^{(n)}$, and also for the numerator and denominator polynomials of the approximants in the upper half of the Padé table. Limiting forms of these results (obtained, e.g., when $a = b = 1$, $q \to 1$) yield all cases in which these numbers and polynomials are known in closed form.

There are other algorithms, notably the <u>$\epsilon$-algorithm</u> and related methods due to Wynn [1956], [1961], [1966a], which operate directly on the entries of the Padé table. Their most important use, probably, is in the calculation of numerical values for a sequence of Padé approximants, e.g., the values at $z = 1$ in an attempt to speed the convergence of $\sum_{k=0}^{\infty} c_k$.

1.4.5. Applications to special functions. The qd-algorithm, either applied to a Taylor series or to an asymptotic expansion, has been used by many authors to obtain the corresponding S-fraction explicitly or numerically. We mention the work of Gargantini and Henrici [1967] on the Bessel function $K_0(z)$ and more general confluent hypergeometric functions, the work of Thacher [1967] on the complex error function, of Cody and Thacher [1968] and Chipman [1972] on the exponential integral $E_1(z)$ and related integrals, of Strecok and Gregory [1972] on the irregular Coulomb wave function along the transition line, and the study of Shenton and Bowman [1971] on the polygamma functions $\psi^{(n)}(z)$. Jacobs and Lambert [1972] apply S-fractions to polylogarithms of a complex argument, while Barlow [1974] does the same to generalized polylogarithms.

Earlier, Fair [1964] uses Lanczos' $\tau$-method for obtaining the J-fraction for functions defined by Riccati differential equations, and applies the technique to confluent hypergeometric functions and Bessel functions of the first and second kind. Fair and Luke [1967] further apply it to incomplete elliptic integrals (cf. also Luke [1969, Vol. II, p. 77ff]).

For large classes of functions, including Gauss hypergeometric functions and the incomplete gamma function, Luke [1969, Vol. II, Chs. XIII and XIV], [1970b], [1971a], [1975] gives explicit expressions for the Padé entries on the diagonal, and immediately above, as well as appraisals of the errors. Those for the incomplete gamma function also serve to approximate the gamma function in the complex plane. See, however, Ng [1975] for a comparison with other methods. Tables of Padé coefficients are given in Luke [1969, Vol. II, p. 402ff] for the exponential, sine, and cosine integrals and for the error function. Golden, McGuire and Nuttall [1973] give an experimental study of the diagonal Padé approximants in the case of Hankel functions of the first and second kind.

Gaussian quadrature, or the equivalent J-fraction in (15), have been used by Todd [1954] for evaluating the complex exponential integral, and by Gautschi [1970] for evaluating the complex error function. In the latter work, the continued fraction approach is combined with a Taylor series approach, there being a gradual transition from one to the other as the complex argument decreases in magnitude.

1.4.6. Error estimates. It is important to have reasonably good estimates of the error due to premature truncation of a continued fraction. One distinguishes between a priori estimates, which are expressed directly in terms of the elements of the continued fraction, and a posteriori estimates, which depend on the knowledge of a finite number (usually two or three) of convergents. Concerning the latter, we mention the elegant work of Henrici [1965] and Henrici and Pfluger [1966] on Stieltjes fractions, in which a sequence of nested lens-shaped regions is constructed the intersection of which contains the value of the continued fraction. For more recent extensions of this work, as well as for other types of estimates, we refer to the survey of Jones [1974].

For a large number of continued fraction expansions of special functions, Wynn [1962a, b] gives "efficiency profiles", i.e., tables from which the order of convergents can be determined as a function of the (real) argument and the accuracy desired.

1.4.7. Generalizations. In view of the contact properties of Padé and continued fraction approximations, one expects these approximations to be best near the point of contact, and to gradually worsen away from it. There is, in fact, a close relationship between the best uniform rational approximants on small discs $|z| \leq \epsilon$, or small intervals $0 \leq z \leq \epsilon$, and the Padé approximant, the former tending to the latter as $\epsilon \to 0$ (Walsh [1964a], [1974], Chui, Shisha and Smith [1974]). The reason for this behavior is largely due to the employment of powers in setting up the Padé table. To obtain a more balanced rational approximation on a given interval, it has been suggested to use systems of orthogonal polynomials instead, and to proceed similarly as in 1.4.1, starting with the appropriate orthogonal expansion of f. It will be noted that the analogue of (2) is still a linear problem, but the analogue of (6) is not. The original work along this line is due to Maehly [1956], [1958] (see also Kogbetliantz [1960], Spielberg [1961b]), who uses Chebyshev polynomials, and is continued by Cheney [1966, p. 177ff], Holdeman [1969] and Fleischer [1972]. These authors use the linear approach. The nonlinear problem, which is closer in spirit to Padé approximation, has only recently been considered (Common [1969], Fleischer [1973a, b], Frankel and Gragg [1973], Clenshaw and Lord [1974], Gragg and Johnson [1974]). The use of Chebyshev polynomials often leads to nearly best rational approximations (Clenshaw [1974]).

In another direction, one might generalize Padé and continued fraction approximation by imposing contact conditions not only at one, but at several points (typically, at the origin and at infinity). See Baker, Rushbrooke and Gilbert [1964] and Baker [1970] for recent attempts in this direction, and McCabe [1974] for an interesting continued fraction approach. The potential of this approach remains largely to be explored.

Finally, we mention generalizations of Padé approximation to functions of two variables by Chisholm [1973a], Hughes Jones and Makinson [1974], Graves-Morris, Hughes Jones and Makinson [1974], Common and Graves-Morris [1974].

1.4.8. Other rational approximations. We already mentioned the $\tau$-method (Lanczos [1956, pp. 464-507]) applied to linear and nonlinear differential equations as a source of rational approximations (Luke [1955], [1958], [1959/60], Guerra [1969], Verbeeck [1970]). Other sources are Maehly's economization of continued fractions and related techniques (Maehly [1960], Spielberg [1961a], Ralston [1963]), Hornecker's method of modifying the Chebyshev expansion (Hornecker [1959a, b], [1960]), the method of Luke and co-workers (Luke [1969, Vol. II, Ch. XI]) on generalized hypergeometric functions and functions representable as Laplace transforms, and the nonlinear sequence-to-sequence transformation of Levin applied to the partial sums of power series (Levin [1973], Longman

[1973]). Integrating Padé approximants for the square root, Luke [1968], [1970a] obtains rational approximations to the three normal forms of incomplete elliptic integrals, including asymptotic estimates of the error. We also mention the curious ad-hoc approximation to the gamma function $\Gamma(z)$ on $\mathrm{Re}\, z \geq 1$ due to Lanczos [1964].

### 1.5. Representation and evaluation of approximations

Once an approximation to a special function has been constructed, it is often possible to represent this approximation in different mathematically equivalent forms. Each form in turn suggests one or several algorithms of evaluation. Although mathematically equivalent, these forms may behave quite differently under evaluation in finite precision. It is important to select a representation, and a corresponding evaluation algorithm, which to the maximum extent possible is invulnerable to the vagaries of finite precision arithmetic.

With regard to representation, what one aims for is well-conditioning. This means that the value of the particular functional form be insensitive to small perturbations in the parameters (coefficients) involved. With regard to algorithms, one strives for economy and stability, i.e., few arithmetic operations and maximum resistance to rounding errors. It is a rare instance where all three of these requirements are in complete harmony with each other.

We discuss some possible representations and algorithms for polynomial and rational approximations, and then consider an algorithm for evaluating approximations in the form of orthogonal sums.

#### 1.5.1. Polynomials

(i) Power form. A polynomial of degree $n$ is most frequently represented in the form

$$p(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n \quad , \tag{1}$$

which can be evaluated rather economically by a scheme ascribed to Horner [1819] (but already known to Newton (Ostrowski [1954])),

$$(2)\qquad \begin{cases} u_n = a_n \\ u_k = xu_{k+1} + a_k, \qquad k = n-1,\ n-2,\ \ldots,\ 0\ , \\ p(x) = u_0\ . \end{cases}$$

The scheme requires $n$ multiplications and $n$ additions. With regard to addition, this is optimal (Ostrowski [1954]). The conditioning of the form (1) (at the point $x$) depends on the relative magnitudes of the quantities $\max_k |a_k x^k|$ and $|p(x)|$. If the former is much larger than the latter, then (1) is ill-conditioned at $x$. Horner's scheme is generally stable, but can be moderately, and in some cases severely, unstable (Wilkinson [1963, p. 36], Reimer and Zeller [1967], Reimer [1968]). The Chebyshev polynomials, of all, are particularly vulnerable (Reimer [1971]).

(ii) Chebyshev polynomial form. Every polynomial of degree $n$ can be represented in terms of Chebyshev polynomials as (cf. 1.2.3(ii))

$$(3)\qquad p(x) = \frac{1}{2}\, a_0 + \sum_{k=1}^{n} a_k\, T_k(x)\ .$$

One of the attractive features of this form is the possibility of obtaining a sequence of approximations of varying accuracy by merely truncating (3) at consecutive terms. For the evaluation of $p(x)$ one has an algorithm due to Clenshaw [1955],

$$(4)\qquad \begin{cases} u_n = a_n,\quad u_{n+1} = 0\,, \\ u_k = 2xu_{k+1} - u_{k+2} + a_k, \qquad k = n-1,\ n-2,\ \ldots,\ 0\ , \\ p(x) = \frac{1}{2}\,(u_0 - u_2)\ , \end{cases}$$

requiring $2n$ additions and $n$ multiplications (cf. 1.5.3). Although more time-consuming than Horner's scheme, Clenshaw's algorithm is often preferred on account of its more favorable stability properties. See Newbery [1974] for a comparative study.

