

APPLICATIONS OF CONTINUED FRACTIONS
IN ONE AND MORE VARIABLES

by

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SUMMARY.

Elementary properties of continued fractions are derived from sets of three-term recurrence relations and approximation methods are developed from this simple approach.

First, a well-known method for numerical inversion of Laplace transforms is modified in two different ways to obtain exponential approximations. Differential-difference equations arising from certain Markov processes are solved by direct application of continued fractions and practical error estimates are obtained. Approximations of a slightly different form are then derived for certain generalised hypergeometric functions using those hypergeometric functions that satisfy three-term recurrence relations and have simple continued fraction expansions. Error estimates are also given in this case.

The class of corresponding sequence algorithms is then described for the transformation of power series into continued fraction form. These algorithms are shown to have very general application and only break down if the required continued fraction does not exist. A continued fraction in two variables is then shown to exist and its correspondence with suitable double power series made feasible by the generalisation of the corresponding sequence method. A convergence theorem, due to Van Vleck, is adapted for use with this type of continued fraction and a comparison is made with Chisholm rational approximants in two variables. Some of these ideas are further generalised to the multivariate case.

Such corresponding fractions are closely related to other fractions that may be used for point-wise bivariate or multivariate interpolation to function values known on a mesh of points. Interpolation algorithms are described and advantages and limitations discussed.

The work presented forms a basis for a wide range of further research and some possible applications in numerical mathematics are indicated.

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M.R. O'Donohoe.

This thesis is based on my own work except for Sections 1.1 and 2.1 which were produced in collaboration with my supervisor, Mr J.A. Murphy. The material in these sections is contained in our paper, "Some Properties of Continued Fractions with Applications in Markov Processes", to appear in the Journal of the I.M.A. Some of the work in Section 2.1 was also submitted by me as a project for the degree of Bachelor of Technology at this University in 1971.

M.R. O'Donohoe.

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NOTATION.

In this thesis I have used various notation conventions which I will now clarify. Within each chapter equations are numbered sequentially, prefixed by the number of the chapter. For example, equation (3.54) is the 54th equation in Chapter 3. The same system applies to theorems, tables, figures, etc. References are generally given by the author's name, followed by the year of publication. Exceptionally, conference proceedings are given by the editor's name, followed by the year of the conference.

The notations $O(z^n)$ and $O(z^{-n})$ are used extensively. Without exception, the positive index denotes an error term of order z^n with additional terms in ascending powers, and the negative index denotes an error of order z^{-n} with additional terms in descending powers of z . Various generalisations of the O -notation are also used but are explained in the text.

Also, when asymptotic expansions are quoted they are generally used as formal expansions only, so that the symbol "=" is used instead of "~".

INTRODUCTION.

Although rarely in the forefront of mathematical research, the theory of continued fractions has a long history and contains contributions by many renowned mathematicians. The origin of the subject is uncertain but Euclid's H.C.F. algorithm is an early example of what is essentially a continued fraction method. Omar Khayam, the 12th Century Persian poet and mathematician, is reputed to have expanded irrational square roots in continued fraction form but the earliest published reference in existence is probably Bombelli's "L'Algebra", printed in Bologna in 1572. In the 17th Century important work was done by Wallis and also Brounker, who obtained a continued fraction for π .

The function theory of continued fractions is more recent in origin and Euler, from 1737 onwards, made the first systematic investigation in a series of papers. Lagrange's method of 1776, for obtaining continued fraction solutions of differential equations, was a major landmark and led to many developments in the next century.

In 1821 Cauchy proposed the use of rational functions as a means of pointwise interpolation to functions of a single variable. This aspect has received little attention, the most notable work being that of Thiele who developed reciprocal differences as a means for forming interpolatory continued fractions and demonstrated the connection between these fractions and analytic expansions.

Towards the end of the 19th Century there was renewed

interest in the field. Laguerre investigated the summation of divergent series in 1879, and published an important paper on differential equations in 1885. Padé's thesis of 1892 formalised the concept of rational approximation and emphasised the connection with continued fraction theory; the idea of Padé approximants is, however, much older. In 1895 Stieltjes began to formulate an analytic theory and valuable work was also contributed by Markov, Pringsheim and others. Van Vleck's papers on the J-fraction and related topics appeared at the turn of the century and most of the classical theory had been developed by 1910.

In 1913 the first modern text book appeared. This was Perron's "Die Lehre von den Kettenbrüchen" which was last edited in 1957 but is still not available in the English language. This is the only major work to include both the arithmetic and the analytic theories of continued fractions. The only comparable work on the analytic theory is by Wall (1948) which includes the matrix theory of continued fractions, developed in the 1920's, and considerable contributions by Wall and his associates over two decades prior to the publication of the book. This is widely regarded as the standard work in the field although its lack of clarity is a frequent criticism. At a more elementary level Wynn's translation of Khovanskii (1963) is a readable account of some of the basic theory, including some generalisations of continued fractions first suggested by Euler in 1771.

The post-war development of electronic computation has led to a revival of interest in continued fractions as a means of

numerical approximation. Accordingly, there have been many advances in the area of numerical analysis over the last twenty years. The well-known quotient-difference algorithm, introduced by Rutishauser in 1954, is a powerful method that may be used to find the roots of a polynomial or the eigenvalues of a matrix, but was first developed for converting a power series to a continued fraction. There are many interesting papers in the numerical field by Wynn, who introduced the ϵ -algorithm, and Gragg, who produced a paper in 1972 surveying the whole field.

The work of Baker, Gammel and others since 1961 has led to a resurgence of interest in Padé approximants, in theoretical physics in particular. Baker and Gammel (1970) have themselves edited a survey book of applications in physics and, in the same field, Graves-Morris has edited the proceedings of a Summer School and Conference at the University of Kent in 1972.

Forseeing the desirability of approximations to functions of more than one variable, Chisholm (1973) has shown how Padé approximants may be generalised to two variables, and it is expected that this is the direction which much future research will take. The generalisation to two variables is not trivial and, as Chisholm points out, can be accomplished in various ways. Bearing in mind the variety of possible applications of such techniques, it is reasonable to suppose that different methods of generalisation will be useful in different situations. In this thesis rational approximants in two variables are obtained by means of continued fractions. These approximants are shown to

be different from Chisholm approximants and advantages and disadvantages of the two methods are discussed. The generalisation to many variables is also described, and analogous techniques are developed for rational interpolation in two or more variables.

In the first part of this thesis exponential approximations are obtained by numerical inversion of Laplace transforms. The process, in which Laplace transforms are expressed as J-fractions and the inversion is performed by a matrix method, was described by Luke (1962) but the idea is probably much older. In this work the technique is modified in two different ways.

The one-to-one correspondence between a continued fraction and a set of three-term recurrence relations is of primary importance throughout this thesis and it is appropriate to begin by using this correspondence to develop some fundamental results for a general continued fraction.

PART I

APPLICATIONS IN ONE VARIABLE

CHAPTER 1.

SOME PROPERTIES OF CONTINUED FRACTIONS.

1.1 Continued Fractions and Recurrence Relations.

By "the continued fraction f_0 " we understand an infinite expression of the type

$$f_0 = \frac{a_1}{b_1 + \frac{a_2}{b_2 + \frac{a_3}{b_3 + \dots + \frac{a_n}{b_n + \dots}}}} \quad (1.1)$$

which we may write in the more convenient form

$$f_0 = \frac{a_1}{b_1} + \frac{a_2}{b_2} + \frac{a_3}{b_3} + \dots + \frac{a_n}{b_n} + \dots \quad (1.2)$$

where the elements $\{a_n\}$ and $\{b_n\}$ are numbers, real or complex.

The n th convergent of f_0 is

$$\frac{A_n}{B_n} = \frac{a_1}{b_1} + \frac{a_2}{b_2} + \frac{a_3}{b_3} + \dots + \frac{a_n}{b_n} \quad (1.3)$$

where A_n and B_n are respectively called the n th numerator and n th denominator of the continued fraction. The numbers a_n and b_n are called the n th partial numerator and n th partial denominator, and the expression a_n/b_n is called the n th partial quotient.

The concept of an infinite continued fraction may be

formalised in various ways. In his standard work on the analytic theory, Wall (1948) introduces a continued fraction in terms of the linear fractional transformations

$$t_n(w) = \frac{a_n}{b_n + w} \quad (1.4)$$

for $n = 1, 2, 3, \dots$. Taking the product of the first n of these transformations and setting $w=0$, we get

$$\frac{A_n}{B_n} = t_1 t_2 \dots t_n(0) \quad (1.5)$$

so that

$$f_0 = \lim_{n \rightarrow \infty} t_1 t_2 \dots t_n(0) \quad (1.6)$$

It may be shown by induction that

$$t_1 t_2 \dots t_n(w) = \frac{A_{n-1} w + A_n}{B_{n-1} w + B_n} \quad (1.7)$$

for $n = 1, 2, 3, \dots$. From (1.7) we can easily obtain the recurrence relations

$$\left. \begin{aligned} A_n &= a_n A_{n-2} + b_n A_{n-1} \\ B_n &= a_n B_{n-2} + b_n B_{n-1} \end{aligned} \right\} \quad (1.8)$$

with initial values $A_0=0$, $A_1=a_1$ and $B_0=1$, $B_1=b_1$. Using

(1.8) we can verify the determinantal forms for the numerators

and denominators,

$$A_n = a_1 \begin{vmatrix} b_2 & 1 & & & \\ -a_3 & b_3 & 1 & & \\ & -a_4 & b_4 & 1 & \\ & & \dots & \dots & \dots \\ & & & \dots & 1 \\ & & & & -a_n & b_n \end{vmatrix} \quad (1.9)$$

for $n = 2, 3, 4, \dots$, and

$$B_n = \begin{vmatrix} b_1 & 1 & & & \\ -a_2 & b_2 & 1 & & \\ & -a_3 & b_3 & 1 & \\ & & \dots & \dots & \dots \\ & & & \dots & 1 \\ & & & & -a_n & b_n \end{vmatrix} \quad (1.10)$$

for $n = 1, 2, 3, \dots$. Also, writing $\alpha_r = \prod_{i=1}^r a_i$ and using (1.8), we can obtain the so-called determinant formula

$$A_{r+1} B_r - A_r B_{r+1} = (-1)^r \alpha_{r+1} \quad (1.11)$$

As an alternative to the fractional transformation approach we may consider the continued fraction (1.2) to be the solution f_0 of the infinite set of recurrence relations

$$\left. \begin{aligned} f_1 &= a_1 - b_1 f_0 \\ f_2 &= a_2 f_0 - b_2 f_1 \\ f_3 &= a_3 f_1 - b_3 f_2 \\ &\dots \\ &\dots \\ f_r &= a_r f_{r-2} - b_r f_{r-1} \\ &\dots \\ &\dots \end{aligned} \right\} \quad (1.12)$$

Dividing the first relation by f_0 and rearranging, we have

$$f_0 = \frac{a_1}{b_1 + \frac{f_1}{f_0}}, \quad (1.13)$$

and dividing the r th relation by f_{r-1} , we have

$$\frac{f_{r-1}}{f_{r-2}} = \frac{a_r}{b_r + \frac{f_r}{f_{r-1}}} \quad (1.14)$$

for $r = 2, 3, 4, \dots$. The results (1.13) and (1.14) lead to the continued fraction (1.2) for which we now establish an elementary convergence result. From the first n relations of (1.12) we obtain, using (1.8),

$$B_n f_0 - A_n = (-1)^n f_n. \quad (1.15)$$

If B_n is non-zero we also have

$$f_0 - \frac{A_n}{B_n} = (-1)^n \frac{f_n}{B_n}. \quad (1.16)$$

If we now choose the sequences $\{a_n\}$ and $\{b_n\}$ in such a way that there exists a suffix N such that B_n is non-zero for all $n > N$ then, from result (1.16), a sufficient condition for the continued fraction (1.2) to converge to a solution of the recurrence relations (1.12) is

$$\lim_{n \rightarrow \infty} \frac{f_n}{B_n} = 0. \quad (1.17)$$

More particularly, a sufficient condition for convergence is

$$\lim_{n \rightarrow \infty} f_n = 0 \quad (1.18)$$

provided there exists N , such that $\inf |B_n| > 0$ for $n > N$.

In this case, if we let a_n and b_n be functions of a complex variable z and if F is the region of the z -plane for which condition (1.18) holds then we can easily prove the following theorem:

Theorem 1.1: The continued fraction (1.2) is convergent in that part of the region F which excludes the zeros of $B_n(z)$ for $n > N$, where N is arbitrarily large.

Similar theorems and some of the results in this section appear in Wall(1948), Perron(1957) and Khovanskii(1963) in which they are usually presented in a different way. The convergence of continued fractions formed from recurrence relations is given an alternative treatment in Nörlund(1924), but Theorem 1.1 is more appropriate for our purposes. In the remainder of this section we assume that condition (1.18) holds so that the continued fraction (1.2) converges.

So far we have shown how continued fractions may be formed from either fractional transformations (1.4) or from recurrence relations (1.12) and some basic properties have been derived using both techniques. It is the main theme of this thesis to show the usefulness of recurrence relations in continued fraction methods, both as a practical means for solving problems in Part I, and as a tool for research in Part II. The simplicity of this approach promotes a deeper

understanding of continued fractions and makes possible their generalisation to two or more variables. Throughout this work the sequence $\{f_r\}$ assumes great importance and it shall be referred to as the corresponding sequence of the continued fraction (1.2). In Chapter 2. we shall relate $\{f_r\}$ to sequences of probability functions and hypergeometric functions, and in Chapter 3. the corresponding sequence will be used as the basis of a class of algorithms which will be generalised in Part II.

We now note that the corresponding sequence $\{f_r\}$ is altered if we perform a similarity transformation on a continued fraction. The values of the continued fraction (1.2) and all its convergents remain unchanged under the transformation

$$f_0 = \frac{c_1 a_1}{c_1 b_1} + \frac{c_1 c_2 a_2}{c_2 b_2} + \frac{c_2 c_3 a_3}{c_3 b_3} + \dots + \frac{c_{r-1} c_r a_r}{c_r b_r} + \dots \quad (1.19)$$

This is equivalent to multiplying the r th equation of the set (1.12) by γ_r , where $\gamma_r = \prod_{i=1}^r c_i$, and forming a new corresponding sequence $\{f'_r\}$, where

$$\left. \begin{aligned} f'_0 &= f_0 \\ f'_r &= \gamma_r f_r \end{aligned} \right\} \quad (1.20)$$

for $r = 1, 2, 3, \dots$

Now, from (1.14) we have the continued fraction

$$\frac{f_n}{f_{n-1}} = \frac{a_{n+1}}{b_{n+1}} + \frac{a_{n+2}}{b_{n+2}} + \frac{a_{n+3}}{b_{n+3}} + \dots \quad (1.21)$$

for $n = 1, 2, 3, \dots$ for which we have the following expression,

using (1.8),

$$f_o = \frac{A_n + \frac{f_n}{f_{n-1}} A_{n-1}}{B_n + \frac{f_n}{f_{n-1}} B_{n-1}} \quad (1.22)$$

for $n = 1, 2, 3, \dots$. Subtracting the n th convergent of f_o and using (1.11) and (1.14) we obtain

$$f_o - \frac{A_n}{B_n} = \frac{(-1)^n \alpha_{n+1}}{B_n (B_{n+1} + \frac{f_{n+1}}{f_n} B_n)} \quad (1.23)$$

Hence we have obtained a continued fraction for the truncation error, $T_n(f_o)$, of f_o ,

$$T_n(f_o) \equiv f_o - \frac{A_n}{B_n} = \frac{(-1)^n \alpha_{n+1}}{B_n B_{n+1}} + \frac{a_{n+2} B_n^2}{b_{n+2}} + \frac{a_{n+3}}{b_{n+3}} + \frac{a_{n+4}}{b_{n+4}} + \dots, \quad (1.24)$$

which we shall call the truncation fraction. This result was essentially obtained by Wall(1948) in connection with matrix theory. Also, by comparison with (1.16) we have another important continued fraction,

$$f_r = \frac{\alpha_{r+1}}{B_{r+1}} + \frac{a_{r+2} B_r}{b_{r+2}} + \frac{a_{r+3}}{b_{r+3}} + \frac{a_{r+4}}{b_{r+4}} + \dots \quad (1.25)$$

The n th denominator of this fraction is B_{r+n} . We denote the n th numerator by $A_n^{(r)}$, where $A_n^{(o)} = A_n$, $A_1^{(r)} = \alpha_{r+1}$ and

$$A_n^{(r)} = a_{r+n} A_{n-2}^{(r)} + b_{r+n} A_{n-1}^{(r)} \quad (1.26)$$

for $n = 2, 3, 4, \dots$. The truncation fraction for f_r

is then

$$T_n(f_r) \equiv f_r - \frac{A_n^{(r)}}{B_{r+n}} = \frac{(-1)^n \alpha_{r+n+1} B_r}{B_{r+n} B_{r+n+1}} + \frac{a_{r+n+2} B_{r+n}^2}{b_{r+n+2}} + \frac{a_{r+n+3}}{b_{r+n+3}} + \dots,$$

$$\text{i.e. } T_n(f_r) = (-1)^n B_r \frac{f_{r+n}}{B_{r+n}}. \quad (1.27)$$

If we now set $f_{r+n} = 0$ then

$$f_0 = \frac{A_{r+n}}{B_{r+n}}, \quad f_r = \frac{A_n^{(r)}}{B_{r+n}},$$

and (1.16) gives

$$\frac{A_{r+n}}{B_{r+n}} - \frac{A_r}{B_r} = \frac{(-1)^r A_n^{(r)}}{B_r B_{r+n}},$$

so we can generalise the determinant formula (1.11) to

$$A_{r+n} B_r - A_r B_{r+n} = (-1)^r A_n^{(r)}. \quad (1.28)$$

We now introduce a generalisation that has a direct application in Chapter 2. Still assuming that condition (1.18) is satisfied we examine a new set of recurrence relations

$$\left. \begin{aligned} f_1^{(m)} &= -b_1 f_0^{(m)} \\ f_2^{(m)} &= a_2 f_0^{(m)} - b_2 f_1^{(m)} \\ f_3^{(m)} &= a_3 f_1^{(m)} - b_3 f_2^{(m)} \\ &\dots \dots \dots \\ &\dots \dots \dots \\ f_m^{(m)} &= a_m f_{m-2}^{(m)} - b_m f_{m-1}^{(m)} \\ f_{m+1}^{(m)} &= a_{m+1} f_{m-1}^{(m)} - b_{m+1} f_m^{(m)} + k_{m+1} \\ f_{m+2}^{(m)} &= a_{m+2} f_m^{(m)} - b_{m+2} f_{m+1}^{(m)} \\ &\dots \dots \dots \\ &\dots \dots \dots \end{aligned} \right\} (1.29)$$

in which the term k_{m+1} occurs in the $(m+1)$ th relation and a_1 is absent unless $m = 0$. Apart from the term k_{m+1} the coefficients are the coefficients of (1.12) and we have, in particular, $k_1 = a_1$ and $f_r^{(0)} = f_r$. We will now derive results for $\{f_r^{(m)}\}$ analogous to those we have developed for $\{f_r\}$.