(iii) Root product form. This is the form obtained by factoring the polynomial into its linear and quadratic factors,

$$(5) \qquad p(x) = a_n \prod_{k=1}^{r} (x-x_k) \prod_{k=r+1}^{r+s} [(x-x_k)^2 + y_k], \quad y_k > 0, \quad r + 2s = n \ .$$

Like Horner's scheme, this form requires $n$ additions and $n$ multiplications. For maximum stability, however, the differences $x - x_k$ must be evaluated with care: Assuming $x$ machine representable (in floating-point arithmetic), and denoting by $x_k^*$ the machine representable part of $x_k$, and by $r_k$ the remainder,

$$x_k = x_k^* + r_k \ ,$$

one should evaluate $x - x_k$ in two steps as $(x - x_k^*) - r_k$, thereby preserving as much significance as possible when $x$ is close to $x_k$. Note that this doubles the number of additions. The construction of the form (5) requires some effort, namely the calculation of all zeros of $p$, but this effort may be rewarded by a well-conditioned representation.

(iv) Newton form. In a sense intermediate between (1) and (5) is Newton's form

$$(6) \qquad \begin{aligned} p(x) = a_0 &+ a_1(x-x_0) + a_2(x-x_0)(x-x_1) + \dots \\ &+ a_n(x-x_0)(x-x_1) \dots (x-x_{n-1}) \ , \end{aligned}$$

which reduces to (1) if all $x_k = 0$, and to (5) (with $s = 0$), if $a_k = 0$ for $k < n$. We have the Horner-type evaluation scheme

$$(7) \qquad \begin{cases} u_n = a_n \ , \\ u_k = (x-x_k)u_{k+1} + a_k, \qquad k = n-1, n-2, \dots, 0 \ , \\ p(x) = u_0 \ , \end{cases}$$

which is quite stable if the differences $x-x_k$ are evaluated as above in (iii), and the parameters $x_k, a_k$ are selected to make the two additive terms on the right of (7) of equal sign. This can always be done (Mesztenyi and Witzgall [1967]). A special form of (6) has proved useful, e.g., in approximating modified Bessel functions (Blair and Edwards [1974])

(v) Lagrange form. Given any $n+1$ distinct real numbers $x_0, x_1, \ldots, x_n$, we may represent a polynomial of degree $n$ in its Lagrange form

$$(8)\qquad p(x) = \sum_{k=0}^{n} a_k \ell_k(x), \quad \ell_k(x) = \prod_{\substack{r=0\\ r\neq k}}^{n} \frac{x-x_r}{x_k-x_r}, \qquad a_k = p(x_k) \ ,$$

familiar from interpolation theory. It is evaluated most conveniently in the barycentric form (see, e.g., Bulirsch and Rutishauser [1968])

$$(9)\qquad p(x) = \frac{\sum_{k=0}^{n} a_k \frac{\lambda_k}{x-x_k}}{\sum_{k=0}^{n} \frac{\lambda_k}{x-x_k}} \qquad (x \neq x_i, \quad i = 0, 1, \ldots, n) \ ,$$

where $\lambda_k = \prod_{r\neq k} (x_k - x_r)^{-1}$ are precomputed constants.

(vi) Ultraeconomic forms. There are a number of representations, due to Motzkin, Belaga, Pan, and others, which require only of the order $n/2$ multiplications and $n$ additions. While these forms are highly interesting from the standpoint of complexity theory, their practical merits are not entirely clear. For one thing, they tend to be poorly conditioned (Rice [1965], Fike [1967]), although this matter deserves further analysis. For another, the time saving gained by fewer multiplications may well be lost on some computers by the need for more memory transactions (Cody [1967]).

1.5.2. Rational functions

(i) Polynomial ratio form. This is the collective name given to all the forms that can be obtained by representing the polynomials $p$ and $q$ in

$$r(x) = \frac{p(x)}{q(x)} \tag{10}$$

in any one of the forms discussed in 1.5.1. Since division is a stable operation, the conditioning and stability properties of $r$ depend entirely on those of $p$ and $q$. Occasionally it is preferable (see, e.g., Cody and Hillstrom [1970, p. 676]) to write the two polynomials in descending powers of $x$.

(ii) Continued fraction forms. Intrinsically different are representations of $r$ in terms of continued fractions. There are many different types of continued fractions that can be used in this connection. We mention only the J-fractions (cf. 1.4.2), which are of the form

$$r(x) = \frac{r_1}{x+s_1+}\ \frac{r_2}{x+s_2+} \cdots \frac{r_n}{x+s_n}, \quad r_k \neq 0 \ \text{ all } k, \tag{11}$$

and refer to Hart et al. [1968, p. 73ff] for others. The continued fraction (11) represents a rational function in $\mathbb{R}_{n,n-1}$. Conversely, a rational function in $\mathbb{R}_{n,n-1}$ can be represented in the form (11), unless certain determinants in the coefficients of $p$ and $q$ happen to vanish (Wall [1948, p. 165]). Conversion algorithms are given in Hart et al. [1968, pp. 155-160].

For the evaluation of (11) one proceeds most easily "from tail to head", according to

$$\begin{cases} u_{n+1} = 0, \\ u_k = \dfrac{r_k}{x+s_k+u_{k+1}}, \qquad k = n, n-1, \ldots, 1, \\ r(x) = u_1. \end{cases} \tag{12}$$

This requires 2n-1 additions and n divisions, which, unless division is very slow, compares favorably with the 2n-1 additions, 2n-1 multiplications, and 1 division, required with Horner's scheme in (10), and even more favorably with the evaluation of the continued fraction by means of the fundamental three-term recurrence relation. The algorithm (12) is not only more economical than Horner's scheme, but also more stable, in general. There are, however, exceptions (Cody and Hillstrom [1967, p. 203]). The stability of evaluation schemes for continued fractions is discussed by Macon and Baskervill [1956], Blanch [1964] and Jones and Thron [1974a, c].

1.5.3. Orthogonal sums. The Chebyshev polynomials $T_k$ in (3) are a special case of orthogonal polynomials, $\{\pi_k\}$, which are known to satisfy a recurrence relation of the form (cf. 1.4.2 (17))

$$\pi_{r+1} = \alpha_r(x)\,\pi_r + \beta_r(x)\,\pi_{r-1}, \quad r = 1, 2, 3, \ldots \quad . \tag{13}$$

Other (nonpolynomial) systems of special functions also satisfy relations of this type. When expanding a given function in terms of $\pi_k$, it is useful to have an efficient algorithm for evaluating a partial sum,

$$s(x) = \sum_{k=0}^{n} a_k\,\pi_k(x) \quad . \tag{14}$$

One such algorithm is Clenshaw's algorithm (Clenshaw [1955]), a generalization of the algorithm in (4),

$$\begin{cases} u_n = a_n, \quad u_{n+1} = 0 \,, \\ u_k = \alpha_k(x)\,u_{k+1} + \beta_{k+1}(x)\,u_{k+2} + a_k \\ \qquad\qquad k = n-1, \; n-2, \; \ldots, \; 0 \,, \\ s(x) = u_0\pi_0(x) + u_1[\pi_1(x) - \alpha_0(x)\,\pi_0(x)] \quad . \end{cases} \tag{15}$$

The validity of (15) is best seen by writing (13) in matrix form (Deuflhard [1974]) as

$$\begin{bmatrix} 1 & & & & O \\ -\alpha_0 & 1 & & & \\ -\beta_1 & -\alpha_1 & 1 & & \\ & \ddots & \ddots & \ddots & \\ O & & -\beta_{n-1} & -\alpha_{n-1} & 1 \end{bmatrix} \begin{bmatrix} \pi_0 \\ \pi_1 \\ \pi_2 \\ \vdots \\ \pi_n \end{bmatrix} = \begin{bmatrix} \pi_0 \\ \pi_1 - \alpha_0 \pi_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

or briefly as $L\pi = \rho$, and noting that the recurrence in (15) is simply $L^T u = a$. Thus,

$$s(x) = a^T \pi = a^T L^{-1} \rho = ((L^T)^{-1} a)^T \rho = u^T \rho \ ,$$

which is the last line of (15). The argument clearly extends to functions $\pi_k$ satisfying recurrence relations of order larger than two. Other possible extensions are considered in Saffren and Ng [1971].

For orthogonal polynomials $\{\pi_k\}$ one has $\pi_1 - \alpha_0(x)\pi_0 = 0$, and the last line in (15) simplifies to $s(x) = u_0 \pi_0$. The derivative $s'(x)$ can be computed by a similar algorithm (Smith [1965], Cooper [1967]).

Applying (15) to the Chebyshev polynomials $T_k$, $U_k$ of the first and second kind, and noting that $T_k(\cos\theta) = \cos k\theta$, $(\sin\theta)\, U_k(\cos\theta) = \sin(k+1)\theta$, one is led to an algorithm for evaluating trigonometric sums, known as <u>Goertzel's algorithm</u> (Goertzel [1958], [1960]), or <u>Watt's algorithm</u> (Watt [1958/59]).