It is easily proved by induction that

$$f_{r-1}^{(m)} = -\frac{B_{r-1}}{B_r} f_r^{(m)} \quad (1.30)$$

for $r = 1, 2, 3, \dots, m$. In particular, when $r = m$ we substitute for $f_{m-1}^{(m)}$ in the $(m+1)$ th relation of (1.29) and obtain

$$f_{m+1}^{(m)} = k_{m+1} - \frac{B_{m+1}}{B_m} f_m^{(m)} \quad (1.31)$$

Now, the relation (1.31) together with the $(m+2)$ th, $(m+3)$ th, $(m+4)$ th, \dots relations of the set (1.29) form a set analogous to (1.12) so that we obtain the continued fraction

$$f_m^{(m)} = \frac{k_{m+1}}{\left(\frac{B_{m+1}}{B_m}\right) + \frac{a_{m+2}}{b_{m+2}} + \frac{a_{m+3}}{b_{m+3}} + \dots} \quad (1.32)$$

or, using (1.19),

$$f_m^{(m)} = \frac{k_{m+1} B_m}{B_{m+1}} + \frac{a_{m+2} B_m}{b_{m+2}} + \frac{a_{m+3}}{b_{m+3}} + \dots \quad (1.33)$$

In fact we have

$$f_m^{(m)} = \frac{k_{m+1}}{\alpha_{m+1}} B_m f_m \quad (1.34)$$

By repeated application of (1.30) to (1.34) we get

$$f_r^{(m)} = (-1)^{m-r} \frac{k_{m+1}}{\alpha_{m+1}} B_r f_m \quad (1.35)$$

for $r \leq m$. Although the continued fraction (1.33) is of a more convenient form, we must be careful to use (1.32) when considering $\{f_r^{(m)}\}$, for $r \geq m$, as the corresponding sequence of $f_m^{(m)}$.

Applying result (1.25) we get

$$f_r^{(m)} = \frac{k_{m+1}}{\alpha_{m+1}} B_m f_r \quad (1.36)$$

for $r \geq m$.

For results (1.35) and (1.36) we have the truncation fractions

$$\begin{aligned} T_n(f_r^{(m)}) &= (-1)^{m-r} \frac{k_{m+1}}{\alpha_{m+1}} B_r T_n(f_m) \\ &= (-1)^{m+n-r} \frac{k_{m+1}}{\alpha_{m+1}} B_r B_m \frac{f_{m+n}}{B_{m+n}} \end{aligned} \quad (1.37)$$

for $r \leq m$, and

$$\begin{aligned} T_n(f_r^{(m)}) &= \frac{k_{m+1}}{\alpha_{m+1}} B_m T_n(f_r) \\ &= (-1)^n \frac{k_{m+1}}{\alpha_{m+1}} B_r B_m \frac{f_{r+n}}{B_{r+n}} \end{aligned} \quad (1.38)$$

for $r \geq m$.

Finally, analogous to (1.19), we can transform the set of relations (1.29) to a more convenient form, constructing a new corresponding sequence $\{f_r^{(m)'}\}$ where

$$\left. \begin{aligned} f_0^{(m)'} &= f_0^{(m)} \\ f_r^{(m)'} &= \gamma_r f_r^{(m)} \end{aligned} \right\} \quad (1.39)$$

and a new term k_{m+1}' where

$$k_{m+1}' = \gamma_{m+1} k_{m+1} \quad (1.40)$$

In this section we have discussed continued fractions in a general way, without reference to particular types of fraction. In the remainder of this chapter we shall examine continued fractions that represent or approximate to functions of a single variable.

1.2 Corresponding Fractions.

In this section we shall describe various well-studied continued fractions which represent a function $f_0(z)$ formally defined by the power series expansion

$$f_0(z) = a_0 + a_1 z + a_2 z^2 + \dots, \quad (1.41)$$

convergent for $|z| < R_1$, or by the expansion

$$f_0(z) = \frac{b_0}{z} + \frac{b_1}{z^2} + \frac{b_2}{z^3} + \dots, \quad (1.42)$$

convergent for $|z| > R_2$. We shall assume that the coefficients $\{a_n\}$ and $\{b_n\}$ are complex, although in most applications they will be real numbers. We also note that it is not always necessary that the series (1.41) and (1.42) converge for a valid continued fraction expansion to exist, as may be seen in examples given by Wall(1948). The continued fractions studied in this section are all of the form

$$F_0(z) = \frac{u_1(z)}{v_1(z)} + \frac{u_2(z)}{v_2(z)} + \frac{u_3(z)}{v_3(z)} + \dots \quad (1.43)$$

where u_n and v_n are polynomials in the complex variable z , so that the n th convergent $U_n(z)/V_n(z)$ is a rational approximation to $f_0(z)$.

For convenience we now define corresponding fractions in a slightly more general way than most definitions given in the literature.

The continued fraction (1.43) is said to correspond to

the power series (1.41) if

$$f_0(z) - \frac{U_n(z)}{V_n(z)} = o(z^{\sigma(n)}) \quad , \quad (1.44)$$

for $n = 1, 2, 3, \dots$ where $\{\sigma(n)\}$ is a non-decreasing sequence of positive integers such that $\sigma(n) \rightarrow \infty$ as $n \rightarrow \infty$. For the continued fraction (1.43) to correspond to the series (1.42) we use the definition (1.44), except that $\{\sigma(n)\}$ must be a non-increasing sequence of negative integers such that $\sigma(n) \rightarrow -\infty$ as $n \rightarrow \infty$. We now proceed to list various types of corresponding fraction.

The continued fraction

$$F_0(z) = \frac{c_0}{1} + \frac{c_1 z}{1} + \frac{c_2 z^2}{1} + \dots + \frac{c_n z^n}{1} + \dots \quad (1.45)$$

corresponds to the series (1.41) if the coefficients $\{c_n\}$ are chosen such that

$$f_0(z) - \frac{U_n(z)}{V_n(z)} = o(z^n) \quad . \quad (1.46)$$

Such a fraction exists provided that the Hankel determinants

$$H_{2n} = \begin{vmatrix} a_0 & a_1 & \dots & a_n \\ a_1 & a_2 & \dots & a_{n+1} \\ & & \dots & \\ & & & \dots \\ a_n & a_{n+1} & & a_{2n} \end{vmatrix} \quad \text{and, } H_{2n+1} = \begin{vmatrix} a_1 & a_2 & \dots & a_{n+1} \\ a_2 & a_3 & \dots & a_{n+2} \\ & & \dots & \\ & & & \dots \\ a_{n+1} & a_{n+2} & & a_{2n+1} \end{vmatrix} \quad (1.47)$$

are non-zero for $n = 0, 1, 2, 3, \dots$. Now, adapting a theorem

given by Khovanskii (1963), if the fraction (1.45) converges uniformly over a domain D including $|z| < R_1$ then it converges to the function $f_0(z)$ inside $|z| < R_1$ so that $F_0(z)$ may be considered as an analytic continuation of $f_0(z)$ into D . Consequently in many applications, particularly in Chapter 3., it is convenient and not ambiguous to use the notation $f_0(z)$ to refer to a power series or to one of its corresponding fractions.

Now, replacing z by $1/z$ in (1.45) and using the transformation (1.19) we obtain a continued fraction of the form

$$f_0(z) = \frac{c_0}{z} + \frac{c_1}{1} + \frac{c_2}{z} + \frac{c_3}{1} + \dots + \frac{c_{2n}}{z} + \frac{c_{2n+1}}{1} + \dots \quad (1.48)$$

which corresponds to the series (1.42) if the coefficients $\{c_n\}$ are chosen such that

$$f_0(z) - \frac{U_n(z)}{V_n(z)} = o(z^{-n-1}) \quad (1.49)$$

The fraction (1.48) was studied by Stieltjes (1894) and is consequently called an S-fraction. Because of the similarity in structure we shall also refer to the fraction (1.45) as an S-fraction.

As stated above, the S-fraction (1.45) does not exist if any of the Hankel determinants (1.47) is zero. A more general fraction which always exists and corresponds to the

series (1.41) is

$$f_0(z) = \frac{c_0}{1} + \frac{c_1 z^{\alpha_1}}{1} + \frac{c_2 z^{\alpha_2}}{1} + \dots + \frac{c_n z^{\alpha_n}}{1} + \dots \quad (1.50)$$

if $a_0 \neq 0$, where the exponents $\{\alpha_n\}$ are positive integers.

If the series represents a rational function then the fraction terminates, and vice versa. Wall (1948) called (1.50) a C-fraction. An example of a C-fraction is

$$\cos z = \frac{1}{1} + \frac{\frac{1}{2}z^2}{1} - \frac{\frac{5}{12}z^2}{1} + \frac{\frac{1}{100}z^2}{1} - \dots, \quad (1.51)$$

in which $\alpha_n = 2$ for $n = 1, 2, 3, \dots$. Alternatively, we could consider (1.51) to be an S-fraction in the variable z^2 .

We now consider the continued fraction

$$f_0(z) = \frac{p_1}{q_1 + z} + \frac{p_2}{q_2 + z} + \dots + \frac{p_n}{q_n + z} + \dots \quad (1.52)$$

which corresponds to the series (1.42) if $\{p_n\}$ and $\{q_n\}$ are chosen such that

$$f_0(z) - \frac{U_n(z)}{V_n(z)} = O(z^{-2n-1}) \quad (1.53)$$

The fraction (1.52) is called a J-fraction because of its connection with J-forms. It is said to be the even part of the S-fraction (1.48) because the n th convergent of (1.52) is identical to the $(2n)$ th convergent of (1.48). The J-fraction has many interesting properties, some of which will be exploited in Chapter 2. In particular, if $\{p_n\}$ and $\{q_n\}$ are real and p_2, p_3, p_4, \dots are all negative,

then the numerators and denominators are each sequences of orthogonal polynomials so that the zeros and poles of the convergents are all real.

The even part of (1.45) is also called a J-fraction and has the form

$$f_o(z) = \frac{p_1}{1+q_1z} + \frac{p_2z^2}{1+q_2z} + \frac{p_3z^2}{1+q_3z} + \dots + \frac{p_nz^2}{1+q_nz} + \dots \quad (1.54)$$

A corresponding fraction that always exists and is always non-terminating was first suggested by Thron (1948).

This has the form

$$f_o(z) = a_o + d_o z + \frac{z}{1+d_1z} + \frac{z}{1+d_2z} + \dots + \frac{z}{1+d_nz} + \dots \quad (1.55)$$

and is called a T-fraction. The convergents satisfy (1.46) if we take $U_1/V_1 = a_o + d_o z$.

Finally, Murphy(1971) constructed a continued fraction that corresponds simultaneously to power series of the form (1.41) and (1.42). This was further studied by McCabe and Murphy (1974) and will be referred to as an M-fraction. This has the form

$$f_o(z) = \frac{p_o}{1+q_o z} + \frac{p_1z}{1+q_1z} + \frac{p_2z}{1+q_2z} + \dots + \frac{p_nz}{1+q_nz} + \dots, \quad (1.56)$$

where the coefficients $\{p_n\}$ and $\{q_n\}$ are chosen such that

conditions (1.46) and (1.49) are both satisfied. We write

$$f_o(z) - \frac{U_n(z)}{V_n(z)} = O(z^n, z^{-n-1}) \quad (1.57)$$

In Chapter 3. we will derive a class of algorithms applicable to S-, C-, J-, T- and M-fractions and to any other corresponding fractions of similar type. Therefore, it is to our advantage to establish a general expression for a corresponding fraction that satisfies (1.44), having all the fractions described above as particular cases. In order to do this we make the following observations about corresponding fractions:

- (i) The two forms of the S-fraction and the J-fraction are equivalent so that, without loss of generality, we need only consider fractions that correspond to series of the form (1.41).
- (ii) All the partial numerators are monomials.
- (iii) The T-fraction has "redundant" terms, i.e. terms that do not directly match up with terms of the series (1.41).
- (iv) If we only consider correspondence with the series (1.41), then the M-fraction also has "redundant" terms.

Observation (ii) requires further explanation as it is a major limitation on the form that a corresponding fraction

can take. We consider the formal expansion

$$e^z = \frac{1+z}{1} - \frac{\frac{1}{2}z^2(1-\frac{2}{3}z)}{1} - \frac{\frac{1}{4}z^2(1+\frac{2}{5}z)}{1} - \frac{\frac{17}{120}z^2(1-\frac{46}{135}z)}{1} - \dots \quad (1.58)$$

which is valid at least near $z = 0$. Now, e^z is a transcendental function and has no zeros in the finite z -plane, whereas the continued fraction (1.58) is zero at $z = -1$ and terminates at the zeros of the partial numerators. Therefore, at $z = +\frac{3}{2}, -\frac{5}{2}, +\frac{1365}{446}, \dots$ the fraction represents a rational function and does not converge to e^z . As e^z has no singularities in the finite z -plane the expansion (1.58) is unsatisfactory and, in general, any formal corresponding fraction whose partial numerators are not monomials will be unsatisfactory for the same reason.

Bearing in mind (i) - (iv), above, we shall now examine the properties of the continued fraction

$$f_0(z) = \frac{p_1}{q_1(z)} + \frac{p_2 z^{v(1)}}{q_2(z)} + \frac{p_3 z^{v(2)}}{q_3(z)} + \dots + \frac{p_n z^{v(n-1)}}{q_n(z)} + \dots \quad (1.59)$$

where $\{v(n)\}$ is a sequence of positive integers and $q_n(z)$ is a polynomial of degree $\mu(n)$. [In all the fractions listed above $\mu(n) = 0$ or 1 .] Without loss of generality, we normalise (1.59) by setting $q_n(0) = 1$ and we choose $p_n \neq 0$ for all n . Now, there are $\mu(n) + 1$ coefficients in the n th partial quotient which must be matched up to $v(n)$ terms of the power series (1.41), so that the number $\lambda(n)$ of "redundant" terms in the n th partial quotient is given by

$$\lambda(n) = \mu(n) - v(n) + 1 \quad . \quad (1.60)$$

If $P_n(z)/Q_n(z)$ is the n th convergent of (1.59) then we must prove that

$$f_0(z) - \frac{P_n(z)}{Q_n(z)} = O(z^{\sigma(n)}) \quad (1.61)$$

where

$$\sigma(n) = \sum_{i=1}^n v(i) \quad (1.62)$$

Now (1.61) may be written

$$Q_n(z)f_0(z) - P_n(z) = z^{\sigma(n)}S_n(z) \quad (1.63)$$

where $S_n(z)$ has a power series representation of the form

$$S_n(z) = \alpha_0^{(n)} + \alpha_1^{(n)}z + \alpha_2^{(n)}z^2 + \dots \quad (1.64)$$

The identity (1.63) may be proved by induction. We first assume that (1.63) holds for both $n-1$ and n , and using (1.8) we have

$$Q_{n+1}f_0 - P_{n+1} = z^{v(n)}p_{n+1}(Q_{n-1}f_0 - P_{n-1}) + q_{n+1}(Q_n f_0 - P_n) \quad (1.65)$$

By our assumption we have

$$Q_{n+1}f_0 - P_{n+1} = z^{v(n)}p_{n+1}z^{\sigma(n-1)}S_{n-1} + q_{n+1}z^{\sigma(n)}S_n \quad (1.66)$$

Using (1.62) we get

$$Q_{n+1}f_0 - P_{n+1} = z^{\sigma(n)}(p_{n+1}S_{n-1} + q_{n+1}S_n) \quad (1.66)$$

Clearly, we can choose p_{n+1} and the first $v(n+1)-1$ coefficients of $q_{n+1}(z)$ so that the first $v(n+1)$ terms of $(p_{n+1}S_{n-1} + q_{n+1}S_n)$ vanish. We can then write (1.66) in the form

$$Q_{n+1}f_0 - P_{n+1} = z^{\sigma(n+1)}S_{n+1} \quad (1.67)$$

so (1.63) holds for $n+1$ provided that it holds for $n-1$ and n . If we choose $\sigma(0) = 0$ then the result holds trivially for $n = 0$ so that to complete the proof we need only verify (1.63) for $n = 1$. In this case we have

$$Q_1 f_0 - P_1 = q_1 f_0 - p_1 . \quad (1.68)$$

Once again we can choose the coefficients so that the first $v(1)$ terms vanish. Thus we have proved that the successive convergents of the continued fraction (1.59) correspond to $\sigma(1), \sigma(2), \sigma(3), \dots$ terms of the power series (1.41).

Clearly, the S- and J-fractions are particular cases of (1.59) and the C-fraction is the case when all the coefficients of $q_n(z)$ are zero. In Chapter 3. we will show that the M-fraction can be treated as a special case. Also, the T-fraction can be adjusted to look like (1.59) but, because of its essentially different structure, it will be treated separately.

In Chapter 3. we will derive algorithms for converting power series to their corresponding fractions. By this means we could, for example, obtain a continued fraction solution to a differential equation by first solving the equation in series and then applying the appropriate algorithm. Corresponding fractions usually converge more quickly than power series and often provide an analytic continuation outside the domain of convergence of the series. Consequently, continued fraction solutions of differential equations are often useful when obtained in this way. However, it is worth noting that, for a certain class of differential equations,

continued fraction solutions may be obtained directly by a method due to Lagrange. We consider the general Riccati equation

$$\alpha_0 w_0' = \beta_0 w_0^2 + \gamma_0 w_0 + \delta_0 \quad (1.69)$$

in which $w_0(z)$ is the dependent variable and $\alpha_0, \beta_0, \gamma_0, \delta_0$ are polynomials in z . It may be shown that, for suitable elements $\{u_n\}$ and $\{v_n\}$, the substitutions

$$w_n = \frac{u_{n+1}}{v_{n+1} + w_{n+1}} \quad (1.70)$$

lead to a sequence of Riccati equations

$$\alpha_n w_n' = \beta_n w_n^2 + \gamma_n w_n + \delta_n \quad (1.71)$$

for $n=0,1,2,3, \dots$. Recursions may be set up between the coefficients of the n th and $(n-1)$ th equations (1.71) and a continued fraction

$$w_0 = \frac{u_1}{v_1} + \frac{u_2}{v_2} + \dots + \frac{u_n}{v_n} + \dots \quad (1.72)$$

can be found, often with the coefficients known in closed form. Khovanskii (1963) has expanded many elementary functions by this method and Wynn (1964) hints, with some justification, that a function has a simple continued fraction expansion only if it satisfies a Riccati equation. Although Wynn does not define his meaning of "simple", we can treat this as a useful qualitative remark. However, Lagrange's method is still applicable to the more general

differential equation

$$\begin{aligned} & (\alpha_o^{(0)} + \alpha_o^{(1)} w_o + \alpha_o^{(2)} w_o^2 + \dots + \alpha_o^{(n)} w_o^n) w_o' \\ & = \beta_o^{(0)} + \beta_o^{(1)} w_o + \beta_o^{(2)} w_o^2 + \dots + \beta_o^{(n+2)} w_o^{n+2}, \quad (1.73) \end{aligned}$$

where $\alpha_o^{(r)}, \beta_o^{(r)}$ are polynomials in z , except that the recursions are more complicated than in the case of (1.69).

In the next section we discuss continued fractions that are also functions of a single variable, but which are defined in an entirely different way.