Floating-point error analyses of Clenshaw's and Goertzel's algorithms are given by Gentleman [1969/70], Newbery [1973] and Cox [unpubl.]. Although usually quite stable, these algorithms are not without pitfalls. Clenshaw's algorithm (15), e.g., should be avoided if $\{\pi_k\}$ is a minimal solution of (13) (cf. 2.2.1). The computation of $s(x)$ in the final step of (15) then likely leads to large cancellation errors (Elliott [1968]). Goertzel's algorithm, in turn, suffers from substantial accumulation of rounding errors if $\theta$ is small modulo $\pi$ (Gentleman [1969/70]). It can be stabilized either by incorporating phase shifts (Newbery [1973]), or by reformulating the recurrence in a manner proposed by Reinsch (Stoer [1972, p. 64]).

For computational experiments with Clenshaw's algorithm see Ng [1968/69].

## §2. Methods based on linear recurrence relations

It is often necessary to compute not just one particular function, but a whole sequence of special functions. The task is considerably simplified if the members of the sequence satisfy a recurrence relation. It is then possible to compute each member recursively in terms of those already computed. The process is not only fast, but also well adapted to modern computing machinery, and may be useful even if only one member of the sequence is desired.

Most recurrences of interest in special functions are linear difference equations. The particular solution desired is often rapidly decaying, but embedded in a family of growing solutions. The question of numerical stability then becomes a central issue. In order to keep the dominant solutions in check, special precautions need to be adopted. The nature of these precautions is the subject of this paragraph.

Computational aspects of recurrence relations have been reviewed by several writers, notably Fox [1965], Gautschi [1967], [1972], Wimp [1970], and Amos [1970].

### 2.1. First-order recurrence relations

The simplest linear recurrence is

$$y_{n+1} = a_n y_n, \qquad n = 0, 1, 2, \dots , \tag{1}$$

where $y_0$ and $a_n \neq 0$ are given numbers. Multiplication being a stable operation, errors due to rounding will essentially accumulate linearly with $n$, making (1) a stable computational process. A classic example is the recurrence relation for the gamma function.

As we proceed to inhomogeneous recurrences,

$$y_{n+1} = a_n y_n + b_n, \qquad n = 0, 1, 2, \ldots \ , \tag{2}$$

the stability characteristics may change significantly. The relation (2) indeed involves repeated additions, thus potentially unstable operations. It suffices that the two terms on the right be nearly equal in magnitude and opposite in sign to cause significant loss of accuracy, due to "cancellation". If this happens repeatedly, the computation may quickly deteriorate, giving rise to numerical instability.

2.1.1. <u>A simple analysis of numerical stability.</u> Suppose $f_n \neq 0$ is a solution of (2) that we wish to compute. It is instructive to examine how a relative error $\epsilon$ in $f_n$, committed at $n = s$ ($s$ for "starting"), affects the value of $f_n$ at $n = t$ ($t$ for "terminal"), where $t \lesseqgtr s$, assuming that no further errors are being introduced. If we denote the perturbed solution by $f_n^*$, so that $f_s^* = (1+\epsilon)f_s$, we find by a simple computation that

$$f_t^* = \left(1 + \frac{\rho_t}{\rho_s}\epsilon\right)f_t \ , \tag{3}$$

where

$$\rho_n = \frac{f_0 h_n}{f_n} \ , \tag{4}$$

and $h_n$ is the solution of the homogeneous recurrence (1), with $h_0 = 1$. Going from $s$ to $t$, the relative error is thus <u>amplified</u> if $|\rho_t| > |\rho_s|$, and <u>damped</u> if $|\rho_t| < |\rho_s|$. In an effort to maintain optimal numerical stability, the recurrence (2), therefore, should be applied in the direction of decreasing $|\rho_n|$, whenever practicable.

An important special case is

$$\lim_{n\to\infty} |\rho_n| = \infty , \tag{5}$$

where $|\rho_n|$ diverges monotonically. The recurrence (2) is then unstable in the forward direction, the ratio $|\rho_t/\rho_s|$ being unbounded for $t > s$, but stable in the backward direction, the same ratio now being bounded by 1. More than that, we can start the recursion arbitrarily with $f_\nu^* = 0$, for some $\nu$ sufficiently large, and recur downward to some fixed $n$, thereby obtaining $f_n$ to arbitrarily high accuracy. This is because the initial error, $\epsilon = -1$, according to (3), will be damped by a factor of $|\rho_n/\rho_\nu|$, which can be made arbitrarily small by choosing $\nu$ large enough. All intermediate rounding errors, moreover, are being consistently damped.

We can interprete (5) by saying that the particular solution of (2) desired is dominated by the "complementary solution" of (2), i.e., the solution of the corresponding homogeneous recurrence (1). It should be clear on intuitive grounds that forward recurrence cannot be stable under these circumstances.

We remark that similar stability considerations apply to general systems of linear difference equations (Gautschi [1972]).

2.1.2. Applications to special functions. Although not many special functions obey relations of the type (2), there are some which do, e.g., certain integrals in the theory of molecular structure (Gautschi [1961]), the incomplete gamma function (Kohútová [1970], Amos and Burgmeier [1973]), in particular the exponential integrals $E_n(z)$ (Gautschi [1973]), and successive derivatives of $f(z)/z$ (Gautschi [1966], [1972], Gautschi and Klein [1970]). The techniques indicated above provide effective schemes of computation in all these cases.

## 2.2. Homogeneous second-order recurrence relations

We assume now, more importantly, that $f_n$ satisfies a three-term recurrence relation

(1) $$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad n = 1, 2, 3, \ldots ,$$

where, for simplicity,

(2) $$f_n \neq 0, \quad b_n \neq 0 \quad \text{for all } n .$$

Given $f_0$ and $f_1$, we can use (1) in turn for $n = 1, 2, \ldots$ to successively calculate $f_2, f_3, \ldots$ . This is quite effective if $f_0$ and $f_1$ are easily calculated and the recurrence (1) is numerically stable. We expect the latter to be the case if no solution of (1) grows faster than $f_n$. An important example of such a recursion is the one for orthogonal polynomials, $f_n = \pi_n$, where the second solution is the sequence of associated orthogonal polynomials, $g_n = \sigma_n$ (cf. 1.4.2), and where by a theorem of Markov the ratios $\sigma_n/\pi_n$ converge to a finite limit, the corresponding Stieltjes integral, at least outside the interval of orthogonality (Perron [1957, p. 198ff]). The recurrence relation is reputed to be stable even on the interval of orthogonality, except possibly in the vicinities of the endpoints.

If there are solutions which grow much faster than $f_n$, then forward recursion on (1), as in 2.1(5), is bound to fail. Such is the case if the solution $f_n$ is minimal.

2.2.1. Minimal solutions. We call a solution $f_n$ of (1) minimal, if for every other, linearly independent, solution $g_n$ we have

(3) $$\lim_{n \to \infty} f_n/g_n = 0 .$$

All solutions $g_n$, for which (3) holds, are called dominant. A minimal solution, if one exists, is unique apart from a constant factor. It can be specified by imposing a single condition, e.g.,

(4) $$f_0 = s ,$$

or more generally,

$$\sum_{m=0}^{\infty} \lambda_m f_m = s \,, \tag{5}$$

where $s$ and $\lambda_m$ are given numbers.

Defining

$$r_n = f_{n+1}/f_n \,, \qquad n = 0, 1, 2, \ldots \,, \tag{6}$$

we have by a result of Pincherle (see, e.g., Perron [1957, Satz 2.46C], Gautschi [1967]) that

$$r_{n-1} = \frac{f_n}{f_{n-1}} = \frac{-b_n}{a_n -} \, \frac{b_{n+1}}{a_{n+1} -} \, \frac{b_{n+2}}{a_{n+2} -} \cdots, \qquad n = 1, 2, 3, \ldots \,, \tag{7}$$

where the continued fractions converge precisely if (1) has a (nonvanishing) minimal solution, $f_n$. In principle, therefore, all ratios $r_{n-1}$ are known, and (5) gives

$$f_0 = \frac{s}{\sum_{m=0}^{\infty} \lambda_m r_0 r_1 \cdots r_{m-1}} \,, \tag{8}$$

from which

$$f_n = r_{n-1} f_{n-1}, \qquad n = 1, 2, 3, \ldots \,, \tag{9}$$

by virtue of (6).

2.2.2. Algorithms for minimal solutions. Any implementation of the approach just described will involve, explicitly or implicitly, the truncated continued fractions

$$r_{n-1}^{(\nu)} = \frac{-b_n}{a_n -} \, \frac{b_{n+1}}{a_{n+1} -} \cdots \frac{b_\nu}{a_\nu} \,, \qquad n = 1, 2, \ldots, \nu \,. \tag{10}$$

We assume they all exist. (They do for $\nu$ sufficiently large.) For simplicity of exposition, we consider the case of prescribed $f_0$, see (4).

(i) Nonlinear backward recursion. Evaluating (10) recursively from behind, and then using an approximate version of (9), we get the algorithm (Gautschi [1967])

$$\text{(11)} \quad \begin{cases} r_\nu^{(\nu)} = 0, \quad r_{n-1}^{(\nu)} = -\dfrac{b_n}{a_n + r_n^{(\nu)}}, & n = \nu, \nu-1, \dots, 1 , \\ f_0^{(\nu)} = f_0, \quad f_n^{(\nu)} = r_{n-1}^{(\nu)} f_{n-1}^{(\nu)}, & n = 1, 2, \dots, \nu . \end{cases}$$

From Pincherle's result it follows that

$$\text{(12)} \qquad \lim_{\nu\to\infty} f_n^{(\nu)} = f_n$$

for any fixed $n$.

The major inconvenience with (11) is the fact that we do not always know an appropriate value of $\nu$ ahead of time, and may have to repeat (11) several times, with increasing $\nu$, until the $f_n^{(\nu)}$ converge to the desired accuracy.

Replacing $r_\nu^{(\nu)} = 0$ in (11) by $r_\nu^{(\nu)} = \rho_\nu$, a suitable approximation of $r_\nu = f_{\nu+1}/f_\nu$, often leads to improved convergence (Gautschi [1967, pp. 38, 40], Scraton [1972]).

(ii) Linear algebraic system. The approximations $f_n^{(\nu)}$ in (11) can be identified with the solution of the tridiagonal system

$$\text{(13)} \qquad \begin{bmatrix} a_1 & 1 & & & O \\ b_2 & a_2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ O & & & b_\nu & a_\nu \end{bmatrix} \begin{bmatrix} f_1^{(\nu)} \\ f_2^{(\nu)} \\ \vdots \\ f_\nu^{(\nu)} \end{bmatrix} = \begin{bmatrix} -b_1 f_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} ,$$

which is formally obtained from (1) by setting $y_{\nu+1} = 0$.

(iii) Miller's backward recurrence algorithm. We may start the recurrence (1) with

$$\eta_\nu = 1, \quad \eta_{\nu+1} = 0 \ , \tag{14}$$

and use it in the backward direction to obtain $\eta_n = \eta_n^{(\nu)}$, $n = \nu-1, \nu-2, \ldots, 1$. In effect, we produce a solution of the linear system (13), where $f_0$ on the right is replaced by $\eta_0^{(\nu)}$. Consequently,

$$f_n^{(\nu)} = \frac{f_0}{\eta_0^{(\nu)}} \eta_n^{(\nu)}, \qquad n = 0, 1, \ldots, \nu \ . \tag{15}$$

Generating $\eta_n^{(\nu)}$ as described, and then $f_n^{(\nu)}$ by (15), is known as Miller's algorithm (British Association for the Advancement of Science [1952, p. xvii]). It has the same disadvantage as noted in (i). In addition, the quantities $\eta_n^{(\nu)}$ may become large enough to cause overflow on a computer.

(iv) Olver's algorithm. Miller's algorithm can be thought of as solving the system (13) by a form of Gauss elimination, in which the elimination is performed backwards, from the last equation to the first, and the solution then obtained by forward substitution. The algorithm proposed by Olver [1967a] uses the more conventional forward elimination followed by back substitution. To describe it, let

$$p_0 = 0, \quad p_1 = 1, \quad e_0 = f_0 \ ,$$

$$\left.\begin{aligned} p_{n+1} &= -a_n p_n - b_n p_{n-1} \\ e_n &= b_n e_{n-1} \end{aligned}\right\} \quad n = 1, 2, \ldots, \nu \ . \tag{16}$$

Then

$$f_{\nu+1}^{(\nu)} = 0, \quad p_{n+1} f_n^{(\nu)} - p_n f_{n+1}^{(\nu)} = e_n, \qquad n = \nu, \nu-1, \ldots, 1 \ , \tag{17}$$

which yields $f_\nu^{(\nu)}, f_{\nu-1}^{(\nu)}, \ldots, f_1^{(\nu)}$ in this order, provided none of the $p_n$ vanishes.

We note from (17) that

$$\frac{f_n^{(\nu)}}{p_n} - \frac{f_{n+1}^{(\nu)}}{p_{n+1}} = \frac{e_n}{p_n p_{n+1}} ,$$

so that

(18) $$f_n^{(\nu)} = p_n \sum_{k=n}^{\nu} \frac{e_k}{p_k p_{k+1}}, \qquad n = 1, 2, \ldots, \nu .$$

In particular, by (12),

(19) $$f_n = p_n \sum_{k=n}^{\infty} \frac{e_k}{p_k p_{k+1}} .$$

It follows that $f_n^{(\nu)}$ has relative error

(20) $$\frac{f_n - f_n^{(\nu)}}{f_n} = \frac{\sum_{k=\nu+1}^{\infty} e_k / p_k p_{k+1}}{\sum_{k=n}^{\infty} e_k / p_k p_{k+1}} \doteq \frac{e_{\nu+1}}{p_{\nu+1} p_{\nu+2}} \Big/ \frac{e_n}{p_n p_{n+1}} ,$$

the approximation on the far right being valid if the series in (19) converges rapidly. (Using the techniques in Olver [1967b] one could estimate the series more carefully and thus obtain a rigorous error bound). If we wish to obtain $f_n$ to within a relative error $\epsilon$, we may thus iterate with (16) until a value of $\nu$ is reached for which

(21) $$\left| \frac{e_{\nu+1}}{p_{\nu+1} p_{\nu+2}} \right| \leq \epsilon \min_n \left| \frac{e_n}{p_n p_{n+1}} \right| ,$$

the minimum being taken over all values $n$ of interest. With $\nu$ so determined, the $f_n^{(\nu)}$ are then obtained as described in (17). It is this feature of automatically determining $\nu$, which makes Olver's algorithm attractive.

(v) Olver's and Miller's algorithm combined. In some applications, the recursion in (16) for $p_n$ is mildly unstable, initially, although ultimately it is always stable. Olver and Sookne [1972] therefore suggest applying the procedure (16), which serves mainly to determine the cutoff-index $\nu$, only in a region $n \geq n_0$ of perfect stability for the p-recursion, starting with $p_{n_0} = 0$, $p_{n_0+1} = 1$ as before, but with $e_{n_0} = 1$. Once $\nu$ is determined, the desired approximations are then obtained by recurring backward, as in Miller's procedure, starting with $f_{\nu+1}^{(\nu)} = 0$, $f_{\nu}^{(\nu)} = e_\nu/p_{\nu+1}$, and by a final normalization, as in (15).

We remark that all algorithms described can be extended to accommodate the more general "normalization condition" (5). This is an important point, inasmuch as the algorithms so extended do not require the calculation of any particular value of $f_n$ (such as $f_0$ above). For details, we refer to the cited references.

2.2.3. Applications to special functions. The algorithms of 2.2.2 have been applied to a large number of special functions. The first major applications involved Bessel functions and Coulomb wave functions, whose recurrence relations are similar in nature. Further applications soon followed, e.g., to Legendre functions, incomplete beta and gamma functions, repeated integrals of the error function, and others. Detailed references, up to about 1965, can be found in Gautschi [1967]. More recently, in connection with Bessel functions, Mechel [1968] and Cylkowski [1971] discuss appropriate choices of the starting index $\nu$ in Miller's algorithm, while Amos [1974] proposes accurate starting values from uniform asymptotic expansions. The latter approach, combined with Taylor expansion where appropriate, is carefully implemented in Amos and Daniel [1973] and Amos, Daniel and Weston [unpubl.]. Ratios of successive Bessel functions (and of other functions, e.g., the repeated integrals of the error function ) can also be computed by an iterative algorithm based on certain inequalities satisfied by these ratios (Amos [1973], [1974]). For Bessel functions, this is implemented in Amos and Daniel [1973]. Still on Bessel functions, we mention the work of Luke

[1972b], which relates Miller's algorithm to certain rational approximations in the theory of hypergeometric functions, and the computer implementation and certification of Olver's algorithm by Sookne [1973a, b, c, d]. Sidonskiĭ [1967] has a related algorithm for Bessel functions of integer order and real argument, furnishing upper and lower bounds. Hitotumatu [1967/68] recommends a nonlinear normalization condition in place of the linear condition (5). On Coulomb wave functions we note a recent improvement by Gautschi [1969] on the recurrence algorithm (i), and refer to Wills [1971] for a procedure very similar to Olver's. Kölbig [1972] gives a survey of computational methods for Coulomb wave functions. Legendre functions are discussed by Fettis [1967] and more recently by Amos and Bulgren [1969] in connection with series expansions for the bivariate t-distribution in statistics. Bardo and Ruedenberg [1971] revisit the repeated integrals of the error function. Temme [1972] applies algorithm (i) to certain Laplace integrals connected with van Wijngaarden's transformation of formal series.

The stability of forward recurrence is analyzed by Wimp [1971/72], and in the case of orthogonal polynomials of the Laguerre and Hermite type, by Baburin and Lebedev [1967].

### 2.3. Inhomogeneous second-order and higher-order recurrence relations

Some of the more esoteric functions are solutions of inhomogeneous second-order recurrence relations,

$$(1) \qquad y_{n+1} + a_n y_n + b_n y_{n-1} = c_n, \qquad n = 1, 2, 3, \ldots .$$

Others satisfy recurrences of even higher order. The latter are also encountered in the computation of expansion coefficients, e.g., the coefficients in a Taylor series or a series in Chebyshev polynomials. Frequently, the solutions of interest are of the recessive type, in which case some of the algorithms described in 2.2.2, suitably extended, are again effective.