1.3 Interpolatory Fractions.

We now consider continued fractions as a means of pointwise interpolation of a function $F(x)$, given at the $(n+1)$ abscissae $x_0, x_1, x_2, \dots, x_n$. Such a fraction is finite and has the form

$$f(x) = c_0 + \frac{x-x_0}{c_1} + \frac{x-x_1}{c_2} + \dots + \frac{x-x_{n-1}}{c_n}, \quad (1.74)$$

where the coefficients $\{c_r\}$ are chosen such that

$$f(x_r) = F(x_r) \quad . \quad (1.75)$$

We define a sequence of functions $\{v_r(x)\}$ by

$$\left. \begin{aligned} v_0(x) &= f(x) \quad , \\ v_r(x) &= v_r(x_r) + \frac{x-x_r}{v_{r+1}(x)} \quad , \end{aligned} \right\} \quad (1.76)$$

so that

$$c_r = v_r(x_r) \quad (1.77)$$

for $r = 0, 1, 2, \dots, n$. From (1.76) we obtain the inverse difference scheme

$$v_{r+1}(x) = \frac{x - x_r}{v_r(x) - v_r(x_r)} \quad (1.78)$$

from which, using (1.75) and (1.77), we may compute the coefficients $\{c_r\}$ by forming the table below.

$$\left. \begin{array}{llll} x_0 & F(x_0) = v_0(x_0) = c_0 & & \\ x_1 & F(x_1) = v_0(x_1) & v_1(x_1) = c_1 & \\ x_2 & F(x_2) = v_0(x_2) & v_1(x_2) & v_2(x_2) = c_2 \\ & & \vdots & \\ & & \vdots & \\ x_n & F(x_n) = v_0(x_n) & v_1(x_n) & v_2(x_n) \dots v_n(x_n) = c_n \end{array} \right\} \quad (1.79)$$

Although the formula (1.74) is not a "best" approximation in any mathematical sense it often provides a much more accurate means of interpolation than the $(n+1)$ -point Lagrange formula. Bearing in mind that we would normally interpolate to values of a transcendental function, we offer two possible explanations of the superiority of rational over polynomial interpolation. Firstly, all the derivatives of a rational function exist, are piecewise continuous and are not identically zero. Therefore, between their poles, rational functions are "smooth" and appear to more nearly imitate the behaviour of transcendental functions than do polynomials, whose derivatives eventually vanish. Secondly, polynomials have no finite singularities and cannot be used to represent such phenomena. In practice, rational interpolation can be used effectively near a singularity when polynomial interpolation is inapplicable.

Although continued fraction interpolation has been shown to be useful empirically, much research has still to be done to establish conditions under which such interpolation is valid. Mayers (1965) gives an account of various computational difficulties that may arise and which complicate the problem. In Part II we shall generalise interpolatory fractions to two or more variables and, as we expect similar difficulties in the more general case, we now give some examples of the breakdown of the single variable method.

A set of points $[x_0, F(x_0)], [x_1, F(x_1)], \dots, [x_n, F(x_n)]$ is said to be unattainable by the continued fraction (1.74) if $f(x_s) \neq F(x_s)$ for at least one $s \in \{0, 1, 2, \dots, n\}$ when the coefficients $\{c_r\}$ have been calculated using the

inverse differences (1.78). As an example we consider a function $F(x)$ given at 3 points

$$\left. \begin{aligned} F(x_0) &= a, \\ F(x_1) &= F(x_2) = b. \end{aligned} \right\} \quad (1.80)$$

Using inverse differences we obtain the interpolatory fraction

$$f(x) = a + \frac{x - x_0}{\left(\frac{x_1 - x_0}{b - a}\right)} + \frac{x - x_1}{b - a}. \quad (1.81)$$

Evaluating this as a rational function and cancelling we get

$$f(x) = b \quad (1.82)$$

which clearly does not satisfy (1.80).

Another difficulty is that of unwanted poles in the domain of interpolation. This can arise in various ways, most notably if x is real and the function values have a large number of changes of sign. If the continued fraction (1.74) is written as a rational function $A_n(x)/B_n(x)$ then $A_n(x)$ has at most k changes of sign, where $k = \frac{1}{2}n$ for n even and $k = \frac{1}{2}(n+1)$ for n odd. Consequently, if the function values $\{F(x_r)\}$ have more than k changes of sign then the continued fraction can only account for this by changing sign at zeros of $B_n(x)$ inside the domain of interpolation. However, unwanted poles may also occur when the function has k or less changes of sign. Inaccurate or insufficient data points is usually the cause and most well-behaved functions can be interpolated if enough accurate values are known.

The example (1.80) of unattainable points may be dealt with by increasing the number of data points. A similar example,

however, indicates a possible failure of inverse differences that is easily overcome. We consider a function $F(x)$ given at n points such that

$$F(x_0) = F(x_1) \quad . \quad (1.83)$$

We see that the first inverse difference

$$v_1(x_1) = \frac{x_1 - x_0}{F(x_1) - F(x_0)} = c_1 \quad (1.84)$$

does not exist. However, if we rearrange the points to start with $[x_k, F(x_k)]$ such that

$$F(x_k) \neq F(x_r) \quad (1.85)$$

for all $r \neq k$ then the first column of inverse differences will all exist, although the scheme may again fail in a subsequent column.

Clearly, the inverse difference is not a symmetric function of its arguments. A symmetric scheme for computing the coefficients $\{c_r\}$ of the interpolatory fraction (1.74) may be obtained by using Thiele's reciprocal differences [see Mayers (1965)] and is unaffected by the order of the points in the difference table.

In Chapter 6. we will show how inverse differences may be generalised to two or more variables in order to form continued fractions that interpolate on a mesh of points.

CHAPTER 2.

THE LAPLACE TRANSFORM METHOD.

In this chapter we investigate some applications of the results of Section 1.1 which were derived from sets of recurrence relations. In each case Laplace transforms are expressed as J-fractions whose convergents are inverted to form exponential approximations. First we examine a problem arising in Markov processes in which three-term recurrence relations occur naturally, and then we adapt the technique to deal with hypergeometric functions which also satisfy three-term relations.

2.1 Application to General Linear Birth-Death Processes.

A birth-death process is a Markov process in which a population, initially of size m , changes to size r after time t by births and deaths. We assume that in an interval $(t, t+\delta t)$ each individual in the population has a probability $\lambda_r \delta t + O\{(\delta t)^2\}$ of giving birth to a new individual and a probability $\mu_r \delta t + O\{(\delta t)^2\}$ of dying. The parameters λ_r and μ_r are respectively called the birth-rate and death-rate when the population has size r , and we denote by $p_r(t)$ the probability that the population has size r at time t . By considering $p_r(t+\delta t)$ in terms of $p_{r-1}(t)$, $p_r(t)$ and $p_{r+1}(t)$ the following set of differential-difference equations may be obtained:

$$\left. \begin{aligned} p_0'(t) &= -\lambda_0 p_0(t) + \mu_1 p_1(t) \\ p_r'(t) &= \lambda_{r-1} p_{r-1}(t) - (\lambda_r + \mu_r) p_r(t) + \mu_{r+1} p_{r+1}(t) \end{aligned} \right\} \quad (2.1)$$

for $r = 1, 2, 3, \dots$ where $0 \leq p_r(t) \leq 1$ and $\sum_{r=0}^{\infty} p_r(t) = 1$,

subject to the initial conditions

$$p_r(0) = \delta_{r,m} \quad (2.2)$$

for some $m \in \{0,1,2, \dots\}$. We note that $\lambda_r > 0$ for $r = 0,1,2, \dots$ and $\mu_0 = 0, \mu_r > 0$ for $r = 1,2,3, \dots$

and we define

$$L_r = \prod_{i=0}^r \lambda_i, \quad M_r = \prod_{i=1}^r \mu_i, \quad (2.3)$$

and $L_{-1} = M_0 = 1$. For details of the derivation of equations (2.1) and a discussion of birth-death processes see Saaty (1961) or Cox and Miller (1965).

The set of equations (2.1) has been solved analytically, for a few particular choices of $\{\lambda_r\}$ and $\{\mu_r\}$, by a generating function method. [See Cox and Miller (1965).] However, we shall solve the equations numerically using a method that is well-known in matrix form in the case $r = m = 0$. The continued fraction approach enables us to find the solutions for other values of r and m , and for any sets of parameters $\{\lambda_r\}$ and $\{\mu_r\}$.

We denote the Laplace transform of $p_r(t)$ by $P_r(s)$ where

$$P_r(s) = \int_0^{\infty} e^{-st} p_r(t) dt \quad (2.4)$$

Laplace transforming (2.1) and rearranging we have

$$\left. \begin{aligned} P_1 &= -\frac{\delta_{0,m}}{\mu_1} - \left(-\frac{\lambda_0 + s}{\mu_1} \right) P_0, \\ P_{r+1} &= -\frac{\lambda_{r-1}}{\mu_{r+1}} P_{r-1} - \left(-\frac{\lambda_r + \mu_r + s}{\mu_{r+1}} \right) P_r - \frac{\delta_{r,m}}{\mu_{r+1}}. \end{aligned} \right\} \quad (2.5)$$

The set (2.5) is now of the form (1.29). However, to convert the resultant continued fraction to a convenient form we apply the transformations (1.39) and (1.40) using $\gamma_r = (-1)^r M_r$.

The set (2.5) then becomes

$$\left. \begin{aligned} f_1^{(m)} &= \delta_{0,m} - (\lambda_0 + s) f_0^{(m)} \\ f_{r+1}^{(m)} &= -\lambda_{r-1} \mu_r f_{r-1}^{(m)} - (\lambda_r + \mu_r + s) f_r^{(m)} + (-1)^m M_m \delta_{r,m} \end{aligned} \right\} (2.6)$$

where $P_0 = f_0^{(m)}$ and

$$P_r = \frac{(-1)^r}{M_r} f_r^{(m)} \quad (2.7)$$

for $r = 1, 2, 3, \dots$. This leads to the continued fraction

$$f_0 = \frac{1}{\lambda_0 + s} - \frac{\lambda_0 \mu_1}{\lambda_1 + \mu_1 + s} - \frac{\lambda_1 \mu_2}{\lambda_2 + \mu_2 + s} - \dots - \frac{\lambda_{r-1} \mu_r}{\lambda_r + \mu_r + s} - \dots \quad (2.8)$$

If we now let $c_r = -1/\mu_r$ and use the transformation (1.19)

then, from (1.20) and (2.7), the sequence $\{P_r\}$ becomes the

corresponding sequence of a continued fraction equal to f_0 .

Since $\sum_{r=0}^{\infty} p_r(t) = 1$, we get from (2.4) that $\sum_{r=0}^{\infty} P_r(s) = 1/s$

which implies that

$$\lim_{r \rightarrow \infty} P_r(s) = 0 \quad (2.9)$$

except when $s=0$. Hence the region F of theorem 1.1 is the

s -plane, excluding the point $s=0$, and we may apply the theorem

if we can find the positions of the zeros of the denominators

of the continued fraction (2.8). From (2.10) we have

$$B_n = \begin{bmatrix} \lambda_0 + s & 1 & & & & \\ \lambda_0 \mu_1 & \lambda_1 + \mu_1 + s & 1 & & & \\ & \lambda_1 \mu_2 & \lambda_2 + \mu_2 + s & 1 & & \\ & & \dots & \dots & \dots & \\ & & & \dots & \dots & 1 \\ & & & & \lambda_{n-2} \mu_{n-1} & \lambda_{n-1} + \mu_{n-1} + s \end{bmatrix} \quad (2.10)$$

which is clearly zero when $-s$ is an eigenvalue of the matrix

$$C_n = \begin{bmatrix} \lambda_0 & 1 & & & & \\ \lambda_0 \mu_1 & \lambda_1 + \mu_1 & 1 & & & \\ & \lambda_1 \mu_2 & \lambda_2 + \mu_2 & 1 & & \\ & & \dots & \dots & \dots & \\ & & & \dots & \dots & 1 \\ & & & & \lambda_{n-2} \mu_{n-1} & \lambda_{n-1} + \mu_{n-1} \end{bmatrix} \quad (2.11)$$

This matrix is quasi-symmetric and may be transformed into a real symmetric matrix by a similarity transformation

$$E_n = D_n^{-1} C_n D_n \quad (2.12)$$

where the matrix $D_n = \text{diag}\{1, \sqrt{L_0 M_1}, \sqrt{L_1 M_2}, \dots, \sqrt{L_{n-2} M_{n-1}}\}$.

The matrix so formed is

$$E_n = \begin{bmatrix} \lambda_0 & \sqrt{\lambda_0 \mu_1} & & & & \\ \sqrt{\lambda_0 \mu_1} & \lambda_1 + \mu_1 & \sqrt{\lambda_1 \mu_2} & & & \\ & \sqrt{\lambda_1 \mu_2} & \lambda_2 + \mu_2 & \sqrt{\lambda_2 \mu_3} & & \\ & & \dots & \dots & \dots & \\ & & & \dots & \dots & \sqrt{\lambda_{n-2} \mu_{n-1}} \\ & & & & \sqrt{\lambda_{n-2} \mu_{n-1}} & \lambda_{n-1} + \mu_{n-1} \end{bmatrix} \quad (2.13)$$

The matrix E_n is a real symmetric positive definite tridiagonal

matrix with non-zero subdiagonal elements. Because of these properties the eigenvalues are real, positive and distinct. [See Wilkinson (1965).] Hence $B_n(s)$ has only simple zeros which all lie on the negative real axis in the s -plane and, from theorem 1.1, we can state that the continued fraction (2.8) converges in the s -plane cut from 0 to ∞ along the negative real axis. The theory of positive definite continued fractions, as given by Wall (1948), is sufficient to prove that the zeros of $B_n(s)$ are real and distinct, but we have used matrix theory in order to show that the zeros are also negative. We are now justified in using the results (1.35) and (1.36) to give the following expressions for $P_r(s)$:

$$P_r = \frac{(-1)^m}{L_{m-1} M_r} B_r f_m \quad (2.14)$$

for $r \leq m$, and

$$P_r = \frac{(-1)^r}{L_{m-1} M_r} B_m f_r \quad (2.15)$$

for $r \geq m$. Writing $P_{r,n}$ for the n th convergent of $P_r(s)$ and using (1.25) we have

$$P_{r,n} = \frac{(-1)^m}{L_{m-1} M_r} B_r \frac{A_n^{(m)}}{B_{m+n}} \quad (2.16)$$

for $r \leq m$, and

$$P_{r,n} = \frac{(-1)^r}{L_{m-1} M_r} B_m \frac{A_n^{(r)}}{B_{r+n}} \quad (2.17)$$

for $r \geq m$. We are also justified in inverting the \mathcal{L} -transform

expressions (2.16) and (2.17) since all the singularities of $P_{r,n}$ lie to the left of the imaginary axis in the s -plane. In general we consider a convergent $K(s)$ such that

$$K(s) = \frac{N(s)}{B_n(s)} \quad (2.18)$$

where $B_n(s)$ is a denominator polynomial of order n in s and $N(s)$ is the numerator polynomial which is of lower order. If we choose $-z_1, -z_2, \dots, -z_n$ to be the real, negative and distinct roots of $B_n(s)$ then we can write

$$B_n(s) = \prod_{i=1}^n (s+z_i) \quad (2.19)$$

Since the roots are distinct we may write $K(s)$ in the partial fraction form

$$K(s) = \sum_{i=1}^n \frac{\omega_i}{s+z_i} \quad (2.20)$$

where $\omega_1, \omega_2, \dots, \omega_n$ are constants given by

$$\omega_i = \frac{N(-z_i)}{B'_n(-z_i)} \quad (2.21)$$

and where $B'_n(-z_i)$ is computed from

$$B'_n(-z_i) = \prod_{\substack{j=1 \\ i \neq j}}^n (z_j - z_i) \quad (2.22)$$

Inverting the Laplace transform, we get

$$\mathcal{L}^{-1}K(s) = \sum_{i=1}^n \omega_i e^{-z_i t} \quad (2.23)$$

which is the form in which the probabilities, $p_r(t)$, are computed.

To greatly reduce the required computation, since we only require the values of $A_n^{(r)}$ at the roots of B_{r+n} , we appeal to the generalised determinant formula (1.28). From this we get that, at a root of B_{r+n} ,

$$A_n^{(r)} = (-1)^r A_{r+n} B_r. \quad (2.24)$$

Hence we need only compute the roots of the numerators and denominators of the continued fraction (2.8) in order to compute the probabilities, $p_r(t)$, for any value of m . The roots of the numerators are also computed as eigenvalues using (1.9).

From (1.37) and (1.38) we have the truncation results

$$T_n(P_r) = \frac{(-1)^{m+n}}{L_{m-1} M_r} B_r B_m \frac{f_{m+n}}{B_{m+n}} \quad (2.25)$$

for $r \leq m$, and

$$T_n(P_r) = \frac{(-1)^{r+n}}{L_{m-1} M_r} B_r B_m \frac{f_{r+n}}{B_{r+n}} \quad (2.26)$$

for $r \geq m$.

We will now derive estimates of the truncation errors in the probabilities, $p_r(t)$, computed from results (2.16) and (2.17). We observe from (2.8) that for $|s|$ large,

$$B_n(s) = (\lambda_0 + s)(\lambda_1 + \mu_1 + s)(\lambda_2 + \mu_2 + s) \dots (\lambda_{n-1} + \mu_{n-1} + s) + O(s^{n-2}) \quad (2.27)$$

for $n = 2, 3, 4, \dots$ and also, from (1.25),

$$f_n = \frac{(-1)^n L_{n-1} M_n}{(\lambda_0 + s)(\lambda_1 + \mu_1 + s) \dots (\lambda_n + \mu_n + s) + O(s^{n-1})} \quad (2.28)$$

for $|s|$ large and $n = 1, 2, 3, \dots$. We set $\sigma_0 = 0$ and

define

$$\sigma_n = \lambda_0 + \sum_{r=1}^{n-1} (\lambda_r + \mu_r) \quad (2.29)$$

for $n \geq 1$ so that, for $|s|$ large, (2.25) may be written

$$P_r - P_{r,n} = \frac{L_{m+n-1} M_{m+n}}{L_{m-1} M_r} \frac{1}{s^{2n+m-r+1}} \left\{ 1 - \frac{\sigma_{m+n}^{+\sigma} \sigma_{m+n+1}^{-\sigma} \sigma_m^{-\sigma} \sigma_r^{-\sigma}}{s} + O\left(\frac{1}{s^2}\right) \right\} \quad (2.30)$$

for $r \leq m$. Inverting, we obtain, for t small,

$$p_r(t) - \mathcal{L}^{-1}\{P_{r,n}\} = \frac{L_{m+n-1} M_{m+n}}{L_{m-1} M_r} \frac{t^{2n+m-r}}{(2n+m-r)!} \cdot \left\{ 1 - \frac{\sigma_{m+n}^{+\sigma} \sigma_{m+n+1}^{-\sigma} \sigma_m^{-\sigma} \sigma_r^{-\sigma}}{2n+m-r+1} t + O(t^2) \right\} \quad (2.31)$$

for $r \leq m$. In (2.31) the dominant term provides an upper bound which is only a useful estimate if n is large. However, we require a useful error estimate for moderate n , not necessarily an error bound. Accordingly, we choose a function which formally agrees with the first two terms of (2.31), is unbounded and is easy to compute. The chosen estimate is

$$p_r(t) - \mathcal{L}^{-1}\{P_{r,n}\} = \frac{L_{m+n-1} M_{m+n}}{L_{m-1} M_r} \frac{t^{2n+m-r}}{(2n+m-r)!} \cdot \left\{ \frac{1}{(1+\rho_{r,m+n} t)^{2n+m-r-1}} + O(t^2) \right\} \quad (2.32)$$

for $r \leq m$ where

$$\rho_{r,m+n} = \frac{\sigma_{m+n}^{+\sigma} \sigma_{m+n+1}^{-\sigma} \sigma_m^{-\sigma} \sigma_r^{-\sigma}}{(2n+m-r+1)(2n+m-r-1)} \quad (2.33)$$

From (2.26) we also have

$$p_r(t) - \mathcal{L}^{-1}\{P_{r,n}\} = \frac{L_{r+n-1} M_{r+n}}{L_{m-1} M_r} \frac{t^{2n+r-m}}{(2n+r-m)!} \cdot \left\{ \frac{1}{(1+\rho_{m,r+n}t)^{2n+r-m-1}} + o(t^2) \right\} \quad (2.34)$$

for $r \geq m$.

Given a value of n and a sufficiently small error ϵ the results (2.32) and (2.34) may be used to estimate a range of t for which this error is not exceeded. A larger value of ϵ could give a very pessimistic estimate for the range of t .

We now consider four examples of birth-death models. The interpretation of the first three will be found in Cox and Miller (1965), who solve the equations (2.1) for models (i) and (ii) analytically by a generating function method.

- (i) An immigration-death process with $\lambda_r = 0.2$ and $\mu_r = 0.4r$ for $r = 0, 1, 2, 3, \dots$. For this model the probabilities tend to steady state values. The results are evaluated in the two cases when the initial population size m is 0 and 1.
- (ii) An immigration-emigration process (Erlang's model) with $\lambda_r = 0.3$ for $r = 0, 1, 2, 3, \dots$, $\mu_0 = 0$ and $\mu_r = 0.1$ for $r = 1, 2, 3, \dots$. In this case there are no steady state values. We choose $m = 0$.

(iii) A three-server queueing model with $\lambda_r = 0.6$

for $r = 0, 1, 2, 3, \dots$, $\mu_0 = 0$, $\mu_1 = \mu_2 = 0.2$,

$\mu_3 = \mu_4 = 0.4$ and $\mu_r = 0.6$ for $r = 5, 6, 7, \dots$.

This represents a queueing system in which the number of servers is dependent on queue size.

The results are evaluated when $m = 0$ and

when $m = 2$.

(iv) An arbitrary process with $\lambda_r = 0.3$ and $\mu_r = 0.1\sqrt{r}$

for $r = 0, 1, 2, 3, \dots$. We choose $m = 0$.

For prescribed errors and selected values of n estimates have been obtained for the range of t from formulae (2.32) and (2.34). These appear in Table 2.1 overleaf, in which the notation $(-k)$ is used to denote 10^{-k} .

TABLE 2.1

Model	n	r	m	Error	Estimated max(t)	Error	Estimated max(t)
(i)	3	0	0	(-4)	2.11	(-3)	3.47
	3	1	0	(-4)	3.04	(-3)	5.00
	3	0	1	(-4)	2.66	(-3)	4.27
	4	0	0	(-5)	2.78	(-4)	4.12
	4	0	1	(-5)	3.30	(-4)	4.84
	5	0	0	(-5)	4.75	(-4)	6.86
	5	0	1	(-5)	5.43	(-4)	7.86
	5	1	1	(-5)	4.26	(-4)	6.34
	10	0	0	(-8)	12.6	(-5)	34.9
	10	0	1	(-8)	13.9	(-5)	42.2
(ii)	3	0	0	(-5)	3.00	(-4)	4.80
	3	1	0	(-5)	4.30	(-4)	6.55
	3	2	0	(-5)	5.72	(-4)	8.37
	4	0	0	(-5)	6.77	(-4)	10.0
	4	1	0	(-5)	8.54	(-4)	12.3
	5	0	0	(-5)	12.0	(-4)	17.0
	5	1	0	(-5)	14.1	(-4)	19.6
	5	2	0	(-5)	16.2	(-4)	22.0
	10	0	0	(-10)	21.4	(-8)	30.2
	10	5	0	(-12)	24.0	(-10)	31.2
(iii)	3	0	0	(-4)	2.09	(-3)	3.49
	3	2	0	(-4)	2.91	(-3)	4.33
	3	0	2	(-4)	4.25	(-3)	6.65
	4	0	0	(-4)	4.07	(-3)	6.23
	4	0	2	(-4)	6.55	(-3)	9.70
	5	0	0	(-4)	6.20	(-3)	8.98
	5	2	0	(-4)	6.81	(-3)	9.30
	5	2	2	(-4)	4.90	(-3)	7.06
	10	0	0	(-8)	9.50	(-5)	16.7
	10	2	2	(-8)	8.43	(-5)	14.7

TABLE 2.1 (continued)

Model	n	r	m	Error	Estimated max(t)	Error	Estimated max(t)
(iv)	3	0	0	(-5)	2.54	(-4)	4.04
	3	1	0	(-5)	3.33	(-4)	5.01
	4	0	0	(-5)	5.38	(-4)	7.88
	4	1	0	(-5)	6.27	(-4)	8.86
	5	0	0	(-5)	8.99	(-4)	12.5
	5	1	0	(-5)	9.87	(-4)	13.4
	5	5	0	(-8)	8.23	(-6)	12.4
	10	0	0	(-8)	19.3	(-6)	27.7
	10	1	0	(-8)	19.9	(-6)	28.1
	10	5	0	(-8)	24.8	(-5)	33.6

By recomputation with larger n , the range estimates in Table 2.1 were all found to be reasonable, though not always lower bounds on the actual range for the chosen accuracy.

As it is impractical to list a complete set of results for any model, a selection of computed values is given in Tables 2.2 - 2.7 for various choices of n , r and m .

Model (i), $m = 0$.

t	n	$p_0(t)$	$p_1(t)$	$p_2(t)$	$p_5(t)$
0	3	1.0 -0.2(-10)	-0.2(-11)	-0.3(-12)	-0.5(-14)
1	3	0.848027	0.13978896	0.11521411(-1)	0.8600868 (-6)
	4	0.84802939	0.13978915	0.11521420(-1)	0.86008701(-6)
	5	0.84802940	0.13978915	0.11521420(-1)	0.86008701(-6)
2	3	0.75924	0.209057	0.287811 (-1)	0.1001268 (-4)
	4	0.7593162	0.20906688	0.28781779(-1)	0.10012746(-4)
	5	0.75931730	0.20906702	0.28781789(-1)	0.10012747(-4)
	6	0.75931732	0.20906703	0.28781789(-1)	0.10012747(-4)
5	3	0.6456	0.2800	0.60596 (-1)	0.81672 (-4)
	5	0.648985	0.2805796	0.6065200 (-1)	0.81686034(-4)
	7	0.64899363	0.28058095	0.60652112(-1)	0.81686052(-4)
	8	0.64899364	0.28058095	0.60652112(-1)	0.81686052(-4)
10	3	0.587	0.2969	0.7343 (-1)	0.14525 (-3)
	6	0.612094	0.3004480	0.7373659 (-1)	0.14533093(-3)
	8	0.61211062	0.30044973	0.73736701(-1)	0.14533094(-3)
	9	0.61211067	0.30044974	0.73736702(-1)	0.14533094(-3)
20	5	0.6050	0.30310	0.757732 (-1)	0.15771204(-3)
	8	0.6066316	0.30321441	0.75778182(-1)	0.15771239(-3)
	9	0.60663236	0.30321445	0.75778183(-1)	0.15771239(-3)
	10	0.60663240	0.30321445	0.75778183(-1)	0.15771239(-3)

TABLE 2.3

Model (i), $m = 1$.

t	n	$p_0(t)$	$p_1(t)$	$p_2(t)$	$p_3(t)$
0	3	-0.3(-11)	1.0 -0.2(-10)	-0.1(-11)	-0.2(-12)
1	3	0.2795779	0.6145310	0.975015 (-1)	0.7931735 (-2)
	4	0.27957829	0.61453675	0.97501846(-1)	0.79317470(-2)
	5	0.27957829	0.61453678	0.97501848(-1)	0.79317470(-2)
2	3	0.41811	0.45617	0.109778	0.143864 (-1)
	4	0.4181338	0.4563078	0.10978897	0.14387105(-1)
	5	0.41813405	0.45631038	0.10978917	0.14387116(-1)
	6	0.41813405	0.45631042	0.10978917	0.14387116(-1)
5	3	0.5600	0.328	0.9017 (-1)	0.15747 (-1)
	6	0.56116181	0.3304398	0.90416215(-1)	0.15766078(-1)
	7	0.56116190	0.33044018	0.90416243(-1)	0.15766080(-1)
	8	0.56116190	0.33044019	0.90416244(-1)	0.15766080(-1)
10	5	0.600845	0.306090	0.778850 (-1)	0.1319372 (-1)
	8	0.60089946	0.30615799	0.77889095(-1)	0.13193929(-1)
	9	0.60089947	0.30615800	0.77889096(-1)	0.13193929(-1)
20	6	0.606410	0.303303	0.7585405 (-1)	0.12646632(-1)
	8	0.60642882	0.30331618	0.75854478(-1)	0.12646646(-1)
	9	0.60642890	0.30331623	0.75854480(-1)	0.12646646(-1)

TABLE 2.4

Model (ii), $m = 0$.

t	n	$p_0(t)$	$p_1(t)$	$p_2(t)$	$p_5(t)$
0	3	1.0 -0.7(-11)	-0.9(-11)	-0.1(-10)	-0.2(-10)
1	3	0.75162213	0.21359074	0.31428619(-1)	0.13862618(-4)
	4	0.75162216	0.21359074	0.31428619(-1)	0.13862618(-4)
2	3	0.5802518	0.31025888	0.89143932(-1)	0.30633442(-3)
	4	0.58025298	0.31025898	0.89143939(-1)	0.30633438(-3)
	5	0.58025298	0.31025898	0.89143939(-1)	0.30633440(-3)
5	3	0.30304	0.330882	0.2164312	0.10368464(-1)
	4	0.3031410	0.33090176	0.21643475	0.10368476(-1)
	5	0.30314223	0.33090195	0.21643478	0.10368476(-1)
	6	0.30314224	0.33090195	0.21643478	0.10368476(-1)
10	3	0.1327	0.2109	0.22840	0.66638 (-1)
	5	0.1339851	0.2113689	0.22856145	0.66641725(-1)
	6	0.13398693	0.21136930	0.22856156	0.66641726(-1)
	7	0.13398697	0.21136931	0.22856156	0.66641726(-1)
20	5	0.4007 (-1)	0.78029 (-1)	0.117795	0.1425965
	7	0.401489 (-1)	0.7806572 (-1)	0.11781223	0.14259765
	8	0.40149257(-1)	0.78065843(-1)	0.11781227	0.14259765
	9	0.40149273(-1)	0.78065848(-1)	0.11781227	0.14259765

Model (iii), $m = 0$.

t	n	$p_0(t)$	$p_1(t)$	$p_2(t)$	$p_5(t)$
0	3	1.0 -0.7(-11)	-0.5(-11)	-0.1(-10)	-0.9(-11)
1	3	0.5802518	0.3102908	0.8994949 (-1)	0.27308603(-3)
	4	0.58025407	0.31029118	0.89949567(-1)	0.27308606(-3)
	5	0.58025408	0.31029118	0.89949567(-1)	0.27308607(-3)
2	3	0.36964	0.346330	0.193443	0.3940806 (-2)
	4	0.3697074	0.3463505	0.19345128	0.39408309(-2)
	5	0.36970848	0.34635089	0.19345140	0.39408311(-2)
	6	0.36970849	0.34635089	0.19345140	0.39408311(-2)
5	3	0.1327	0.2167	0.2659	0.4989 (-1)
	5	0.135121	0.2182407	0.2672703	0.4992800 (-1)
	7	0.13513614	0.21824977	0.26727570	0.49928072(-1)
	8	0.13513617	0.21824978	0.26727571	0.49928072(-1)
10	7	0.45426 (-1)	0.97643 (-1)	0.1892308	0.12459100
	10	0.45438498(-1)	0.97653500(-1)	0.18923896	0.12459135
	11	0.45438507(-1)	0.97653505(-1)	0.18923896	0.12459135
	12	0.45438507(-1)	0.97653505(-1)	0.18923896	0.12459135
20	10	0.149398 (-1)	0.39698 (-1)	0.102491	0.1442428
	13	0.14948354(-1)	0.3970612 (-1)	0.10250008	0.14424374
	14	0.14948388(-1)	0.39706229(-1)	0.10250011	0.14424374
	15	0.14948393(-1)	0.39706233(-1)	0.10250011	0.14424374

TABLE 2.6

Model (iii), $m = 2$.

t	n	$p_0(t)$	$p_1(t)$	$p_2(t)$	$p_3(t)$
0	3	-0.5(-12)	-0.2(-11)	1.0 -0.2(-10)	-0.1(-10)
1	3	0.9994388 (-2)	0.971657 (-1)	0.530393	0.2694086
	4	0.99943963(-2)	0.97166057(-1)	0.53040470	0.26940995
	5	0.99943963(-2)	0.97166059(-1)	0.53040477	0.26940996
2	3	0.214937 (-1)	0.108857	0.36133	0.289623
	4	0.21494587(-1)	0.10887427	0.3616308	0.2896887
	5	0.21494600(-1)	0.10887458	0.36163757	0.28968992
	6	0.21494601(-1)	0.10887459	0.36163767	0.28968993
5	3	0.2955 (-1)	0.835 (-1)	0.1999	0.2227
	6	0.29697276(-1)	0.845638 (-1)	0.2078358	0.22622438
	7	0.29697301(-1)	0.84564108(-1)	0.20783960	0.22622547
	8	0.29697301(-1)	0.84564119(-1)	0.20783976	0.22622551
10	6	0.21018, (-1)	0.5478 (-1)	0.13543	0.16756
	9	0.21026545(-1)	0.5483809 (-1)	0.13578424	0.16773158
	10	0.21026551(-1)	0.54838142(-1)	0.13578471	0.16773175
	11	0.21026551(-1)	0.54838146(-1)	0.13578474	0.16773177
20	10	0.113879 (-1)	0.31638 (-1)	0.86161 (-1)	0.117797
	13	0.11388898(-1)	0.31643164(-1)	0.8618939 (-1)	0.11781223
	14	0.11388901(-1)	0.31643183(-1)	0.86189513(-1)	0.11781229
	15	0.11388901(-1)	0.31643186(-1)	0.86189530(-1)	0.11781230

Model (iv), $m = 0$.

t	n	$p_0(t)$	$p_1(t)$	$p_2(t)$	$p_5(t)$
0	3	1.0 -0.7(-11)	-0.1(-10)	-0.7(-11)	-0.7(-11)
1	3	0.75163272	0.21400784	0.31088306(-1)	0.13151107(-4)
	4	0.75163278	0.21400785	0.31088306(-1)	0.13151101(-4)
2	3	0.5803683	0.31255174	0.8769737 (-1)	0.27766232(-3)
	4	0.58037098	0.31255218	0.87697416(-1)	0.27766234(-3)
	5	0.58037099	0.31255218	0.87697416(-1)	0.27766234(-3)
5	3	0.30461	0.34409	0.215083	0.852036 (-2)
	4	0.304825	0.3441707	0.2151049	0.85204967(-2)
	5	0.30483024	0.34417241	0.21510533	0.85204985(-2)
	6	0.30483033	0.34417243	0.21510534	0.85204985(-2)
10	4	0.14030	0.24032	0.245715	0.516900 (-1)
	6	0.1405344	0.24045918	0.24577259	0.51691720(-1)
	7	0.14053508	0.24045949	0.24577271	0.51691722(-1)
	8	0.14053510	0.24045951	0.24577271	0.51691722(-1)
20	6	0.5227 (-1)	0.11684	0.168214	0.1268917
	9	0.5235771 (-1)	0.11690943	0.16825762	0.12689585
	10	0.52357796(-1)	0.11690949	0.16825765	0.12689585
	11	0.52357803(-1)	0.11690950	0.16825766	0.12689585

For small n , r and m the eigenvalues were computed using an algorithm based on that given by Bowdler, et. al. (1968). However, this was found to be impractical for larger values of n , r and m because some of the calculations become ill-conditioned.

We consider the set $\{z_i\}$ of eigenvalues of the matrix E_n . It was found that the first n eigenvalues of E_{n+1} could be expressed as $\{z_i + \epsilon_i\}$ where $|\epsilon_i|$ was small for the smaller eigenvalues. Some of the calculations depend critically on the values $\{\epsilon_i\}$ and it was found that for, roughly, $n + \max(r, m) > 20$ some of the values $\{\epsilon_i\}$ were negligible compared to z_i in computations using 20 significant figures. This drawback can be overcome at the expense of computing time by the following means. For the eigenvector \underline{x}_i we have

$$E_{n+1} \underline{x}_i = (z_i + \epsilon_i) \underline{x}_i \quad (2.35)$$

so that

$$(E_{n+1} - z_i I) \underline{x}_i = \epsilon_i \underline{x}_i \quad (2.36)$$

If $|\epsilon_i|$ is small then ϵ_i is the eigenvalue of smallest modulus of the matrix $(E_{n+1} - z_i I)$. Unfortunately, each of the small values $\{\epsilon_i\}$ must be computed separately. The efficiency of the method would be greatly improved if it were possible to find all the values $\{\epsilon_i\}$ simultaneously.

Finally, we have shown how to solve sets of equations of the form

$$\left. \begin{aligned} p_0'(t) &= v_0 p_0(t) + \mu_1 p_1(t) \\ p_r'(t) &= \lambda_{r-1} p_{r-1}(t) + v_r p_r(t) + \mu_{r+1} p_{r+1}(t) \end{aligned} \right\} (2.37)$$

for $r = 1, 2, 3, \dots$ in the case where

$$\left. \begin{aligned} v_0 &= -\lambda_0 \\ v_r &= -(\lambda_r + \mu_r) \end{aligned} \right\} (2.38)$$

for $r = 1, 2, 3, \dots$. It should be stated that, if v_r is real for $r = 0, 1, 2, 3, \dots$, the method will still work in the more general case when condition (2.38) is relaxed, except that the eigenvalues of E_n will be real but not necessarily all positive.

2.2 Approximations for Hypergeometric Functions.

We shall now derive approximations for the hypergeometric function ${}_2F_1(a,b;c;z)$ for suitable real values of the parameters a , b and c using a special case of the continued fraction of Gauss, given by Wall (1948). We shall then extend the method to the confluent hypergeometric functions ${}_1F_1(a;c;z)$ and ${}_2F_0(a,b;z)$, and show how approximations may be constructed for some generalised hypergeometric functions. We shall use the Laplace transform as an algebraic operation instead of a method for solution of differential equations.