2.3.1. Subdominant solutions of inhomogeneous second-order recurrence relations. Assume that the homogeneous recurrence associated with (1) has a pair of linearly independent solutions $g_n$ and $h_n$, of which $g_n$ is minimal (with $g_0 \neq 0$), hence $h_n$ dominant. We then call a solution $f_n$ of (1) subdominant if

$$\lim_{n\to\infty} f_n/h_n = 0 \quad . \tag{2}$$

A subdominant solution may or may not dominate the minimal solution $g_n$. If it does, neither forward nor backward recurrence is entirely satisfactory.

In analogy to 2.2(13) we consider the linear algebraic system

$$\begin{bmatrix} a_1 & 1 & & & O \\ b_2 & a_2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ O & & & b_\nu & a_\nu \end{bmatrix} \begin{bmatrix} f_1^{(\nu)} \\ f_2^{(\nu)} \\ \vdots \\ f_\nu^{(\nu)} \end{bmatrix} = \begin{bmatrix} c_1 - b_1 f_0 \\ c_2 \\ \vdots \\ c_\nu \end{bmatrix} \quad . \tag{3}$$

If this system has a solution for all $\nu$ sufficiently large, and if $f_n$ is a subdominant solution of (1), then by a result of Olver [1967a],

$$\lim_{\nu\to\infty} f_n^{(\nu)} = f_n \quad . \tag{4}$$

The algorithms of Olver and Olver and Sookne (cf. 2.2.2(iv), (v)) thus extend readily to the case of subdominant solutions. So does in particular Olver's device for determining the appropriate $\nu$ and estimating the error (Olver [1967a, b]). Related algorithms are also discussed in Amos and Burgmeier [1973].

Olver applies his algorithm to Anger-Weber and Struve functions, while Amos and Burgmeier apply theirs to numerous other special functions, including incomplete Laplace transforms, and moments, of Bessel and Struve functions, the incomplete gamma function and Lommel functions. Sadowski and Lozier [1972] give an interesting application of Olver's algorithm to certain definite integrals in plasma physics, involving Chebyshev polynomials. Similar integrals are also treated by Piessens and Branders [1973].

2.3.2. Higher-order recurrence relations. Miller's algorithm is applicable to recurrence relations of arbitrary order, but, unless substantially modified, is effective only for solutions which are "sufficiently minimal". For a penetrating study of this we refer to Wimp [1969]. There are applications to hypergeometric and confluent hypergeometric functions in Wimp [1969], as well as in Wimp [1974], and another application in Wimp and Luke [1969]. Thacher [1972] discusses Miller's algorithm in connection with the solution in power series of linear differential equations with polynomial coefficients and relates minimality of the expansion coefficients to the singularities of the differential equation.

Given enough information about the growth pattern of fundamental solutions, approaches via boundary value problems appear to be more widely applicable. By imposing the right boundary conditions, it is sometimes possible to filter out a desired solution which is neither minimal nor dominant. The principal references in this direction are Oliver [1966/67], [1968a, b].

## §3. Nonlinear recurrence algorithms for elliptic integrals and elliptic functions

Some functions of several variables, notably elliptic integrals, have the remarkable property that their values remain unchanged as the variables undergo certain nonlinear transformations. Repeated application of these transformations, moreover, causes the variables to converge rapidly to certain limiting values, for which the functions can be evaluated by elementary means. These invariance properties thus give rise to interesting and powerful recursive algorithms for computing the functions in question.

### 3.1. Elliptic integrals and Jacobian elliptic functions

3.1.1. Definitions and special values. The best known functions enjoying invariance properties of the type indicated are the elliptic integrals of the first, second, and third kind. In Legendre's canonical form, they are, respectively,

(1) $$F(\varphi, k) = \int_0^{\varphi} \frac{d\theta}{\sqrt{1-k^2 \sin^2 \theta}} ,$$

(2) $$E(\varphi, k) = \int_0^{\varphi} \sqrt{1-k^2 \sin^2 \theta}\, d\theta ,$$

(3) $$\Pi(\varphi, n, k) = \int_0^{\varphi} \frac{d\theta}{(1+n \sin^2 \theta)\sqrt{1-k^2 \sin^2 \theta}} .$$

The variable $k$ is known as the modulus; we assume it in the interval $0 \leq k \leq 1$. The complementary modulus $k'$ is defined by

(4) $$k' = \sqrt{1 - k^2} .$$

The variable $\varphi$ is called the amplitude, and we assume that $0 \leq \varphi \leq \pi/2$. The variable $n$ in (3) may take on arbitrary values, provided the integral is interpreted in the sense of a Cauchy principal value, should $n$ be negative and $1 + n \sin^2 \varphi < 0$.

The integrals (1)-(3) are called complete, or incomplete, depending on whether $\varphi = \pi/2$, or $\varphi < \pi/2$. The complete elliptic integrals are usually denoted by

(5) $$\mathbb{K}(k) = F(\tfrac{\pi}{2}, k), \quad \mathbb{E}(k) = E(\tfrac{\pi}{2}, k), \quad \Pi(n, k) = \Pi(\tfrac{\pi}{2}, n, k) .$$

As $k \downarrow 0$, or $k \uparrow 1$, we have the limiting values

(6) $$\lim_{k \downarrow 0} F(\varphi, k) = \lim_{k \downarrow 0} E(\varphi, k) = \varphi \quad ,$$

(7) $$\lim_{k \uparrow 1} F(\varphi, k) = \tanh^{-1}(\sin\varphi) \quad (0 \leq \varphi < \pi/2), \quad \lim_{k \uparrow 1} E(\varphi, k) = \sin\varphi \quad .$$

Similar, but more complicated formulas hold for $\Pi(\varphi, n, k)$ (see, e.g., Byrd and Friedman [1971, p. 10]). We also note

(8) $$F(\varphi, k) \sim \ln \frac{4}{\cos\varphi + \sqrt{1-k^2\sin^2\varphi}}, \quad E(\varphi, k) \sim 1 \quad \text{as } k \uparrow 1, \; \varphi \uparrow \pi/2 \quad ,$$

where the first relation is given by Carlson [1965, p. 39]; see also Nellis and Carlson [1966, p. 228].

Considering $k$ fixed, the function $u = F(\varphi, k)$ is monotone in $\varphi$, and thus possesses an inverse function,

(9) $$\varphi = \text{am}\, u \quad ,$$

the amplitude function. In terms of it one defines Jacobian elliptic functions by

(10) $$\text{sn}\, u = \sin\varphi, \quad \text{cn}\, u = \cos\varphi, \quad \text{dn}\, u = \sqrt{1-k^2\sin^2\varphi} \quad .$$

3.1.2. Gauss transformations vs. Landen transformations. One distinguishes between Gauss transformations and Landen transformations, and for each between descending and ascending transformations. (Terminology, however, varies). In a descending transformation, the modulus $k$ always decreases; in an ascending transformation, it always increases.

In a Gauss transformation, the amplitude $\varphi$ varies in parallel with k (i.e., $\varphi$ and k both increase or both decrease), while in a Landen transformation they vary in opposite directions. Repeated application of a descending transformation causes k to converge down to zero, while $\varphi$ converges down to some limiting value $\varphi_\infty$ in a Gauss transformation and up to $\infty$ in a Landen transformation. The former, therefore, eventually invokes the equations in (6). Repeated application of an ascending transformation, instead, causes k to converge upward to 1, while $\varphi$ converges upward to $\pi/2$ in a Gauss transformation and down to some limiting value $\varphi_\infty$ in a Landen transformation. The former, therefore, eventually invokes the relations in (8), the latter those in (7).

In describing these transformations, we limit ourselves to elliptic integrals of the first kind, and must refer to the literature for the others. An early treatment of computational algorithms for elliptic functions and integrals is King [1924]. We follow more closely the work of Carlson [1965], who develops the algorithms in a unified way, at least for integrals of the first two kinds. Hofsommer and van de Riet [1963] have ALGOL programs for integrals of the first and second kind, using Landen transformations, as well as programs for elliptic functions, based on ascending Landen and descending Gauss transformations. See also Neuman [1969/70a, b] and Kami, Kiyoto and Arakawa [1971a, b]. Descending transformations for integrals of the third kind are discussed by Ward [1960] in the case of complete integrals, and by Fettis [1965] in the case of incomplete integrals. A thorough treatment of descending Gauss and Landen transformations for integrals of all three kinds, complete with ALGOL procedures, is given in Bulirsch [1965a, b], and more definitively, especially as regards integrals of the third kind, in Bulirsch [1969a, b]. In the latter work, more general transformations, ascribed to Bartky, and extensions thereof, are used effectively. A good introduction into these developments is Bulirsch and Stoer [1968]. For the theory of elliptic integrals and elliptic functions we refer to the books of Neville [1944], [1971] and Tricomi [1948], [1951].

We begin with Gauss' process of the arithmetic-geometric mean, which underlies all algorithms for elliptic functions.

3.2. Gauss' algorithm of the arithmetic-geometric mean

Starting with $a_0 > b_0 > 0$, Gauss' algorithm generates two sequences $\{a_n\}$, $\{b_n\}$ by compounding the arithmetic and the geometric mean in the following manner,

$$\text{(1)} \qquad \begin{cases} a_{n+1} = \frac{1}{2}(a_n + b_n)\,, \\ \\ b_{n+1} = \sqrt{a_n b_n}\,, \end{cases} \qquad n = 0, 1, 2, \ldots\,.$$

Since the iteration functions are homogeneous of degree 1, only the ratio $b_0/a_0$ matters.