However, before we consider the more general case, we examine a degenerate form of the hypergeometric function. The hypergeometric differential equation is

$$z(1-z) y'' + [c-(a+b+1)z] y' - ab y = 0 \quad (2.39)$$

and the hypergeometric function ${}_2F_1(a,b;c;z)$ is defined, subject to normalisation, as the solution of (2.39) that is regular at the origin. For a discussion of hypergeometric functions see Erdelyi, et. al. (1953). Bearing in mind that the parameters a and b are interchangeable, we consider the case $b = 1$, for which the equation (2.39) may be integrated directly to give

$$z(1-z) y' + (c-1-az) y = c-1. \quad (2.40)$$

This is a Riccati equation, i.e. it is an equation of the form (1.69), and we expect the solution ${}_2F_1(a,1;c;z)$ to have

a simple continued fraction expansion. Now, hypergeometric functions satisfy the three-term recurrence relation

$${}_2F_1(a,b;c;z) = {}_2F_1(a,b+1;c+1;z) - \frac{a(c-b)}{c(c+1)} z {}_2F_1(a+1,b+1;c+2;z) \quad (2.41)$$

from which we may obtain a continued fraction for the ratio ${}_2F_1(a,b+1;c+1;z)/{}_2F_1(a,b;c;z)$, known as the continued fraction of Gauss. Noting that ${}_2F_1(a,0;c;z) \equiv 1$, we have the particular case

$${}_2F_1(a,1;c;z) = \frac{1}{1} - \frac{h_1 z}{1} - \frac{(1-h_1)h_2 z}{1} - \frac{(1-h_2)h_3 z}{1} - \dots \quad (2.42)$$

where

$$h_{2r-1} = \frac{a+r-1}{c+2r-2}, \quad h_{2r} = \frac{r}{c+2r-1}. \quad (2.43)$$

If we let $\{f_r(z)\}$ be the corresponding sequence of the S-fraction (2.42), and if α_n is defined as in Chapter 1., then we can show that

$$\left. \begin{aligned} f_{2n-2}(z) &= \alpha_{2n-1} {}_2F_1(a+n-1,n;c+2n-2;z), \\ f_{2n-1}(z) &= \alpha_{2n} {}_2F_1(a+n,n;c+2n-1;z), \end{aligned} \right\} \quad (2.44)$$

for $n = 1, 2, 3, \dots$. So we can use the expression (1.25) to obtain two expansions for ${}_2F_1(a,n;c;z)$. These are

$${}_2F_1(a,n;c;z) = \frac{1}{P_{2n-1}} + \frac{p_{2n-1} z P_{2n-2}}{1} + \frac{p_{2n} z}{1} + \frac{p_{2n+1} z}{1} + \dots \quad (2.45)$$

and

$${}_2F_1(a,n;c;z) = \frac{1}{Q_{2n}} + \frac{q_{2n} z Q_{2n-1}}{1} + \frac{q_{2n+1} z}{1} + \frac{q_{2n+2} z}{1} + \dots \quad (2.46)$$

where $\{p_r\}$ are the coefficients and $\{P_r\}$ the denominators of the S-fraction

$${}_2F_1(a-n+1, 1; c-2n+2; z) = \frac{1}{1} + \frac{p_1 z}{1} + \frac{p_2 z^2}{1} + \dots \quad (2.47)$$

and $\{q_r\}$ are the coefficients and $\{Q_r\}$ the denominators of the S-fraction

$${}_2F_1(a-n, 1; c-2n+1; z) = \frac{1}{1} + \frac{q_1 z}{1} + \frac{q_2 z^2}{1} + \dots \quad (2.48)$$

The coefficients $\{p_r\}$ and $\{q_r\}$ are determined by comparison with (2.42). It may be shown that ${}_2F_1(a, b; c; z)$ satisfies a Riccati equation only if a or b is a positive integer. However, this equation is not particularly simple as the degree of the polynomial coefficients increases with n .

We have shown that when b is a positive integer a continued fraction expression of the form (2.45) or (2.46) may be found for ${}_2F_1(a, b; c; z)$. If b is a negative integer then the hypergeometric function reduces to a polynomial so that approximations are not usually required. We are left to deal with the case when neither a nor b is an integer and the coefficients of the corresponding S-fraction are not known in closed form.

We start from the Taylor series expansion

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{r=0}^{\infty} \frac{\Gamma(a+r)\Gamma(b+r)}{\Gamma(c+r)} \frac{z^r}{r!}, \quad (2.49)$$

convergent for $|z| < 1$, and compare this with the Taylor series for the confluent hypergeometric function ${}_1F_1(a; c; z)$.

This is

$${}_1F_1(a; c; z) = \frac{\Gamma(c)}{\Gamma(a)} \sum_{r=0}^{\infty} \frac{\Gamma(a+r)}{\Gamma(c+r)} \frac{z^r}{r!}, \quad (2.50)$$

convergent for all finite z . Here we are only concerned with (2.49) and (2.50) as formal expansions so that domains of convergence are unimportant. We define the Laplace transform of a function $f(z)$ by

$$\mathcal{L}\{f(z)\} = \int_0^{\infty} e^{-st} f(t) dt \quad (2.51)$$

and note that for $k > 0$,

$$\mathcal{L}\{z^{k-1}\} = \frac{\Gamma(k)}{s^k}. \quad (2.52)$$

Multiplying (2.50) by z^{b-1} and taking the Laplace transform we get

$$\mathcal{L}\{z^{b-1} {}_1F_1(a; c; z)\} = \frac{\Gamma(c)}{\Gamma(a)} \sum_{r=0}^{\infty} \frac{\Gamma(a+r)}{\Gamma(c+r)} \frac{1}{r!} \mathcal{L}\{z^{b+r-1}\}. \quad (2.53)$$

Using (2.52) and comparing with (2.49) we have

$$\mathcal{L}\{z^{b-1} {}_1F_1(a; c; z)\} = \frac{\Gamma(b)}{s^b} {}_2F_1(a, b; c; \frac{1}{s}), \quad (2.54)$$

and in particular

$$\mathcal{L}\{{}_1F_1(a; c; z)\} = \frac{1}{s} {}_2F_1(a, 1; c; \frac{1}{s}). \quad (2.55)$$

We may write (2.42) in the form

$${}_2F_1(a, 1; c; z) = \frac{1}{1} - \frac{\lambda_0 z}{1} - \frac{\mu_1 z}{1} - \frac{\lambda_1 z}{1} - \frac{\mu_2 z}{1} - \frac{\lambda_2 z}{1} - \dots \quad (2.56)$$

Now, taking the even part and replacing z by $1/s$ we obtain

$$\frac{1}{s} {}_2F_1(a, 1; c; \frac{1}{s}) = -\frac{1}{\lambda_0^{-s}} - \frac{\lambda_0 \mu_1}{\lambda_1 + \mu_1^{-s}} - \frac{\lambda_1 \mu_2}{\lambda_2 + \mu_2^{-s}} - \dots, \quad (2.57)$$

using (1.19). Now we have a J-fraction for $\mathcal{L}\{{}_1F_1(a; c; z)\}$ of similar form to (2.8) that we derived for the birth-death process. Thus we can obtain an approximation of the form

$${}_1F_1(a; c; z) = \sum_{i=1}^n \omega_i e^{\alpha_i z} + \epsilon_{11}^{(n)}(z) \quad (2.58)$$

where $\{\alpha_i\}$ are the roots of the n th denominator of (2.57) and $\epsilon_{11}^{(n)}(z)$ is the error committed by the n th approximation.

Naturally, we only expect this approximation to be useful when $\text{Re}(\alpha_i z) \leq 0$ for each i . Again, multiplying (2.58) by z^{b-1} and taking the Laplace transform we get

$$\mathcal{L}\{z^{b-1} {}_1F_1(a; c; z)\} = \sum_{i=1}^n \omega_i \mathcal{L}\{z^{b-1} e^{\alpha_i z}\} + \mathcal{L}\{z^{b-1} \epsilon_{11}^{(n)}(z)\}. \quad (2.59)$$

Using (2.54) we have

$$\frac{\Gamma(b)}{s^b} {}_2F_1(a, b; c; \frac{1}{s}) = \sum_{i=1}^n \omega_i \frac{\Gamma(b)}{(s - \alpha_i)^b} + \mathcal{L}\{z^{b-1} \epsilon_{11}^{(n)}(z)\}. \quad (2.60)$$

Finally, replacing s by $1/z$ we obtain

$${}_2F_1(a, b; c; z) = \sum_{i=1}^n \frac{\omega_i}{(1 - \alpha_i z)^b} + \epsilon_{21}^{(n)}(z) \quad (2.61)$$

where the new error term $\epsilon_{21}^{(n)}(z)$ is given by

$$\epsilon_{21}^{(n)}(z) = \frac{1}{\Gamma(b) z^b} \mathcal{L}\{z^{b-1} \epsilon_{11}^{(n)}(z)\}_{s=1/z}. \quad (2.62)$$

Thus, we have obtained a form of exponential approximation (2.61) for ${}_2F_1(a,b;c;z)$ and we can use (2.62) to derive an estimate of the truncation error $\epsilon_{21}^{(n)}(z)$. Some of the results of Section 2.1 can be applied in this case. In particular, we adapt result (2.31) to the error $\epsilon_{11}^{(n)}(z)$ of the approximation (2.58). We have

$$\epsilon_{11}^{(n)}(z) = L_{n-1} M_n \frac{z^{2n}}{(2n)!} \left\{ 1 + \frac{\sigma_n + \sigma_{n+1}}{2n+1} z + o(z^2) \right\} \quad (2.63)$$

where L_{n-1}, M_n are defined by (2.3) and

$$\sigma_n = \lambda_0 + \sum_{r=1}^{n-1} (\lambda_r + \mu_r) \quad (2.64)$$

Using (2.62) and (2.63) we get a similar expression for $\epsilon_{21}^{(n)}(z)$.

We have

$$\epsilon_{21}^{(n)}(z) = L_{n-1} M_n \frac{\Gamma(b+2n)}{\Gamma(b)} \frac{z^{2n}}{(2n)!} \left\{ 1 + \frac{\sigma_n + \sigma_{n+1}}{2n+1} (b+2n) z + o(z^2) \right\} \quad (2.65)$$

Adapting (2.32) we have the error estimate

$$\epsilon_{11}^{(n)}(z) = L_{n-1} M_n \frac{z^{2n}}{(2n)!} \left\{ \frac{1}{(1-\theta_n z)^{2n-1}} + o(z^2) \right\} \quad (2.66)$$

where

$$\theta_n = \frac{\sigma_n + \sigma_{n+1}}{(2n+1)(2n-1)} \quad (2.67)$$

The analogous estimate for $\epsilon_{21}^{(n)}(z)$ is

$$\epsilon_{21}^{(n)}(z) = L_{n-1} M_n \frac{\Gamma(b+2n)}{\Gamma(b)} \frac{z^{2n}}{(2n)!} \left\{ \frac{1}{(1-\phi_n z)^{2n-1}} + o(z^2) \right\} \quad (2.68)$$

where

$$\phi_n = (b+2n) \theta_n \quad (2.69)$$

Unfortunately, these estimates are no easier to compute than those in Section 2.1 although they depend only on the parameters a , b and c . However, they do give useful estimates for the range of z , on the negative real axis, over which a given error is not exceeded.

Although the approximations (2.58) and (2.61) are valid more generally, we are particularly interested in determining conditions under which the computations are easily performed. It may be verified that the n th denominator $B_n(s)$ of the J-fraction (2.57) can be expressed in the form

$$B_n(s) = (-s)^n {}_2F_1\left(-n, 1-a-n; 2-c-2n; \frac{1}{s}\right) \quad (2.70)$$

where the right-hand side is a hypergeometric polynomial. If the denominators have complex roots they may still be computed by a QR algorithm, although the faster, more stable method given in Section 2.1 may be applied when the roots are real. We have shown that a sufficient condition for the roots of $B_n(s)$ to be real is that all the partial numerators, except the first, of the fraction (2.57) are negative. That is, we require

$$\lambda_{r-1} \mu_r > 0 \quad (2.71)$$

for $r = 1, 2, 3, \dots$, or

$$\left. \begin{aligned} (1-h_1)h_1h_2 &> 0, \\ (1-h_{2r-2})(1-h_{2r-1})h_{2r-1}h_{2r} &> 0, \end{aligned} \right\} \quad (2.72)$$

for $r = 2, 3, 4, \dots$. Using (2.43) this condition reduces to

$$c > a > 0 \quad (2.73)$$

This is not too restrictive as many well-known hypergeometric functions satisfy (2.73), bearing in mind that the parameters a and b are interchangeable. Also, under condition (2.73) all singularities of the approximations (2.61) lie on the interval $(1, \infty)$ of the real axis in the z -plane.

We now formally define the generalised hypergeometric function by the Taylor series expansion

$${}_m F_n(\{a_i\}; \{c_j\}; z) = \frac{\prod_{j=1}^n \Gamma(c_j)}{\prod_{i=1}^m \Gamma(a_i)} \sum_{r=0}^{\infty} \frac{\prod_{i=1}^m \Gamma(a_i+r)}{\prod_{j=1}^n \Gamma(c_j+r)} \frac{z^r}{r!}, \quad (2.74)$$

where there are m parameters $\{a_i\}$ and n parameters $\{c_j\}$. It is easily verified that result (2.54) may be written more generally as

$$\mathcal{L}\{z^{b-1} {}_m F_n(\{a_i\}; \{c_j\}; z)\} = \frac{\Gamma(b)}{s^b} {}_{m+1} F_n(\{a_i\}, b; \{c_j\}; \frac{1}{s}), \quad (2.75)$$

where b becomes the $(m+1)$ th parameter on the right-hand side.

In particular, for the confluent hypergeometric functions

we have

$$\mathcal{L}\{z^{b-1} {}_0 F_1(c; z)\} = \frac{\Gamma(b)}{s^b} {}_1 F_1(b; c; \frac{1}{s}), \quad (2.76)$$

and

$$\mathcal{L}\{z^{b-1} {}_1 F_0(a; z)\} = \frac{\Gamma(b)}{s^b} {}_2 F_0(a, b; \frac{1}{s}). \quad (2.77)$$

To form approximations for ${}_1 F_1(b; c; z)$ and ${}_2 F_0(a, b; z)$ we must find the roots of the denominators of the J -fractions for

$\frac{1}{s} {}_1F_1(1; c; \frac{1}{s})$ and $\frac{1}{s} {}_2F_0(a, 1; \frac{1}{s})$ respectively. Each of these

J-fractions can be expressed in the form (2.57) where, for

$$\frac{1}{s} {}_1F_1(1; c; \frac{1}{s}) ,$$

$$\left. \begin{aligned} \lambda_0 &= \frac{1}{c} , \\ \lambda_r &= \frac{c+r-1}{(c+2r-1)(c+2r)} , \\ \mu_r &= -\frac{r}{(c+2r-2)(c+2r-1)} , \end{aligned} \right\} \quad (2.78)$$

for $r = 1, 2, 3, \dots$ and, for $\frac{1}{s} {}_2F_0(a, 1; \frac{1}{s})$,

$$\left. \begin{aligned} \lambda_0 &= a , \\ \lambda_r &= (a + r) , \\ \mu_r &= r , \end{aligned} \right\} \quad (2.79)$$

for $r = 1, 2, 3, \dots$. These J-fractions may be obtained from the S-fraction (2.42). We observe that the coefficients (2.79) satisfy condition (2.71) if $a > 0$, which is a sufficient condition for the roots of the denominators of the J-fraction for $\frac{1}{s} {}_2F_0(a, 1; \frac{1}{s})$ to be real. Unfortunately, the coefficients (2.78) do not satisfy condition (2.71) for any values of c , but we do have the alternative approximation (2.58) in this case. However, the approximations to be derived from (2.78) may be of use in cases when (2.58) is inapplicable. As the J-fractions for $\frac{1}{s} {}_1F_1(1; c; \frac{1}{s})$ and $\frac{1}{s} {}_2F_0(a, 1; \frac{1}{s})$ can both be expressed in the form (2.57), the error estimation formula (2.68) is valid in each case.

Now, suppose we wish to find approximations for ${}_3F_1(a, b, d; c; z)$. We start with the p th approximation

$${}_2F_1(a, b; c; z) = \sum_{i=1}^p \frac{A_i}{(1-\alpha_i z)^b} + \epsilon_{21}^{(p)}(z) \quad (2.80)$$

Multiplying by z^{d-1} and taking the Laplace transform we have

$$\mathcal{L}\{z^{d-1} {}_2F_1(a, b; c; z)\} = \sum_{i=1}^p A_i \mathcal{L}\left\{\frac{z^{d-1}}{(1-\alpha_i z)^b}\right\} + \mathcal{L}\{z^{d-1} \epsilon_{21}^{(p)}(z)\} \quad (2.81)$$

By comparing series expansions, we observe that

$${}_1F_0(b; \alpha_i z) \equiv (1-\alpha_i z)^{-b} \quad (2.82)$$

so we may apply result (2.77) to (2.81) to obtain

$$\mathcal{L}\{z^{d-1} {}_2F_1(a, b; c; z)\} = \frac{\Gamma(d)}{s^d} \sum_{i=1}^p A_i {}_2F_0(b, d; \frac{\alpha_i}{s}) + \mathcal{L}\{z^{d-1} \epsilon_{21}^{(p)}(z)\} \quad (2.83)$$

But, from (2.75), we also have

$$\mathcal{L}\{z^{d-1} {}_2F_1(a, b; c; z)\} = \frac{\Gamma(d)}{s^d} {}_3F_1(a, b, d; c; \frac{1}{s}) \quad (2.84)$$

Comparing (2.83) and (2.84) we have

$${}_3F_1(a, b, d; c; \frac{1}{s}) = \sum_{i=1}^p A_i {}_2F_0(b, d; \frac{\alpha_i}{s}) + \frac{s^d}{\Gamma(d)} \mathcal{L}\{z^{d-1} \epsilon_{21}^{(p)}(z)\} \quad (2.85)$$

We now use the q th approximation

$${}_2F_0(b, d; z) = \sum_{j=1}^q \frac{B_j}{(1-\beta_j z)^b} + \epsilon_{20}^{(q)}(z) \quad (2.86)$$

Replacing s by $1/z$ in (2.85) and using (2.86) we get

the (p,q) th approximation

$${}_3F_1(a,b,d;c;z) = \sum_{i=1}^p A_i \sum_{j=1}^q \frac{B_j}{(1-\alpha_i \beta_j z)^b} + \epsilon_{31}^{(p,q)}(z), \quad (2.87)$$

where

$$\epsilon_{31}^{(p,q)}(z) = \sum_{i=1}^p A_i \epsilon_{20}^{(q)}(\alpha_i z) + \frac{1}{z^d \Gamma(d)} \mathcal{L}\{z^{d-1} \epsilon_{21}^{(p)}(z)\}_{s=1/z}. \quad (2.88)$$

Clearly the computation of error estimates, like those we have derived earlier, will be too time-consuming to be of value here. We note that if $c > a > 0$ and $d > 0$ then all the values $\{\alpha_i\}$ and $\{\beta_j\}$ will be real.

We have constructed single series approximations for the ${}_1F_1$, ${}_2F_0$ and ${}_2F_1$ functions and a double series approximation for the ${}_3F_1$ function. Similarly, we can form double series approximations for the ${}_3F_0$ function, and triple series approximations could then be derived for the ${}_4F_0$ and ${}_4F_1$ functions, and so on. Approximations of different forms can also be obtained for other generalised hypergeometric functions, although not all such functions can be treated in this way.

In Tables 2.8 - 2.14, below, numerical results are given for the following examples:

- (i) ${}_2F_1(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z)$, using the approximation (2.61).
- (ii) ${}_1F_1(\frac{1}{2}; \frac{3}{2}; z)$, using (2.58).
- (iii) ${}_1F_1(\frac{1}{2}; \frac{3}{2}; z)$, using (2.78).
- (iv) $\frac{1}{2}\pi {}_2F_1(\frac{1}{2}, \frac{1}{2}; 1; m)$, using (2.61).
- (v) $\frac{1}{2}\pi {}_2F_1(\frac{1}{2}, -\frac{1}{2}; 1; m)$, using (2.61).

$$(vi) \quad {}_1F_1\left(\frac{1}{2}; 1; z\right), \text{ using (2.58).}$$

$$(vii) \quad {}_2F_0\left(\frac{1}{2}, \frac{1}{2}; z\right), \text{ using (2.79).}$$

$$(viii) \quad {}_3F_1\left(\frac{1}{2}, \frac{1}{2}, 1; 2; z\right), \text{ using (2.87).}$$

Each of the hypergeometric functions above may be expressed in terms of special functions as follows:

$$(i) \quad z {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; -z^2\right) = \sinh^{-1} z.$$

$$(ii) \ \& \ (iii) \quad 2z^{\frac{1}{2}} {}_1F_1\left(\frac{1}{2}; \frac{3}{2}; -z\right) = \gamma\left(\frac{1}{2}, z\right), \text{ where}$$

γ is the incomplete gamma function.

$$(iv) \quad \frac{1}{2}\pi {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; m\right) = K(m), \text{ the complete elliptic integral of the first kind.}$$

$$(v) \quad \frac{1}{2}\pi {}_2F_1\left(\frac{1}{2}, -\frac{1}{2}; 1; m\right) = E(m), \text{ the complete elliptic integral of the second kind.}$$

$$(vi) \quad e^{-z} {}_1F_1\left(\frac{1}{2}; 1; 2z\right) = I_0(z), \text{ the modified Bessel function of the first kind.}$$

$$(vii) \quad \pi^{\frac{1}{2}}(2z)^{-\frac{1}{2}}e^{-z} {}_2F_0\left(\frac{1}{2}, \frac{1}{2}; -\frac{1}{2z}\right) = K_0(z), \text{ the modified Bessel function of the second kind.}$$

$$(viii) \quad \pi^{\frac{1}{2}}z {}_3F_1\left(\frac{1}{2}, \frac{1}{2}, 1; 2; -z\right) = \int_0^z t^{-\frac{1}{2}}e^{\frac{1}{2t}} K_0\left(\frac{1}{2t}\right) dt.$$

For further details of the above functions see Abramowitz and Stegun (1964).

In Table 2.8, below, are listed estimates of suitable ranges of z , on the real axis, for prescribed errors and various values of n . The estimates are valid for $z < 0$ and, as before, the notation $(-k)$ denotes an absolute error of 10^{-k} .

TABLE 2.8

Example	n	Error	Estimated min(z)	Error	Estimated min(z)
(i)	3	(-4)	-1.98	(-3)	-4.51
	4	(-5)	-2.30	(-4)	-4.44
	5	(-5)	-4.37	(-4)	-9.43
	8	(-8)	-4.17	(-6)	-12.7
	10	(-8)	-9.41	(-7)	-18.4
(ii)	3	(-4)	-2.94	(-3)	-4.80
	4	(-5)	-4.21	(-4)	-6.10
	5	(-7)	-4.14	(-5)	-7.39
	8	(-10)	-7.74	(-8)	-11.2
	10	(-10)	-13.7	(-8)	-18.8
(iii)	3	(-4)	-2.06	(-3)	-3.54
	4	(-5)	-2.78	(-4)	-4.17
	5	(-7)	-2.59	(-5)	-4.80
	8	(-10)	-4.55	(-8)	-6.69
	10	(-10)	-7.94	(-8)	-11.1
(vi)	3	(-4)	-2.83	(-3)	-4.63
	4	(-5)	-4.10	(-4)	-5.95
	5	(-8)	-3.09	(-5)	-7.25
	8	(-8)	-11.1	(-4)	-26.5
	10	(-10)	-13.6	(-6)	-26.6
(vii)	3	(-3)	-1.11	(-2)	-5.09
	4	(-3)	-3.41	(-2)	-24.1
	5	(-4)	-2.47	(-3)	-15.0
	8	(-6)	-4.90	(-5)	-36.4
	10	(-8)	-2.82	(-7)	-16.9

The estimates in Table 2.8, above, were found to be reasonable and a selection of computed results for Examples (i) - (viii) is given in Tables 2.9 - 2.14, below. In these tables the last convergent listed, for each value of z , is generally accurate to the number of figures shown, and these values may often be verified by reference to Abramowitz and Stegun (1964). Without loss of generality, the imaginary part of z is chosen to be non-negative as the moduli of the real and imaginary parts of all the approximations are symmetric about the real axis.

TABLE 2.9

Example (i).					${}_2F_1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z\right)$				
Re z	Im z	n	Re F(z)	Im F(z)	Re z	Im z	n	Re F(z)	Im F(z)
-0.5	0	3	0.9312295	0	0	5	6	0.70746	0.24223
		4	0.9312298	0			8	0.707525	0.2421520
		5	0.9312298	0			9	0.7075187	0.2421516
							10	0.7075181	0.2421530
-1	0	3	0.881365	0	0	10	10	0.582693	0.242611
		4	0.8813733	0			13	0.5826797	0.2425952
		5	0.8813736	0			17	0.5826799	0.2425964
							18	0.5826799	0.2425963
-2	0	4	0.810489	0	-2	1	3	0.801124	0.05651
		5	0.8104965	0			5	0.8011345	0.0563142
		6	0.8104969	0			6	0.8011337	0.0563135
		7	0.8104970	0			7	0.8011336	0.0563135
-5	0	5	0.69067	0	-1	1	3	0.86228	0.081307
		6	0.690708	0			4	0.862233	0.0812989
		7	0.6907135	0			5	0.8622313	0.0813006
		8	0.6907145	0			6	0.8622313	0.0813007
-10	0	5	0.5904	0	1	1	5	1.02205	0.2723083
		8	0.590879	0			7	1.022007	0.2723083
		10	0.5908871	0			8	1.022006	0.2723083
		11	0.5908876	0			9	1.022006	0.2723083
0	1	3	0.944766	0.136085	2	1	11	0.976318	0.445834
		4	0.9447981	0.1360665			14	0.9763356	0.4458673
		5	0.9447967	0.1360661			19	0.9763372	0.4458648
							20	0.9763371	0.4458647
0	2	4	0.863718	0.197569	1	0.1	8	2.13189	0.2498
		5	0.8637632	0.1975208			11	2.13216	0.250043
		6	0.8637574	0.1975178			18	2.132091	0.2500334
		7	0.8637572	0.1975178			19	2.132090	0.2500334

TABLE 2.10

Comparison of examples (ii) and (iii).				${}_1F_1\left(\frac{1}{2}; \frac{3}{2}; z\right)$			
(a) z real, $F(z)$ real.							
z	n	Ex.(ii) $F(z)$	Ex.(iii) $F(z)$	z	n	Ex.(ii) $F(z)$	Ex.(iii) $F(z)$
-1	3	0.7468238	0.7468270	1	3	1.4626509	1.462673
	4	0.7468241	0.7468241		4	1.4626517	1.4626517
-2	3	0.598131	0.59822	2	3	2.36437	2.3686
	4	0.5981439	0.5981429		4	2.3644539	2.3644545
	5	0.5981440	0.5981440		6	2.3644539	2.3644539
-5	3	0.3947	0.3977	5	4	17.169	14.5
	4	0.39569	0.39555		5	17.172109	17.37
	5	0.3957119	0.395721		7	17.172158	17.17238
	7	0.3957123	0.3957123		9	17.172158	17.172158
(b) z imaginary, $F(z)$ complex.							
Re z	Im z	n	Example(ii) Re $F(z)$ Im $F(z)$		Example(iii) Re $F(z)$ Im $F(z)$		
0	1	3	0.9045247	0.3102685	0.9045204	0.3102623	
		4	0.9045242	0.3102683	0.9045242	0.3102683	
0	2	3	0.66762	0.498837	0.66776	0.49845	
		4	0.6675968	0.4988117	0.6675996	0.498806	
		5	0.6675968	0.4988119	0.6675969	0.4988118	
		6	0.6675968	0.4988119	0.6675968	0.4988119	
0	5	4	0.18423	0.26102	0.1828	0.2658	
		5	0.1840972	0.261162	0.18399	0.26152	
		6	0.1840997	0.2611598	0.1840944	0.261177	
		8	0.1840996	0.2611598	0.1840997	0.2611598	

TABLE 2.11

Examples (iv) and (v).				$\frac{1}{2}\pi {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; m\right)$			
m	n	K(m)	E(m)	m	n	K(m)	E(m)
0.1	3	1.61244135	1.53075764	0.7	4	2.075319	1.2416722
					6	2.0753629	1.24167057
0.2	3	1.65962358	1.48903506	0.7	7	2.07536311	1.24167057
	4	1.65962360	1.48903506		9	2.07536314	1.24167057
0.3	3	1.71388906	1.44536309	0.8	5	2.25715	1.178491
					7	2.2572043	1.17848994
					8	2.25720519	1.17848993
					10	2.25720532	1.17848992
0.4	3	1.7775160	1.39939238	0.9	7	2.578006	1.1047758
	4	1.77751932	1.39939214		11	2.5780918	1.10477474
	5	1.77751937	1.39939214		12	2.57809202	1.10477473
0.5	3	1.854053	1.3506453	0.95	10	2.90824	1.0604743
					13	2.9083319	1.06047375
					17	2.90833713	1.06047373
					21	2.90833725	1.06047373
0.6	3	1.94945	1.298435	1.0*	11	4.6	1.00085
	4	1.9495626	1.29842825		14	4.8	1.00052
	6	1.94956774	1.29842804		17	5.0	1.00036
	7	1.94956775	1.29842804		20	5.2	1.00026

*K(1.0) = ∞ , E(1.0) = 1.0

TABLE 2.12

Example (vi).			${}_1F_1\left(\frac{1}{2}; 1; z\right)$									
Re z	Im z	n	Re F(z)	Im F(z)	Re z	Im z	n	Re F(z)	Im F(z)			
-10	0	4	0.182542	0	0	1	3	0.8235853	0.4499267			
		6	0.182538	0			4	0.8235847	0.4499264			
		7	0.1825407	0			3	0.413461	0.64393			
		8	0.1825408	0			4	0.4134380	0.6438915			
-5	0	3	0.2690	0	0	5	5	0.4134381	0.6438917			
		4	0.270018	0			4	0.038961	-0.02910			
		5	0.2700460	0			5	0.038759	-0.0289537			
		6	0.2700464	0			6	0.0387624	-0.0289564			
-1	0	3	0.6450349	0	0	10	7	0.0387624	-0.0289563			
		4	0.6450353	0			6	-0.05042	0.17045			
1	0	3	1.7533865	0			7	-0.0503759	0.170297			
		4	1.7533877	0			8	-0.0503775	0.1703020			
3	0	4	7.380078	0			9	-0.0503775	0.1703019			
		5	7.3801012	0			-2	1	3	0.42921	0.119745	
		6	7.3801013	0			4	0.4291879	0.1197210			
5	0	4	40.0742	0			5	0.4291877	0.1197210			
		5	40.078373	0			-1	1	3	0.5665358	0.2231414	
		6	40.078445	0			4	0.5665342	0.2231443			
10	0	5	4041.4	0	1	1	3	1.3424713	0.9681422			
		6	4042.696	0			4	1.3424757	0.9681344			
		7	4042.7535	0			2	1	3	2.4581	2.19063	
		8	4042.7554	0						4	2.4578438	2.1905864
										5	2.4578432	2.1905852

TABLE 2.13

Example (vii).					${}_2F_0\left(\frac{1}{2}, \frac{1}{2}; z\right)$				
Re z	Im z	n	Re F(z)	Im F(z)	Re z	Im z	n	Re F(z)	Im F(z)
-0.1	0	3	0.9773562	0	0	0.2	3	0.990519	0.046570
		4	0.9773567	0			5	0.9905619	0.0465577
		5	0.9773567	0			7	0.9905604	0.0465577
							8	0.9905605	0.0465578
-0.2	0	3	0.958209	0	0	0.5	5	0.96046	0.09623
		4	0.9582198	0			9	0.9605958	0.0961556
		6	0.9582210	0			15	0.9605901	0.0961579
							18	0.9605902	0.0961578
-0.5	0	4	0.91308	0	0	0.7	7	0.93914	0.011908
		6	0.9131440	0			12	0.9392172	0.0118978
		9	0.9131492	0			14	0.9392118	0.0118979
		11	0.9131494	0	22	0.9392116	0.0118982		
-0.8	0	5	0.87883	0	0.1	0.5	5	0.97355	0.1082
		7	0.878932	0			8	0.973668	0.10788
		12	0.8789500	0			14	0.9736431	0.1079014
		15	0.8789504	0	21	0.9736432	0.1079004		
-1.0	0	6	0.85977	0	-0.1	0.5	4	0.94748	0.08604
		9	0.859875	0			5	0.947502	0.08627
		14	0.8598861	0			8	0.9475949	0.0863096
		18	0.8598866	0	17	0.9475939	0.0863030		
0	0.1	3	0.9973397	0.0244733	-0.3	0.5	5	0.922844	0.07105
		4	0.9973401	0.0244717			7	0.9228018	0.071114
		5	0.9973400	0.0244717			11	0.9228081	0.0711248
							15	0.9228086	0.0711245

TABLE 2.14

Example (viii).				${}_3F_1\left(\frac{1}{2}, \frac{1}{2}, 1; 2; z\right)$			
(a) $\text{Re } z = -0.5, \text{Im } z = 0.$				(b) $\text{Re } z = 0, \text{Im } z = 0.3.$			
p	q	Re F(z)	Im F(z)	p	q	Re F(z)	Im F(z)
3	3	0.951807	0	3	3	0.993123	0.034817
3	5	0.9518452	0	3	5	0.9931483	0.0348274
3	7	0.9518467	0	3	7	0.9931476	0.0348263
3	8	0.9518468	0	3	8	0.9931476	0.0348264
4	4	0.9518470	0	4	4	0.9931488	0.0348309
4	6	0.9518541	0	4	5	0.9931520	0.0348277
4	7	0.9518541	0	4	6	0.9931516	0.0348268
4	8	0.9518541	0	4	8	0.9931513	0.0348268
5	5	0.9518531	0	5	5	0.9931520	0.0348275
5	8	0.9518546	0	5	6	0.9931517	0.0348265
5	9	0.9518547	0	5	9	0.9931513	0.0348266
6	6	0.9518543	0	6	6	0.9931516	0.0348265
7	7	0.9518546	0	7	7	0.9931514	0.0348265
8	8	0.9518547	0	8	8	0.9931513	0.0348265
9	9	0.9518547	0	9	9	0.9931513	0.0348266

TABLE 2.14 (continued)

(c) $\text{Re } z = 0.1, \text{Im } z = 0.3$				(d) $\text{Re } z = -0.5, \text{Im } z = 0.3$			
p	q	Re F(z)	Im F(z)	p	q	Re F(z)	Im F(z)
3	3	1.003702	0.039303	3	3	0.9495728	0.02295
3	4	1.003760	0.039274	3	5	0.9495693	0.0228742
3	7	1.0037490	0.0392607	3	7	0.9495669	0.0228714
3	9	1.0037498	0.0392609	3	9	0.9495666	0.0228713
4	4	1.003764	0.0392639	4	4	0.9495705	0.0228716
4	5	1.0037573	0.0392514	4	5	0.9495665	0.0228603
4	6	1.0037535	0.0392521	4	7	0.9495641	0.0228576
4	9	1.0037537	0.0392536	4	9	0.9495638	0.0228574
5	5	1.0037569	0.0392510	5	5	0.9495658	0.0228594
5	6	1.0037528	0.0392518	5	6	0.9495641	0.0228571
5	8	1.0037529	0.0392535	5	9	0.9495631	0.0228565
6	6	1.0037528	0.0392519	6	6	0.9495640	0.0228570
7	7	1.0037526	0.0392532	7	7	0.9495633	0.0228566
8	8	1.0037529	0.0392535	8	8	0.9495631	0.0228565
9	9	1.0037531	0.0392535	9	9	0.9495630	0.0228565
10	10	1.0037531	0.0392534	10	10	0.9495630	0.0228565

CHAPTER 3.

THE CORRESPONDING SEQUENCE ALGORITHMS.

In this chapter we examine the problem of converting a given power series to an appropriate continued fraction. We shall define a class of algorithms based on the corresponding sequence of a continued fraction, giving examples and making comparisons with algorithms of the quotient-difference type. The idea of corresponding sequence algorithms is not new, although a short paper by Watson (1972) may well be the only published work on the subject. Notably, these algorithms are not included in the monumental survey paper of Wynn (1960). In Part II we will show that the use of corresponding sequence algorithms makes possible the generalisation of corresponding fractions to two and more variables. We begin with a general approach to the problem in one variable.

3.1 The General Algorithm.

We consider a function $f_0(z)$ formally defined by the power series

$$f_0(z) = a_0 + a_1 z + a_2 z^2 + a_3 z^3 + \dots \quad (3.1)$$

and we assume that a corresponding fraction of the form

$$f_0(z) = \frac{p_1}{q_1(z)} + \frac{p_2 z^{v(1)}}{q_2(z)} + \frac{p_3 z^{v(2)}}{q_3(z)} + \dots + \frac{p_n z^{v(n-1)}}{q_n(z)} + \dots \quad (3.2)$$

exists, i.e. a fraction of the form (1.59) that we described

in Section 1.2 . The recurrence relations that give rise to the fraction (3.2) are

$$f_n(z) = z^{v(n-1)} p_n f_{n-2}(z) - q_n(z) f_{n-1}(z) \quad (3.3)$$

for $n = 1, 2, 3, \dots$ where we set $v(0) = 0$ and $f_{-1}(z) = 1$.

We shall consider the function $f_n(z)$ as a formal power series in z and we write

$$f_n(z) = z^{\sigma(n)} \{ a_0^{(n)} + a_1^{(n)} z + a_2^{(n)} z^2 + \dots + a_r^{(n)} z^r + \dots \} \quad (3.4)$$

where

$$\sigma(n) = \sum_{i=1}^n v(i) \quad (3.5)$$

and, in particular, we have $a_r^{(0)} = a_r$ for all r . Now, equating powers of z in (3.3) we obtain

$$a_r^{(n)} = E^{v(n)} \{ p_n a_r^{(n-2)} - q_n(E^{-1}) a_r^{(n-1)} \} \quad (3.6)$$

where the shift operator E is defined by

$$E^m a_r^{(n)} = a_{r+m}^{(n)} \quad (3.7)$$

for all integer values of m . We require that the relation (3.6) holds for $n = 1, 2, 3, \dots$ and $r = -v(n), -v(n)+1, \dots, -2, -1, 0, 1, 2, 3, \dots$ so we choose $a_r^{(n)} = 0$ for $r < 0$, $a_0^{(-1)} = 1$ and $a_r^{(-1)} = 0$ for $r \neq 0$. Now the relation (3.6) summarises an algorithm for obtaining the coefficients of the continued fraction (3.2) from the sequence $\{a_r\}$. We call this algorithm the corresponding sequence algorithm, or CS algorithm, for the continued fraction (3.2). The equations summarised by (3.6) form a "triangular" system so there is no problem of solution as we shall see in the next two sections.

3.2 Algorithms for S-Fractions and Padé Approximants.

We consider an S-fraction of the form

$$f_0(z) = \frac{c_0}{1} + \frac{c_1 z}{1} + \frac{c_2 z^2}{1} + \dots + \frac{c_n z^n}{1} + \dots \quad (3.8)$$

and, to simplify the calculations, we adjust the series coefficients so that $a_0 = c_0 = 1$. Comparing (3.8) with (3.2) we can write the summarised CS algorithm (3.6) as

$$a_r^{(n)} = c_{n-1} a_{r+1}^{(n-2)} - a_{r+1}^{(n-1)} \quad (3.9)$$

for all r and n or, written in full,

$$\left. \begin{aligned} c_0 &= 1, \\ a_r^{(1)} &= -a_{r+1}, \quad r = 0, 1, 2, 3, \dots, \\ c_n &= \frac{a_0^{(n)}}{a_0^{(n-1)}}, \quad n = 1, 2, 3, \dots, \\ a_r^{(n)} &= c_{n-1} a_{r+1}^{(n-2)} - a_{r+1}^{(n-1)}, \quad r = 0, 1, 2, 3, \dots, \\ & \quad n = 2, 3, 4, \dots \end{aligned} \right\} \quad (3.10)$$

In the case of the S-fraction it is also useful to define a modified CS algorithm. First we perform a similarity transformation on the S-fraction (3.8), with $c_0 = 1$, to obtain

$$f_0(z) = \frac{k_1}{k_1} + \frac{k_1 k_2 c_1 z}{k_2} + \frac{k_2 k_3 c_2 z^2}{k_3} + \dots + \frac{k_n k_{n+1} c_n z^n}{k_{n+1}} + \dots, \quad (3.11)$$

forming a new corresponding sequence $\{F_n(z)\}$ satisfying

the recurrence relations

$$F_n(z) = k_n \{ k_{n-1} c_{n-1} z F_{n-2}(z) - F_{n-1}(z) \} \quad (3.12)$$

for $n = 1, 2, 3, \dots$ where $F_0(z) = f_0(z)$ and we set $F_{-1}(z) = 1/z$.