The arithmetic mean being larger than the geometric mean, we have $a_n > b_n$ for all $n$, and therefore $b_0 < a_{n+1} < a_n$, $b_n < b_{n+1} < a_0$. It follows that $\{a_n\}$ and $\{b_n\}$ both converge monotonically to certain limits, which, by letting $n \to \infty$ in (1), are readily found to be equal. The common limit is denoted by $M = M(a_0, b_0)$, and called the arithmetic-geometric mean of $a_0$ and $b_0$. Clearly, $b_0 < M(a_0, b_0) < a_0$.

In order to discuss the rate of convergence, it is convenient to introduce

$$\text{(2)} \qquad \epsilon_n = \frac{a_n - b_n}{a_n + b_n}\,.$$

One finds by a simple computation that

$$\text{(3)} \qquad \epsilon_{n+1} = \left(\frac{\epsilon_n}{1 + \sqrt{1 - \epsilon_n^2}}\right)^2, \qquad n = 0, 1, 2, \ldots\,.$$

The sequence $\{\epsilon_n\}$, therefore, converges monotonically and quadratically to zero. Since

(4) $$0 < a_n - M < (a_0 + M)\epsilon_n, \quad 0 < M - b_n < 2M\epsilon_n ,$$

we see that also $\{a_n\}$ and $\{b_n\}$ converge quadratically. We note from (2) that

(5) $$\frac{b_n}{a_n} = 1 - 2\epsilon_n + O(\epsilon_n^2), \quad n \to \infty .$$

Quadratic convergence is a common feature of more general processes of compounding means (Lehmer [1971]). For variants of Gauss' algorithm (none of which quadratically convergent, however), and for many historical notes, see also Carlson [1971]. For complex variables, the algorithm is discussed by Fettis and Caslin [1969] and Morita and Horiguchi [1972/73].

In applications to elliptic integrals, the ratio $b_0/a_0$ will be identified with either the modulus $k$, or the complementary modulus $k'$. The algorithm (1) then generates a sequence of transformed moduli $k_n = b_n/a_n$, or $k'_n = b_n/a_n$, respectively, where in the former case

(6) $$k_{n+1} = \frac{2\sqrt{k_n}}{1+k_n}, \quad n = 0, 1, 2, \ldots, \quad k_0 = k ,$$

and in the latter,

(7') $$k'_{n+1} = \frac{2\sqrt{k'_n}}{1+k'_n}, \quad n = 0, 1, 2, \ldots, \quad k'_0 = k' .$$

An equivalent form of (7') is

(7) $$k_{n+1} = \frac{1-k'_n}{1+k'_n}, \quad n = 0, 1, 2, \ldots, \quad k_0 = k .$$

Since the modulus increases in (6), and decreases in (7), we call (6) an ascending and (7) a descending transformation. The convergence is to 1 and 0, respectively, and quadratic in both cases.

The choice of the transformation is dictated by the speed of convergence, which depends on the magnitude of $\epsilon_0 = (1-b_0/a_0)/(1+b_0/a_0)$. Since we want $\epsilon_0$ small, we choose an ascending transformation if $k^2 > \frac{1}{2}$, and a descending transformation otherwise, so that in either case $1 > (b_0/a_0)^2 \geq \frac{1}{2}$, and thus

$$\epsilon_0 \leq \frac{1-2^{-\frac{1}{2}}}{1+2^{-\frac{1}{2}}} < .172 \; .$$

From (3) we then find that

$$\text{(8)} \qquad \epsilon_{n+1} = \left( \frac{\epsilon_n}{1+\sqrt{1-\epsilon_n^2}} \right)^2 < \frac{\epsilon_n^2}{(1+\sqrt{1-\epsilon_0^2})^2} < \frac{\epsilon_n^2}{3.94} \;,$$

and so,

$$\text{(9)} \quad \epsilon_1 < .00751, \quad \epsilon_2 < 1.44 \times 10^{-5}, \quad \epsilon_3 < 5.27 \times 10^{-11}, \quad \epsilon_4 < 7.05 \times 10^{-22}, \ldots ,$$

illustrating the quadratic nature of convergence.

### 3.3. Computational algorithms based on Gauss and Landen transformations

3.3.1. Descending Gauss transformation. We define

$$\text{(1)} \qquad \begin{cases} a_0 = 1, \quad b_0 = k', \quad t_0 = \csc \varphi \;, \\ a_{n+1} = \frac{1}{2}(a_n + b_n) \;, \\ b_{n+1} = \sqrt{a_n b_n} \;, \qquad\qquad n = 0, 1, 2, \ldots \;. \\ t_{n+1} = \frac{1}{2}(t_n + \sqrt{t_n^2 - a_n^2 + b_n^2}) \;, \end{cases}$$

One verifies without difficulty that $t_n$ and $a_n/t_n$ both decrease. Hence, $a_n/t_n \leq 1$, and $t_n$ must converge,

$$t_n \downarrow T, \quad n \to \infty ,$$

where $T \geq M$. The speed of convergence is comparable to that of $\epsilon_n$, in the sense

$$(2) \qquad t_n - T \sim \frac{M^2}{T}\epsilon_n, \quad n \to \infty .$$

To see this, observe from the last relation in (1), and from 3.2(5), that

$$t_{n+1} = \frac{1}{2} t_n \left\{ 1 + \sqrt{1 - \left(\frac{a_n}{t_n}\right)^2 \left[1 - \left(\frac{b_n}{a_n}\right)^2\right]} \right\} = \frac{1}{2} t_n \left\{ 1 + \sqrt{1 - \left(\frac{a_n}{t_n}\right)^2 \left[4\epsilon_n + O(\epsilon_n^2)\right]} \right\}$$

$$= \frac{1}{2} t_n \left\{ 1 + 1 - 2\left(\frac{M}{T}\right)^2 \epsilon_n + o(\epsilon_n) \right\} = t_n \left\{ 1 - \left(\frac{M}{T}\right)^2 \epsilon_n + o(\epsilon_n) \right\} ,$$

from which

$$t_n - t_{n+1} = \frac{M^2}{T}\epsilon_n + o(\epsilon_n) .$$

Since $\epsilon_n$ converges quadratically, in particular $\epsilon_{n+1} < \epsilon_n^2$, we easily obtain, for any $p \geq 0$,

$$t_n - t_{n+p+1} = \frac{M^2}{T}\epsilon_n + o(\epsilon_n) ,$$

from which (2) follows by letting $p \to \infty$.

We now set

$$(3) \qquad \frac{a_n}{t_n} = \sin \varphi_n \ (0 < \varphi_n < \tfrac{\pi}{2}), \quad \frac{b_n}{a_n} = k_n', \qquad n = 0, 1, 2, \ldots ,$$

which for $n = 0$ is consistent with the first relations in (1) (if $\varphi_0 = \varphi$, $k_0' = k'$). The last relation in (1) can then be written in trigonometric form as

$$\sin \varphi_{n+1} = \frac{(1+k_n') \sin \varphi_n}{1 + \sqrt{1 - k_n^2 \sin^2 \varphi_n}}, \qquad n = 0, 1, 2, \ldots .$$

If in the integral $F(\varphi_n, k_n) = \int_0^{\varphi_n} (1 - k_n^2 \sin^2 \theta)^{-\frac{1}{2}} d\theta$ we make the change of variables

$$\sin \lambda = \frac{(1+k_n') \sin \theta}{1 + \sqrt{1 - k_n^2 \sin^2 \theta}}, \quad 0 < \theta \leq \varphi_n ,$$

we find, after a little computation, that

$$(4) \qquad \frac{1}{a_n} F(\varphi_n, k_n) = \frac{1}{a_{n+1}} F(\varphi_{n+1}, k_{n+1}), \qquad n = 0, 1, 2, \ldots .$$

This is the <u>descending Gauss transformation</u> for elliptic integrals $F(\varphi, k)$. Since $k_n \downarrow 0$, and recalling 3.1(6), we conclude

$$(5) \qquad F(\varphi, k) = \lim_{n \to \infty} \frac{1}{a_n} F(\varphi_n, k_n) = \frac{1}{M} \sin^{-1} \frac{M}{T} .$$

Thus, $F(\varphi, k)$ may be approximated by evaluating $a_n^{-1} \sin^{-1}(a_n/t_n)$ for some $n$ sufficiently large. Observing that

$$0 < \frac{a_n}{t_n} - \frac{M}{T} = \frac{(a_n - M)T + M(T - t_n)}{t_n T} < \frac{a_n - M}{T} ,$$

and using Taylor's theorem, and 3.2(4), we find

$$\left| \frac{1}{M} \sin^{-1} \frac{M}{T} - \frac{1}{a_n} \sin^{-1} \frac{a_n}{t_n} \right| \leq \frac{M+1}{M^2} \left(\frac{\pi}{2} + \sec \varphi\right) \epsilon_n .$$

For $a_n^{-1} \sin^{-1}(a_n/t_n)$ to be an acceptable approximation to $F(\varphi, k)$, it suffices, therefore, that $\epsilon_n$ be sufficiently small [which for most purposes will be the case when $n = 3$ or $n = 4$; cf. 3.2(9)].