For convenience we choose

$$k_n = c_n^{-1} \quad (3.13)$$

for $n = 1, 2, 3, \dots$ and writing

$$F_n(z) = z^n (b_0^{(n)} + b_1^{(n)} z + b_2^{(n)} z^2 + \dots + b_r^{(n)} z^r + \dots) \quad (3.14)$$

we obtain the modified CS algorithm, summarised by

$$b_r^{(n)} = \frac{1}{c_n} \{ b_{r+1}^{(n-2)} - b_{r+1}^{(n-1)} \} \quad (3.15)$$

for all r and n . We note that $b_0^{(n)} = 1$, for all n , and need not be stored. Written in full, this algorithm is

$$\left. \begin{aligned} c_0 &= 1, \quad c_1 = -a_1, \\ b_r^{(1)} &= -\frac{a_{r+1}}{c_1}, \quad r = 1, 2, 3, \dots, \\ c_n &= b_1^{(n-2)} - b_1^{(n-1)}, \quad n = 2, 3, 4, \dots, \\ b_r^{(n)} &= \frac{1}{c_n} \{ b_{r+1}^{(n-2)} - b_{r+1}^{(n-1)} \}, \quad r = 1, 2, 3, \dots, \\ & \quad n = 2, 3, 4, \dots \end{aligned} \right\} \quad (3.16)$$

As an example we perform each algorithm on the power series expansion

$$e^{-z} = 1 - z + \frac{1}{2} z^2 - \frac{1}{6} z^3 + \frac{1}{24} z^4 - \frac{1}{120} z^5 + \dots \quad (3.17)$$

TABLE 3.1

Ordinary CS algorithm (3.10)
for the S-fraction.

a_5	$-\frac{1}{120}$	$a_r^{(1)}$ ↓	$a_r^{(2)}$ ↓	$a_r^{(3)}$ ↓	$a_r^{(4)}$ ↓	$a_r^{(5)}$ ↓
a_4	$\frac{1}{24}$	$\frac{1}{120}$	$\frac{1}{30}$	$-\frac{1}{80}$	$-\frac{1}{120}$	$\frac{1}{720}$
a_3	$-\frac{1}{6}$	$-\frac{1}{24}$	$-\frac{1}{8}$	$\frac{1}{24}$	$-\frac{1}{120}$	$\frac{1}{720}$
a_2	$\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{8}$	$-\frac{1}{80}$	$-\frac{1}{120}$	$\frac{1}{720}$
a_1	-1	$-\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{24}$	$-\frac{1}{120}$	$\frac{1}{720}$
a_0	1	1	$-\frac{1}{2}$	$-\frac{1}{12}$	$\frac{1}{72}$	$\frac{1}{720}$
	1	1	$-\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{6}$	$\frac{1}{10}$
	c_0	c_1	c_2	c_3	c_4	c_5

TABLE 3.2

Modified CS algorithm (3.16)
for the S-fraction.

a_5	$-\frac{1}{120}$	$b_r^{(1)}$ ↓	$b_r^{(2)}$ ↓	$b_r^{(3)}$ ↓	$b_r^{(4)}$ ↓
a_4	$\frac{1}{24}$	$\frac{1}{120}$	$-\frac{1}{15}$	$\frac{3}{20}$	$-\frac{3}{5}$
a_3	$-\frac{1}{6}$	$-\frac{1}{24}$	$-\frac{1}{15}$	$\frac{3}{20}$	$-\frac{3}{5}$
a_2	$\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{3}{20}$	$-\frac{3}{5}$
a_1	-1	$-\frac{1}{2}$	$-\frac{2}{3}$	$-\frac{1}{2}$	$-\frac{3}{5}$
a_0	1	1	$-\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{6}$
	1	1	$-\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{6}$
	c_0	c_1	c_2	c_3	c_4

Each algorithm indicates the S-fraction expansion

$$e^{-z} = \frac{1}{1} + \frac{z}{1} - \frac{\frac{1}{2}z}{1} + \frac{\frac{1}{6}z}{1} - \frac{\frac{1}{6}z}{1} + \frac{\frac{1}{120}z}{1} - \dots \quad (3.18)$$

The modified algorithm (3.16) commends itself for hand calculation as it is simple to use and easy to remember. Also, the coefficients $\{b_r^{(n)}\}$ in the modified algorithm are usually easier to work with than the coefficients $\{a_r^{(n)}\}$ in the ordinary algorithm, as may be seen in the example above in which the coefficients $\{a_r^{(n)}\}$ become small more quickly.

We will now consider the importance of the S-fraction and its CS algorithm in relation to the more general field of Padé approximants. This was the subject of the paper by Watson (1972), mentioned above, who suggested the use of the algorithm for performing operations, such as differentiation and integration, on Padé approximants expressed in terms of S-fractions. In such applications the CS algorithm is also used in its equally convenient reverse form, i.e. to convert the continued fraction coefficients $\{c_n\}$ to the series coefficients $\{a_n\}$.

We define the $[M/N]$ Padé approximant to the function $f_0(z)$, formally defined by (3.1), to be $A_M(z)/B_N(z)$ where $A_M(z)$ and $B_N(z)$ are polynomials of degree M and N , respectively, such that

$$B_N(z) f_0(z) - A_M(z) = O(z^{M+N+1}) \quad (3.19)$$

For a given series (3.1) the $[M/N]$ Padé approximant is unique, if it exists, and the "staircase" sequence of approximants

$$\begin{array}{cc} [L-1/0] & [L/0] \\ & [L/1] \quad [L+1/1] \\ & & [L+1/2] \quad [L+2/2] \\ & & & \dots \\ & & & & \dots \end{array} \quad (3.20)$$

is given by the successive convergents of the corresponding fraction

$$f_0(z) = a_0 + a_1 z + a_2 z^2 + \dots + a_{L-1} z^{L-1} + a_L z^L \left\{ \frac{1}{1} + \frac{c_1^{(L)} z}{1} + \frac{c_2^{(L)} z}{1} + \dots \right\} \quad (3.21)$$

Also, the "staircase" sequence of Padé approximants

$$\begin{array}{cccc} [0/L-1] & & & \\ [0/L] & [1/L] & & \\ & [1/L+1] & [2/L+1] & \\ & & [2/L+2] & \dots \dots \dots \end{array} \quad (3.22)$$

is given by the successive convergents of the corresponding fraction

$$f_0(z) = \frac{1}{d_0 + d_1 z + \dots + d_{L-1} z^{L-1} + d_L z^L \left\{ \frac{1}{1} + \frac{g_1^{(L)} z}{1} + \frac{g_2^{(L)} z}{1} + \dots \right\}} \quad (3.23)$$

By suitable choice of L , we can express any Padé approximant as a convergent of one of the fractions (3.21) and (3.23). In (3.21) the first $(L+1)$ coefficients are identical to those of the series (3.1) and the coefficients $c_1^{(L)}, c_2^{(L)}, c_3^{(L)}, \dots$ may be obtained by applying the modified CS algorithm to the sequence $a_{L+1}/a_L, a_{L+2}/a_L, a_{L+3}/a_L, \dots$. In (3.23) the series $d_0 + d_1 z + d_2 z^2 + \dots$ is the power series of the reciprocal of $f_0(z)$ and its coefficients may be computed from the relation

$$d_n = -d_0 \sum_{r=1}^n d_{n-r} a_r \quad (3.24)$$

for $n = 1, 2, 3, \dots$ and where $d_0 = a_0^{-1}$. The coefficients $g_1^{(L)}, g_2^{(L)}, g_3^{(L)}, \dots$ are then obtained by applying the modified CS algorithm to the sequence $d_{L+1}/d_L, d_{L+2}/d_L, d_{L+3}/d_L, \dots$.

Padé approximants may, of course, be obtained without reference to continued fractions. [See, for example, Baker and Gammel (1970), Graves-Morris (1972a, 1972b).] However, in problems which give rise to power series the continued fraction approach is far simpler.

As an example, setting $L = 2$ in (3.23), we have in particular the $[2/3]$ Padé approximant

$$\frac{A_2(z)}{B_3(z)} = \frac{1}{d_0 + d_1 z} + \frac{d_2 z^2}{1} + \frac{g_1^{(2)} z}{1} + \frac{g_2^{(2)} z}{1} + \frac{g_3^{(2)} z}{1} \quad (3.25)$$

If we write

$$\left. \begin{aligned} A_2(z) &= p_0 + p_1 z + p_2 z^2, \\ B_3(z) &= 1 + q_1 z + q_2 z^2 + q_3 z^3, \end{aligned} \right\} \quad (3.26)$$

and equate coefficients of powers of z in (3.19) we must solve six equations in the six unknowns $p_0, p_1, p_2, q_1, q_2, q_3$ to find the Padé approximant in rational function form. However, the application of the modified CS algorithm to find the approximant in the form (3.25) is comparatively trivial. Again taking $f_0(z) = e^{-z}$, we already know the reciprocal series

$$e^z = 1 + z + \frac{1}{2} z^2 + \frac{1}{6} z^3 + \frac{1}{24} z^4 + \frac{1}{120} z^5 + \dots \quad (3.27)$$

so that we have

$$\frac{d_3}{d_2} = \frac{1}{3}, \quad \frac{d_4}{d_2} = \frac{1}{12}, \quad \frac{d_5}{d_2} = \frac{1}{60} \quad (3.28)$$

and we apply the modified CS algorithm to these values.

d_5/d_2	$\frac{1}{60}$			
d_4/d_2	$\frac{1}{12}$	$\frac{1}{20}$		
d_3/d_2	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{2}{5}$	
	1	$-\frac{1}{3}$	$\frac{1}{12}$	$-\frac{3}{20}$
		$g_1^{(2)}$	$g_2^{(2)}$	$g_3^{(2)}$

TABLE 3.3

Modified CS algorithm (3.16)

for Padé approximants.

Thus, the [2/3] Padé approximant to e^{-z} is

$$e^{-z} = \frac{1}{1+z} + \frac{\frac{1}{2}z^2}{1} - \frac{\frac{1}{3}z}{1} + \frac{\frac{1}{12}z}{1} - \frac{\frac{3}{20}z}{1} + O(z^6) \quad (3.29)$$

This is one of the simplest methods for obtaining a Padé approximant and is easily accomplished by a minimum of computation.

It is interesting to compare this algorithm with that of Longman (1971). Longman's algorithm computes the coefficients of Padé approximants in rational function form. An advantage of the continued fraction approach is that, by computing just one more coefficient, we can progress from one approximant to another. Whilst Longman's algorithm is useful for computing the whole Padé table, we can use the CS algorithm to calculate high order approximants without computing the whole of the preceding table. As fewer computational steps are necessary we may suppose that there is less build-up of rounding error with the CS algorithm.

3.3 Algorithms for Other Corresponding Fractions.

We now consider a power series

$$f_0(z) = 1 + a_1 z + a_2 z^2 + a_3 z^3 + \dots \quad (3.30)$$

that does not have an S-fraction expansion. However, as stated in Section 1.2, this series always has a C-fraction expansion of the form

$$f_0(z) = \frac{1}{1 + \frac{c_1 z^{v(1)}}{1} + \frac{c_2 z^{v(2)}}{1} + \dots + \frac{c_n z^{v(n)}}{1} + \dots} \quad (3.31)$$

in which the exponents $\{v(n)\}$ are positive integers. In particular, if $a_1 = a_2 = \dots = a_k = 0$ then $v(1) = k+1$, and in general many of the coefficients $\{a_r\}$ may be zero. Proceeding as in Section 3.2 we can obtain a modified CS algorithm, summarised by

$$b_r^{(n)} = \frac{1}{c_n} \left\{ b_{r+v(n)}^{(n-2)} - b_{r+v(n)}^{(n-1)} \right\}, \quad (3.32)$$

which is similar to the relation (3.15) that we derived for the S-fraction. In practice the algorithm is the same as that for the S-fraction except that the indices $\{v(n)\}$ must also be computed. In order to do this all the zero coefficients are stored and the number of zeros at the bottom of the n th column gives $v(n)-1$. The only other difference is that the n th column must be displaced by $v(n-1)$ places compared with the $(n-1)$ th column, as indicated in Table 3.4 below. The example below is for a suitable arbitrary function $f_0(z)$ whose power

series expansion begins

$$f_0(z) = 1 + 2z^3 + z^5 + z^7 + \dots \quad (3.33)$$

a_7	1				
a_6	0	} 3 places			
a_5	1				
a_4	0				
a_3	2	$\frac{1}{2}$	} 2 places		
a_2	0	0			
a_1	0	0	-4	$-\frac{1}{8}$	
	1	-2	$-\frac{1}{2}$	4	$-\frac{31}{8}$
		3	2	1	1

$v(1) \quad v(2) \quad v(3) \quad v(4)$

TABLE 3.4

Modified CS algorithm (3.16)

adapted for the C-fraction.

Table 3.4 indicates a C-fraction expansion which begins

$$f_0(z) = \frac{1}{1} - \frac{2z^3}{1} - \frac{\frac{1}{2}z^2}{1} + \frac{4z}{1} - \frac{\frac{31}{8}z}{1} + \dots \quad (3.34)$$

We now consider the J-fraction

$$f_0(z) = \frac{p_1}{1+q_1z} + \frac{p_2z^2}{1+q_2z} + \frac{p_3z^2}{1+q_3z} + \dots + \frac{p_nz^2}{1+q_nz} + \dots \quad (3.35)$$

which is the even part of the S-fraction (3.8). Adapting result (3.6) for the fraction (3.35) we get

$$a_r^{(n)} = p_n a_{r+2}^{(n-2)} - a_{r+2}^{(n-1)} - q_n a_{r+1}^{(n-1)} \quad (3.36)$$

which leads to the computational scheme

$$\begin{aligned}
 p_1 &= a_0, \quad q_1 = -\frac{a_1}{a_0}, \\
 a_r^{(1)} &= -\{ a_{r+2} + q_1 a_{r+1} \}, \quad r = 0, 1, 2, 3, \dots, \\
 p_n &= \frac{a_0^{(n-1)}}{a_0^{(n-2)}}, \quad n = 2, 3, 4, \dots, \\
 q_n &= \frac{1}{a_0^{(n-1)}} \{ p_n a_1^{(n-2)} - a_1^{(n-1)} \}, \quad n = 2, 3, 4, \dots, \\
 a_r^{(n)} &= p_n a_{r+2}^{(n-2)} - a_{r+2}^{(n-1)} - q_n a_{r+1}^{(n-1)}, \quad r = 0, 1, 2, 3, \dots, \\
 &\quad n = 2, 3, 4, \dots.
 \end{aligned} \tag{3.37}$$

The algorithm (3.37) may also be applied to convert a power series of the form

$$f_o(z) = \frac{a_0}{z} + \frac{a_1}{z^2} + \frac{a_2}{z^3} + \dots \tag{3.38}$$

to a J-fraction of the form

$$f_o(z) = \frac{p_1}{q_1+z} + \frac{p_2}{q_2+z} + \dots + \frac{p_n}{q_n+z} + \dots \tag{3.39}$$

The fact that corresponding fractions have two interchangeable forms provides the simplest method for obtaining the CS algorithm for the M-fraction.

The M-fraction, described in Section 1.2, is of the form

$$f_o(z) = \frac{p_0}{1+q_0 z} + \frac{p_1 z}{1+q_1 z} + \frac{p_2 z}{1+q_2 z} + \dots + \frac{p_n z}{1+q_n z} + \dots \tag{3.40}$$

and corresponds simultaneously to the two power series expansions

$$f_o(z) = a_0 + a_1 z + a_2 z^2 + \dots \quad (3.41)$$

for $|z|$ small and

$$f_o(z) = \frac{b_0}{z} + \frac{b_1}{z^2} + \frac{b_2}{z^3} + \dots \quad (3.42)$$

for $|z|$ large. Adapting the general algorithm (3.6) we obtain an algorithm

$$a_r^{(n)} = p_{n-1} a_{r+1}^{(n-2)} - a_{r+1}^{(n-1)} - q_{n-1} a_r^{(n-1)} \quad (3.43)$$

for converting the series (3.41) to the M-fraction (3.40).

However, (3.43) summarises only half of the CS algorithm as we have not yet considered correspondence with the series (3.42).

Now, by a similarity transformation, we can write the fraction (3.40) in the form

$$f_o(z) = \frac{p_0 \frac{1}{z}}{q_0 + \frac{1}{z}} + \frac{p_1 \frac{1}{z}}{q_1 + \frac{1}{z}} + \frac{p_2 \frac{1}{z}}{q_2 + \frac{1}{z}} + \dots + \frac{p_n \frac{1}{z}}{q_n + \frac{1}{z}} + \dots, \quad (3.44)$$

and replacing $1/z$ by z we obtain

$$f_o\left(\frac{1}{z}\right) = \frac{p_0 z}{q_0 + z} + \frac{p_1 z}{q_1 + z} + \frac{p_2 z}{q_2 + z} + \dots + \frac{p_n z}{q_n + z} + \dots \quad (3.45)$$

Also, replacing $1/z$ by z in (3.42) we get

$$f_o\left(\frac{1}{z}\right) = b_0 z + b_1 z^2 + b_2 z^3 + \dots \quad (3.46)$$

so we can again apply the general algorithm (3.6) to the fraction (3.45) to obtain

$$b_r^{(n)} = p_{n-1} b_{r+1}^{(n-2)} - q_{n-1} b_{r+1}^{(n-1)} - b_r^{(n-1)} . \quad (3.47)$$

Now, the relations (3.43) and (3.47) together lead to the computational scheme

$$\left. \begin{aligned} p_0 &= a_0, \quad q_0 = \frac{a_0}{b_0}, \\ a_r^{(1)} &= - \{ a_{r+1} + q_0 a_r \}, \quad r = 0, 1, 2, 3, \dots, \\ b_r^{(1)} &= - \{ q_0 b_{r+1} + b_r \}, \quad r = 0, 1, 2, 3, \dots, \\ p_n &= \frac{a_0^{(n)}}{a_0^{(n-1)}}, \quad n = 1, 2, 3, \dots, \\ q_n &= p_n \frac{b_0^{(n-1)}}{b_0^{(n)}}, \quad n = 1, 2, 3, \dots, \\ a_r^{(n)} &= p_{n-1} a_{r+1}^{(n-2)} - a_{r+1}^{(n-1)} - q_{n-1} a_r^{(n-1)}, \quad r = 0, 1, 2, 3, \dots, \\ &\quad n = 2, 3, 4, \dots, \\ b_r^{(n)} &= p_{n-1} b_{r+1}^{(n-2)} - q_{n-1} b_{r+1}^{(n-1)} - b_r^{(n-1)}, \quad r = 0, 1, 2, 3, \dots, \\ &\quad n = 2, 3, 4, \dots \end{aligned} \right\} (3.48)$$

As a numerical example we consider Dawson's integral

$$u(z) = e^{-z^2} \int_0^z e^{t^2} dt \quad (3.49)$$

and choose the function $f_0(z) = \sqrt{2/z} u(\sqrt{z/2})$ which has the

two series expansions

$$f_0(z) = 1 - \frac{z}{3} + \frac{z^2}{15} - \frac{z^3}{105} + \frac{z^4}{945} - \dots \quad (3.50)$$

for $|z|$ small, and

$$f_0(z) = \frac{1}{z} + \frac{1}{z^2} + \frac{3}{z^3} + \frac{15}{z^4} + \frac{105}{z^5} + \dots \quad (3.51)$$

for $|z|$ large. Table 3.5, below, is the layout for computing the coefficients $\{p_n\}$ and Table 3.6 is the layout for computing $\{q_n\}$, although the two sets of calculations are interrelated.

a_4	$\frac{1}{945}$				
a_3	$-\frac{1}{105}$	$\frac{8}{945}$			
a_2	$\frac{1}{15}$	$-\frac{2}{35}$	$\frac{16}{945}$		
a_1	$-\frac{1}{3}$	$\frac{4}{15}$	$-\frac{8}{105}$	$\frac{64}{4725}$	
a_0	1	$-\frac{2}{3}$	$\frac{8}{45}$	$-\frac{16}{525}$	$\frac{128}{33075}$
	1	$-\frac{2}{3}$	$-\frac{4}{15}$	$-\frac{6}{35}$	$-\frac{8}{63}$
	p_0	p_1	p_2	p_3	p_4

TABLE 3.5

CS algorithm (3.48) for the M-fraction:

$a_r^{(n)}$ -array.

b_4	105				
b_3	15	- 120			
b_2	3	- 18	48		
b_1	1	- 4	8	$-\frac{64}{5}$	
b_0	1	- 2	$\frac{8}{3}$	$-\frac{16}{5}$	$\frac{128}{35}$
	1	$\frac{1}{3}$	$\frac{1}{5}$	$\frac{1}{7}$	$\frac{1}{9}$
	q_0	q_1	q_2	q_3	q_4

TABLE 3.6

CS algorithm (3.48) for the M-fraction:

$b_r^{(n)}$ -array.