3.3.2. Ascending Landen transformation. We define

$$(6)\qquad \begin{cases} a_0 = 1, \quad b_0 = k, \quad s_0 = \cot\varphi\ , \\ a_{n+1} = \frac{1}{2}(a_n + b_n)\ , \\ b_{n+1} = \sqrt{a_n b_n}\ , & n = 0, 1, 2, \ldots\ . \\ s_{n+1} = \frac{1}{2}\left(s_n + \sqrt{s_n^2 + a_n^2 - b_n^2}\right), \end{cases}$$

Clearly, $s_n$ increases, while $a_n/s_n$ decreases. An argument similar to the one surrounding (2) shows that $s_n \uparrow S$, where $S < \infty$, and in fact,

$$(7)\qquad S - s_n \sim \frac{M^2}{S}\epsilon_n, \qquad n \to \infty\ .$$

Letting

$$(8)\qquad \frac{a_n}{s_n} = \tan\varphi_n \ (0 < \varphi_n < \frac{\pi}{2}), \quad \frac{b_n}{a_n} = k_n, \qquad n = 0, 1, 2, \ldots\ ,$$

we can recast the last relation in (6) in the trigonometric form

$$\tan\varphi_{n+1} = \frac{(1+k_n)\tan\varphi_n}{1 + \sqrt{1 + k_n'^2 \tan^2\varphi_n}}, \qquad n = 0, 1, 2, \ldots\ .$$

Similarly as in 3.3.1, it follows that

$$(9)\qquad \frac{1}{a_n} F(\varphi_n, k_n) = \frac{1}{a_{n+1}} F(\varphi_{n+1}, k_{n+1}), \qquad n = 0, 1, 2, \ldots\ ,$$

which is known as the ascending Landen transformation. Making use of 3.1(7), we now obtain

(10) $$F(\varphi, k) = \lim_{n\to\infty} \frac{1}{a_n} F(\varphi_n, k_n) = \frac{1}{M} \sinh^{-1} \frac{M}{S} \quad .$$

When $S$ is small, there is some loss of significant figures in computing $s_n^2 + a_n^2 - b_n^2$ . We can avoid this by introducing

(11) $$d_n = \sqrt{a_n^2 - b_n^2} \quad ,$$

and computing $s_n^2 + a_n^2 - b_n^2 = s_n^2 + d_n^2$, where the $d_n$ are generated recursively by

(12) $$d_{n+1} = \frac{d_n^2}{4a_{n+1}}, \qquad n = 0, 1, 2, \ldots \quad .$$

3.3.3. Ascending Gauss transformation. We define

(13) $$\begin{cases} a_0 = 1, \quad b_0 = k, \quad q_0 = \csc\varphi \quad , \\ a_{n+1} = \frac{1}{2}(a_n + b_n) \quad , \\ b_{n+1} = \sqrt{a_n b_n} \quad , & n = 0, 1, 2, \ldots \quad . \\ q_{n+1} = \frac{1}{2}\left(q_n + \frac{a_n b_n}{q_n}\right) \quad , \end{cases}$$

One verifies without difficulty that $q_n \geq a_n$ for all $n$ . Consequently, $q_{n+1} < q_n$, and the sequence $\{q_n\}$, being monotone decreasing and bounded from below by $M$, converges to some limit. It is easily seen that the limit is $M$ ,

$$q_n \downarrow M, \quad n \to \infty \quad .$$

We set

(14) $$\frac{a_n}{q_n} = \sin\varphi_n \quad (0 < \varphi_n < \frac{\pi}{2}), \quad \frac{b_n}{a_n} = k_n, \qquad n = 0, 1, 2, \ldots ,$$

and rewrite the last relation in (13) as

$$\sin\varphi_{n+1} = \frac{(1+k_n)\sin\varphi_n}{1+k_n\sin^2\varphi_n}, \qquad n = 0, 1, 2, \ldots ,$$

which shows that $\varphi_n$ indeed increases. The ascending Gauss transformation takes the form

(15) $$\frac{1}{2^n a_n} F(\varphi_n, k_n) = \frac{1}{2^{n+1} a_{n+1}} F(\varphi_{n+1}, k_{n+1}), \qquad n = 0, 1, 2, \ldots .$$

In contrast to the previous transformations, $F(\varphi_n, k_n)$ no longer remains bounded as $n \to \infty$. Indeed, simultaneously $\varphi_n \uparrow \pi/2$ and $k_n \uparrow 1$, and so, by 3.1(8),

$$F(\varphi_n, k_n) \sim \ln \frac{4}{\cos\varphi_n + \sqrt{1-k_n^2\sin^2\varphi_n}}, \quad n \to \infty .$$

From (15) we obtain

(16) $$F(\varphi, k) = \frac{1}{M} \lim_{n\to\infty} \left\{ 2^{-n} \ln \frac{2q_n + 2a_n}{\sqrt{q_n^2 - a_n^2} + \sqrt{q_n^2 - b_n^2}} \right\} .$$

It suffices to evaluate the expression on the right for $n$ large enough so that $\epsilon_n$ is negligible compared to $1$.

The denominator

$$e_n = \sqrt{q_n^2 - a_n^2} + \sqrt{q_n^2 - b_n^2}$$

can be computed without loss of significance by means of

$$4q_n e_{n+1} = e_n^2 + (a_n - b_n)^2 \quad ,$$

where the second term on the right is substantially smaller than the first, $(a_n - b_n)^2 \leq \epsilon_n e_n^2$ . The cancellation error incurred in computing $a_n - b_n$, therefore, is of no consequence.

3.3.4. Descending Landen transformation. We define

$$(17) \qquad \begin{cases} a_0 = 1, \quad b_0 = k_0', \quad p_0 = \cot\varphi \ , \\ a_{n+1} = \frac{1}{2}(a_n + b_n) \ , \\ b_{n+1} = \sqrt{a_n b_n} \ , & n = 0, 1, 2, \ldots \ . \\ p_{n+1} = \frac{1}{2}\left(p_n - \frac{a_n b_n}{p_n}\right) \ , \end{cases}$$

This time, $p_n$ cannot possibly tend to a finite limit $P$, as this would imply $P^2 = -M^2$, which is absurd. Neither need $p_n$ preserve its sign.

Letting

$$(18) \qquad \frac{a_n}{p_n} = \tan\varphi_n, \quad \frac{b_n}{a_n} = k_n', \qquad n = 0, 1, 2, \ldots \ ,$$

and writing the last relation of (17) in trigonometric form,

$$\tan\varphi_{n+1} = \frac{(1+k_n')\tan\varphi_n}{1 - k_n' \tan^2\varphi_n}, \qquad n = 0, 1, 2, \ldots \ ,$$

we find however that $\varphi_n$ increases, if we take (Carlson [1965])

$$(19) \qquad i_n \frac{\pi}{2} < \varphi_n \leq (i_n + 1)\frac{\pi}{2} \ ,$$

where

(20) $$i_0 = 0, \quad i_n = \begin{cases} 2i_{n-1} & \text{if } p_n \geq 0 , \\ 2i_{n-1}+1 & \text{if } p_n < 0 \text{ or } p_n = \infty . \end{cases}$$

The descending Landen transformation states that

(21) $$\frac{1}{2^n a_n} F(\varphi_n, k_n) = \frac{1}{2^{n+1} a_{n+1}} F(\varphi_{n+1}, k_{n+1}), \qquad n = 0, 1, 2, \ldots ,$$

and consequently, since $k_n \downarrow 0$, that

(22) $$F(\varphi, k) = \frac{1}{M} \lim_{n\to\infty} 2^{-n} \varphi_n, \qquad \varphi_n = \tan^{-1} \frac{a_n}{p_n} .$$

The branch of the inverse tangent is to be taken in conformity with (19) and (20).

### 3.4. Complete elliptic integrals

All four transformations discussed in 3.3 apply equally for complete integrals. Some of them, however, simplify.

Thus, in the descending Gauss transformation, we find that $t_n = a_n$ for all $n$, which reduces the algorithm 3.3(1), and 3.3(5), to

(1) $$\begin{cases} a_0 = 1, \quad b_0 = k' , \\ a_{n+1} = \frac{1}{2}(a_n + b_n) , \\ b_{n+1} = \sqrt{a_n b_n} , \\ \mathbb{K}(k) = \frac{\pi}{2M} . \end{cases} \qquad n = 0, 1, 2, \ldots ,$$

The arithmetic-geometric mean $M = M(1, k')$ is thus seen to be related to the complete elliptic integral of the first kind, $\mathbb{K}(k)$ .

Similarly, in the descending Landen transformation, we have $p_0 = 0$ , and thus $p_n = \infty$ for all $n \geq 1$, which, by 3.3(20) has the consequence that $i_n = 2^n - 1$. By 3.3(19), therefore, $\varphi_n = 2^{n-1}\pi$, and 3.3(22) then reestablishes (1). The descending Gauss and Landen transformations thus become identical.

Not so for the ascending transformations. In the <u>ascending Gauss transformation</u>, we find $q_n = a_n$ for all $n$, and 3.3(13), together with 3.3(16), where $n$ is conveniently replaced by $n + 1$, simplify to

$$(2) \qquad \begin{cases} a_0 = 1, \quad b_0 = k, \\ a_{n+1} = \frac{1}{2}(a_n + b_n), \\ b_{n+1} = \sqrt{a_n b_n}, \\ \mathbb{K}(k) = \frac{1}{2M} \lim_{n\to\infty} \left(2^{-n} \ln \frac{4}{\epsilon_n}\right). \end{cases} \qquad n = 0, 1, 2, \ldots,$$

The <u>ascending Landen transformation</u>, finally, neither simplifies, nor does it preserve the completeness of the integral.

### 3.5. Jacobian elliptic functions

All four algorithms of 3.3, suitably reversed, yield algorithms for computing Jacobian elliptic functions. We recall that, by definition,

$$(1) \qquad \operatorname{sn} u = \sin\varphi, \quad \text{where } u = F(\varphi, k), \quad 0 \leq u \leq \mathbb{K}(k).$$

In the case of the <u>descending Gauss transformation</u>, e.g., we need to compute $\operatorname{sn} u = 1/t_0$ in 3.3(1), knowing that $T = \lim_{n\to\infty} t_n = M/\sin(Mu)$ by virtue of 3.3(5). We accomplish this by using the Gauss arithmetic-geometric mean process to compute $M$, hence $T$, and then reversing the recursion for $t_n$ in 3.3(1) to compute $t_0$. Thus (Salzer [1962], Hofsommer and van de Riet [1963], Carlson [1965]),

$$
(2)\quad \begin{cases}
a_0 = 1, \quad b_0 = k' , \\
\left.\begin{aligned} a_{n+1} &= \frac{1}{2}(a_n + b_n) \\ b_{n+1} &= \sqrt{a_n b_n} \end{aligned}\right\} \quad n = 0, 1, \ldots, \nu-1 , \\
t_\nu^{(\nu)} = a_\nu / \sin(a_\nu u) , \\
t_{n-1}^{(\nu)} = t_n^{(\nu)} + \dfrac{a_{n-1}^2 - b_{n-1}^2}{4t_n^{(\nu)}}, \qquad n = \nu, \nu-1, \ldots, 1 , \\
\operatorname{sn} u = \dfrac{1}{t_0^{(\nu)}}, \quad \operatorname{cn} u = \sqrt{[t_0^{(\nu)}]^2 - 1}\, \operatorname{sn} u, \quad \operatorname{dn} u = (2t_1^{(\nu)} - t_0^{(\nu)}) \operatorname{sn} u ,
\end{cases}
$$

where $\nu$ is chosen large enough for $a_\nu - M$ to be negligible. (By 3.2(4), this will be the case if $\epsilon_\nu$ is negligible compared to $1/2$ ). A simpler form of the t-recursion results from using 3.3.2(11) and (12),

$$
(2')\qquad t_{n-1}^{(\nu)} = t_n^{(\nu)} + \frac{a_n d_n}{t_n^{(\nu)}}, \qquad n = \nu, \nu-1, \ldots, 1 .
$$

From the ascending Landen transformation we obtain (Southard [1963], Hofsommer and van de Riet [1963], Carlson [1965]), similarly,

$$
(3)\quad \begin{cases}
a_0 = 1, \quad b_0 = k , \\
\left.\begin{aligned} a_{n+1} &= \frac{1}{2}(a_n + b_n) \\ b_{n+1} &= \sqrt{a_n b_n} \end{aligned}\right\} \quad n = 0, 1, \ldots, \nu-1 , \\
s_\nu^{(\nu)} = a_\nu / \sinh(a_\nu u) , \\
s_{n-1}^{(\nu)} = s_n^{(\nu)} - \dfrac{a_n d_n}{s_n^{(\nu)}}, \qquad n = \nu, \nu-1, \ldots, 1 , \\
\operatorname{sn} u = \dfrac{1}{\sqrt{1 + [s_0^{(\nu)}]^2}}, \quad \operatorname{cn} u = s_0^{(\nu)} \operatorname{sn} u, \quad \operatorname{dn} u = (2 s_1^{(\nu)} - s_0^{(\nu)}) \operatorname{sn} u .
\end{cases}
$$

According to the discussion at the end of 3.2, the ascending algorithm (3) is faster than the descending algorithm (2) when $k^2 > \frac{1}{2}$.

## §4. Computer software for special functions

Good numerical methods need to be made easily accessible to the interested user. One way of doing this is by providing computer programs written in one of the higher-level languages such as FORTRAN or ALGOL. For special functions, as well as for many other mathematical problem areas, a great number of such programs are in fact available, and have been so for some time. There are published algorithms in specialized journals (e.g., Comm. ACM, Numer. Math., BIT, Computer Physics Comm., Applied Statistics, and ACM Trans. Mathematical Software), and many others in user's group libraries, commercial libraries, local subroutine libraries, etc. Unfortunately, the quality of these algorithms and programs varies enormously. It has been felt, therefore, in recent years, that libraries should be established by selecting a few algorithms, known for their outstanding quality, implementing them carefully into reliable and thoroughly tested pieces of computer software, integrating the pieces into larger, well-streamlined, and easy-to-use collections of subroutines, and finally releasing these collections to the computing public, with provisions for updating them at regular intervals.

This is not the place to enter into a discussion of the many design objectives and desirable attributes of such packages, nor of explaining the considerable difficulties in trying to attain them; we refer for this to Rice [1971] and Cody [1974]. We would like to draw attention, however, to two current efforts in this direction, one in the United States known as the NATS project (National Activity to Test Software), the other in England, known as the NAG project (Numerical Algorithms Group, formerly Nottingham Algorithms Group). The former's original objective is to produce high-quality software for two restricted problem areas, namely matrix eigensystem problems, and special functions, for which initial packages have been released in 1972 and 1973 under the names EISPACK and FUNPACK, respectively. The latter's objectives are similar, but embrace a wider problem area – essentially all the major numerical analysis problems. The most recent version ("mark 4") was completed in 1973. For a general description of the NATS project we refer to Boyle et al. [1972] and Smith, Boyle and Cody [1974], and for a discussion of the NAG project to Ford and Hague [1974] and Ford and Sayers [1974]. We briefly compare the two efforts, as far as they concern special functions.

### 4.1. NATS software for special functions

The special function package of the NATS project – FUNPACK – is developed and maintained under the direction of Cody at Argonne National Laboratory (Cody [1975]). His principal decisions in designing FUNPACK are, first of all, to adopt FORTRAN as the exclusive language of the package, and, secondly, to limit the programs to three different lines of computers, namely the IBM 360-370 series, the CDC6000-7000 series, and Univac 1108. Accordingly, only three accuracy requirements have to be dealt with, roughly 14 significant decimal digits on CDC equipment, and 16, respectively 18, decimal digits for the hardware double-precision arithmetic on IBM and Univac equipment. The package, therefore, is designed to perform well on these particular machines, and is not expected, nor intended, to be easily transportable to other machines.

The limitation to three different precisions has a major influence in the selection of approximation methods. Most attractive, under the circumstances, are rational Chebyshev approximations, both by virtue of their efficiency and uniform accuracy. This, in fact, is the choice made in FUNPACK. The current version I includes subroutines for six special functions – the exponential integral, the complete elliptic integrals of the first and second kind, Dawson's integral, and the Bessel functions $K_0$ and $K_1$. All of them are computed from appropriate best rational approximations. Plans are underway to extend the package to include sequences of functions and multivariate functions.

All the programming of the package, as well as the initial testing, was done at Argonne National Laboratory, which has IBM equipment. Similar tests were run on CDC equipment at the University of Texas, and on Univac equipment at the University of Wisconsin. After this initial testing and "tuning" of the routines, they were subjected to additional field tests on the same type of computers, running, however, with different FORTRAN compilers and under a variety of operating systems, some in batch mode, others in time sharing mode. Only after successful completion of all field tests, in September of 1973, was the first version of the package released.

## 4.2. NAG software for special functions

The special function chapter of the NAG library is being developed by Schonfelder at the University of Birmingham (Schonfelder [1974a, b]). While the basic objectives, and methods of testing, are similar to those of the NATS project, there are some significant differences. For one, all programs in the NAG library are written separately in two languages, FORTRAN and ALGOL. For another, the library is designed to be highly portable, i.e., to run, with a minimal amount of changes, on a wide variety of different machines. Finally, coverage is hoped to eventually include all the major functions in Abramowitz and Stegun [1964] – roughly fifty separate functions. At the moment (Schonfelder [1975]), the list of functions for the forthcoming edition ("mark 5") is to include the exponential, sine, and cosine integral, the gamma function, the error function and Fresnel integrals, and the Bessel functions $J_0$, $J_1$, $Y_0$, $Y_1$, $I_0$, $I_1$, $K_0$, $K_1$. Plans exist to cover functions of several variables, and of complex variables, but implementation appears to be several years in the future (Schonfelder [1975]).

The choices made for the methods of computation reflect the multi-machine character of the NAG library. Preference, in fact, is given to expansions in Chebyshev polynomials, which can be truncated easily to fit various machine precisions, although they may be somewhat inferior in efficiency compared to rational approximations.

### 4.3. Other software for special functions

Good subroutines for special functions can be found in other mathematical subroutine libraries, e.g., the Boeing library and handbook (Newbery [1971]), containing programs in FORTRAN, and the NUMAL library (Numerical procedures in ALGOL 60) developed at the Mathematical Centre in Amsterdam (den Heijer et al. [1974]). The latter has appeared in seven volumes, volume 6 being devoted to special functions. In addition, there are a number of commercial subroutine packages. IBM offers SSP (Scientific Subroutine Package), currently in its 5th edition, and SLMATH (Subroutine Library Mathematics) and its PL/1 version, PLMATH, while IMSL (International Mathematical Statistical Libraries) regularly issues revised editions of its library.

We listed only those library projects, relevant to special functions, which are most familiar to us, realizing that there are undoubtedly many others.

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