The resulting M-fraction is thus

$$f_0(z) = \frac{1}{1+z} - \frac{\frac{2}{3}z}{1+\frac{1}{3}z} - \frac{\frac{4}{15}z}{1+\frac{1}{5}z} - \frac{\frac{6}{35}z}{1+\frac{1}{7}z} - \frac{\frac{8}{63}z}{1+\frac{1}{9}z} - \dots \quad (3.52)$$

or, using a similarity transformation,

$$f_0(z) = \frac{1}{1+z} - \frac{2z}{3+z} - \frac{4z}{5+z} - \frac{6z}{7+z} - \frac{8z}{9+z} - \dots \quad (3.53)$$

This expansion may be verified by applying Lagrange's method to the Riccati equation

$$2z f_0' = -(1+z) f_0 + 1 \quad (3.54)$$

Finally, we consider the T-fraction

$$f(z) = 1 + d_0 z + \frac{z}{1+d_1 z} + \frac{z}{1+d_2 z} + \dots + \frac{z}{1+d_n z} + \dots \quad (3.55)$$

which, as stated in Section 1.2, is not a particular case of the general corresponding fraction (3.2) so we must derive its CS algorithm by considering the special form of its corresponding sequence. We first set

$$f_0(z) = f(z) - (1 + d_0 z) \quad (3.56)$$

so that

$$f_0(z) = \frac{z}{1+d_1 z} + \frac{z}{1+d_2 z} + \dots + \frac{z}{1+d_n z} + \dots, \quad (3.57)$$

which is the fractional part of (3.55). We formally define $f(z)$ by the series expansion

$$f(z) = 1 + a_1 z + a_2 z^2 + a_3 z^3 + \dots \quad (3.58)$$

so that

$$d_0 = a_1 - 1. \quad (3.59)$$

The recurrence relations that give rise to the fraction (3.57) are

$$f_n(z) = z f_{n-2}(z) - (1 + d_n z) f_{n-1}(z) \quad (3.60)$$

for $n = 1, 2, 3, \dots$ and where we set $f_{-1}(z) = 1$. Each member of the corresponding sequence $\{f_n\}$ may be expressed as a series of the form

$$f_n(z) = z^{n+1} \{1 + a_1^{(n)} z + a_2^{(n)} z^2 + \dots + a_r^{(n)} z^r + \dots\}, \quad (3.61)$$

where the first coefficient is always unity, and we can equate coefficients of powers of z in (3.60) to obtain

$$a_r^{(n)} = a_{r+1}^{(n-2)} - a_{r+1}^{(n-1)} - d_n a_r^{(n-1)}. \quad (3.62)$$

This leads to the computational scheme

$$\left. \begin{aligned} d_0 &= a_1 - 1, \quad d_1 = -a_2 - 1, \\ a_r^{(0)} &= a_{r+1}, \quad r = 1, 2, 3, \dots, \\ a_r^{(1)} &= -a_{r+2} - d_1 a_{r+1}, \quad r = 1, 2, 3, \dots, \\ d_n &= a_1^{(n-2)} - a_1^{(n-1)} - 1, \quad n = 2, 3, 4, \dots, \\ a_r^{(n)} &= a_{r+1}^{(n-2)} - a_{r+1}^{(n-1)} - d_n a_r^{(n-1)}, \quad r = 1, 2, 3, \dots, \\ & \quad n = 2, 3, 4, \dots \end{aligned} \right\} \quad (3.63)$$

We note, in particular, that $a_r^{(0)} \neq a_r$ in this algorithm.

For an example we return to the series (3.17) for e^{-z} . The

working is shown in Table 3.7 below.

a_5	$-\frac{1}{120}$	$a_r^{(0)}$ ↓				
a_4	$\frac{1}{24}$	$-\frac{1}{120}$	$a_r^{(1)}$ ↓			
a_3	$-\frac{1}{6}$	$\frac{1}{24}$	$\frac{17}{240}$	$a_r^{(2)}$ ↓		
a_2	$\frac{1}{2}$	$-\frac{1}{6}$	$-\frac{7}{24}$	$-\frac{637}{1440}$	$a_r^{(3)}$ ↓	
a_1	-1	$\frac{1}{2}$	$\frac{11}{12}$	$\frac{205}{144}$	$\frac{238049}{103680}$	
	1	-2	$-\frac{3}{2}$	$-\frac{17}{12}$	$-\frac{217}{144}$	$-\frac{194129}{103680}$
		d_0	d_1	d_2	d_3	d_4

TABLE 3.7

CS algorithm (3.63)

for the T-fraction.

This example indicates the continued fraction expansion

$$e^{-z} = 1 - 2z + \frac{z}{1 - \frac{3}{2}z} + \frac{z}{1 - \frac{17}{12}z} + \frac{z}{1 - \frac{217}{144}z} + \frac{z}{1 - \frac{194129}{103680}z} + \dots$$

(3.64)

3.4 Comparison with the Quotient-Difference Algorithm.

The powerful quotient-difference algorithm, or QD algorithm, of Rutishauser (1954) has many applications in numerical mathematics which have been investigated by Henrici (1958) and others. However, the algorithm was originally designed as a means for converting the coefficients of a power series to those of the corresponding S-fraction. In this application the QD algorithm has two disadvantages when compared to the CS algorithm:

- (i) The QD algorithm breaks down in some cases when the required S-fraction exists. The CS algorithm breaks down if and only if the required S-fraction does not exist.
- (ii) The QD algorithm is more difficult to generalise to other corresponding fractions, whereas the CS algorithm works equally well with all types of corresponding fraction.

We will now derive the QD algorithm to illustrate these disadvantages more clearly. We consider a function $g_0(z)$ formally defined by the power series

$$g_0(z) = a_0 + a_1 z + a_2 z^2 + a_3 z^3 + \dots \quad (3.65)$$

and we wish to find the corresponding S-fraction expansion

which we write in the form

$$g_0(z) = \frac{a_0}{1} - \frac{q_1^{(0)} z}{1} - \frac{e_1^{(0)} z}{1} - \frac{q_2^{(0)} z}{1} - \frac{e_2^{(0)} z}{1} - \dots$$

$$\dots - \frac{q_r^{(0)} z}{1} - \frac{e_r^{(0)} z}{1} - \dots \quad (3.66)$$

where the coefficients $\{q_r^{(0)}\}$ and $\{e_r^{(0)}\}$ are to be determined. Now, to form the CS algorithm we considered the corresponding sequence of functions $\{f_n(z)\}$ connected by a set of recurrence relations. To form the QD algorithm we use the sequence of functions $\{g_n(z)\}$ where we formally define

$$g_n(z) = a_n + a_{n+1}z + a_{n+2}z^2 + \dots \quad (3.67)$$

so that we have the simple recurrence relations

$$g_n(z) = a_n + z g_{n+1}(z) \quad (3.68)$$

for $n = 0, 1, 2, 3, \dots$. Whereas for the CS algorithm we manipulated the power series expressions for the sequence $\{f_n(z)\}$, we suppose for the QD algorithm that S-fractions exist for each member of the sequence $\{g_n(z)\}$ and manipulate the coefficients of these fractions. We write

$$g_n(z) = \frac{a_n}{1} - \frac{q_1^{(n)} z}{1} - \frac{e_1^{(n)} z}{1} - \frac{q_2^{(n)} z}{1} - \frac{e_2^{(n)} z}{1} - \dots$$

$$\dots - \frac{q_r^{(n)} z}{1} - \frac{e_r^{(n)} z}{1} - \dots \quad (3.69)$$

Now, the odd part of the fraction (3.69) is

$$\begin{aligned}
 g_n(z) = & a_n + \frac{a_n q_1^{(n)} z}{1 - \{q_1^{(n)} + e_1^{(n)}\}z} - \frac{e_1^{(n)} q_2^{(n)} z^2}{1 - \{q_2^{(n)} + e_2^{(n)}\}z} - \\
 & \frac{e_2^{(n)} q_3^{(n)} z^2}{1 - \{q_3^{(n)} + e_3^{(n)}\}z} - \dots - \frac{e_{r-1}^{(n)} q_r^{(n)} z^2}{1 - \{q_r^{(n)} + e_r^{(n)}\}z} - \dots,
 \end{aligned}
 \tag{3.70}$$

i.e. the J-fraction whose convergents are the odd numbered convergents of (3.69). Using (3.68) we obtain

$$\begin{aligned}
 g_{n+1}(z) = & \frac{a_n q_1^{(n)}}{1 - \{q_1^{(n)} + e_1^{(n)}\}z} - \frac{e_1^{(n)} q_2^{(n)} z^2}{1 - \{q_2^{(n)} + e_2^{(n)}\}z} - \\
 & \frac{e_2^{(n)} q_3^{(n)} z^2}{1 - \{q_3^{(n)} + e_3^{(n)}\}z} - \dots - \frac{e_{r-1}^{(n)} q_r^{(n)} z^2}{1 - \{q_r^{(n)} + e_r^{(n)}\}z} - \dots.
 \end{aligned}
 \tag{3.71}$$

Also, replacing n by $(n+1)$ in (3.69) and taking the even part we get

$$\begin{aligned}
 g_{n+1}(z) = & \frac{a_{n+1}}{1 - q_1^{(n+1)} z} - \frac{e_1^{(n+1)} q_1^{(n+1)} z^2}{1 - \{q_2^{(n+1)} + e_1^{(n+1)}\}z} - \\
 & \frac{e_2^{(n+1)} q_2^{(n+1)} z^2}{1 - \{q_3^{(n+1)} + e_2^{(n+1)}\}z} - \dots - \frac{e_{r-1}^{(n+1)} q_{r-1}^{(n+1)} z^2}{1 - \{q_r^{(n+1)} + e_{r-1}^{(n+1)}\}z} - \dots.
 \end{aligned}
 \tag{3.72}$$

Now, (3.71) and (3.72) both represent the unique J-fraction expansion of $g_{n+1}(z)$ so we can equate coefficients between the

two expressions. By this means we obtain the QD algorithm

$$\left. \begin{aligned}
 q_1^{(n)} &= \frac{a_{n+1}}{a_n}, \quad n = 0, 1, 2, 3, \dots, \\
 e_1^{(n)} &= q_1^{(n+1)} - q_1^{(n)}, \quad n = 0, 1, 2, 3, \dots, \\
 q_r^{(n)} &= q_{r-1}^{(n+1)} \frac{e_{r-1}^{(n+1)}}{e_{r-1}^{(n)}}, \quad r = 2, 3, 4, \dots, \\
 &\quad n = 0, 1, 2, 3, \dots, \\
 e_r^{(n)} &= e_{r-1}^{(n+1)} + q_r^{(n+1)} - q_r^{(n)}, \quad r = 2, 3, 4, \dots, \\
 &\quad n = 0, 1, 2, 3, \dots.
 \end{aligned} \right\} (3.73)$$

The algorithm breaks down if, at any stage, we need to divide by a zero quantity. Clearly, this will occur in the algorithm (3.73) if any of the coefficients $\{a_n\}$ or $\{e_r^{(n)}\}$ is zero. This means that if any of the S-fraction expansions of the sequence $\{g_n(z)\}$ does not exist then the QD algorithm will fail.

As an example we consider a function $g_0(z)$ having a power series expansion that begins

$$g_0(z) = 1 + \frac{2}{3}z + \frac{1}{2}z^2 + \frac{1}{4}z^3 + \frac{1}{8}z^4 + \dots \quad (3.74)$$

The modified CS algorithm below yields the S-fraction coefficients.

a_4	$\frac{1}{8}$				
a_3	$\frac{1}{4}$	$\frac{3}{16}$			
a_2	$\frac{1}{2}$	$\frac{3}{8}$	$-\frac{3}{4}$		
a_1	$\frac{2}{3}$	$\frac{3}{4}$	$-\frac{3}{2}$	$\frac{1}{2}$	
	1	$-\frac{2}{3}$	$-\frac{1}{12}$	$\frac{9}{4}$	- 2
		c_1	c_2	c_3	c_4

TABLE 3.8

Modified CS algorithm (3.16)

for the S-fraction.

Thus the S-fraction expansion exists and begins

$$g_0(z) = \frac{1}{1} - \frac{\frac{2}{3}z}{1} - \frac{\frac{1}{12}z}{1} + \frac{\frac{9}{4}z}{1} - \frac{2z}{1} + \dots \quad (3.75)$$

However, we find that the series

$$g_2(z) = \frac{1}{2} + \frac{1}{4}z + \frac{1}{8}z^2 + \dots \quad (3.76)$$

has no S-fraction expansion because its Hankel determinant H_2 is zero. [See Section 1.2 .] Consequently, the QD algorithm fails for the series (3.74) when the CS algorithm works.

Further, we note from (3.16) that the modified CS algorithm for the S-fraction fails if and only if any of the coefficients $\{c_n\}$ is zero, in which case the S-fraction does not exist.

However, considering the effect of rounding errors in the series coefficients $\{a_n\}$ on the continued fraction coefficients $\{c_n\}$, we have no simple criterion for preferring one algorithm over the other. The CS and QD algorithms involve roughly the same number of similar arithmetic operations which prompts us to conjecture that the two algorithms are approximately equivalent in respect of rounding error.

In Sections 3.1 - 3.3 we have developed CS algorithms in quite a general way and we have illustrated the simplicity of their application. Algorithms of the quotient-difference type may also be constructed for other corresponding fractions although the same drawback is present as for the S-fraction. Notably, McCabe and Murphy (1974) have constructed a QD-type algorithm

for the M-fraction

$$f_0(z) = \frac{a_0}{1+q_0^{(0)}z} + \frac{p_1^{(0)}z}{1+q_1^{(0)}z} + \frac{p_2^{(0)}z}{1+q_2^{(0)}z} + \dots + \frac{p_n^{(0)}z}{1+q_n^{(0)}z} + \dots, \quad (3.77)$$

using two arrays of coefficients $\{p_r^{(n)}\}$ and $\{q_r^{(n)}\}$. The fraction (3.77) corresponds to the two series expansions

$$f_0(z) = a_0 + a_1z + a_2z^2 + \dots \quad (3.78)$$

for $|z|$ small and

$$f_0(z) = \frac{b_0}{z} + \frac{b_1}{z^2} + \frac{b_2}{z^3} + \dots \quad (3.79)$$

for $|z|$ large. The QD algorithm for the M-fraction is

$$\left. \begin{aligned} q_0^{(0)} &= \frac{a_0}{b_0}, \\ p_0^{(n)} &= p_0^{(-n)} = 0, \quad n = 0, 1, 2, 3, \dots, \\ q_0^{(n)} &= -\frac{a_n}{a_{n-1}}, \quad q_0^{(-n)} = -\frac{b_{n-1}}{b_n}, \quad n = 1, 2, 3, \dots, \\ p_r^{(n)} &= p_{r-1}^{(n+1)} + q_{r-1}^{(n+1)} - q_{r-1}^{(n)}, \quad r = 1, 2, 3, \dots, \\ &\quad n = 0, \underline{+1}, \underline{+2}, \underline{+3}, \dots, \\ q_r^{(n)} &= q_{r-1}^{(n-1)} \frac{p_r^{(n)}}{p_r^{(n-1)}}, \quad r = 1, 2, 3, \dots, \\ &\quad n = 0, \underline{+1}, \underline{+2}, \underline{+3}, \dots. \end{aligned} \right\} (3.80)$$

This algorithm fails if any of the coefficients $\{a_r\}$, $\{b_r\}$ or $\{p_r^{(n)}\}$ is zero so that, for the M-fraction at least, the problem is magnified. McCabe and Murphy (1974) have devised an ingenious method for overcoming the difficulty of zero coefficients but at

the expense of much additional computation and a resulting loss of accuracy. We now show that the CS algorithm for the M-fraction breaks down only if the M-fraction does not exist. It is clear from (3.48) that the algorithm fails only if one of the coefficients $\{a_o^{(n)}\}$ or $\{b_o^{(n)}\}$ is zero. From (3.48) we have the recursions

$$\left. \begin{aligned} a_o^{(n)} &= p_n a_o^{(n-1)}, \\ b_o^{(n)} &= \frac{p_n}{q_n} b_o^{(n-1)}, \end{aligned} \right\} \quad (3.81)$$

with the starting values $a_o^{(0)} = p_o$ and $b_o^{(0)} = p_o/q_o$ so that

$$\left. \begin{aligned} a_o^{(n)} &= p_n p_{n-1} \cdots p_2 p_1 p_o, \\ b_o^{(n)} &= \frac{p_n p_{n-1} \cdots p_2 p_1 p_o}{q_n q_{n-1} \cdots q_2 q_1 q_o}. \end{aligned} \right\} \quad (3.82)$$

Clearly, $\{a_o^{(n)}\}$ and $\{b_o^{(n)}\}$ are non-zero only if all the coefficients $\{p_n\}$ are non-zero, which is a necessary condition for the existence of the M-fraction.

For completeness, we now show that the general CS algorithm (3.6) breaks down only if the fraction

$$f_o(z) = \frac{p_1}{q_1(z)} + \frac{p_2 z^{v(1)}}{q_2(z)} + \frac{p_3 z^{v(2)}}{q_3(z)} + \cdots + \frac{p_n z^{v(n-1)}}{q_n(z)} + \cdots \quad (3.83)$$

does not exist. We write

$$q_n(z) = 1 + q_{n1} z + q_{n2} z^2 + \cdots + q_{n, v(n)-1} z^{v(n)-1} \quad (3.84)$$

and put $r = -v(n), -v(n)+1, \dots, -2, -1$ in (3.6) to obtain

$$\begin{aligned}
 p_n &= \frac{a_0^{(n-1)}}{a_0^{(n-2)}}, \\
 q_{n1} &= \frac{1}{a_0^{(n-1)}} \{ p_n a_1^{(n-2)} - a_1^{(n-1)} \}, \\
 q_{n2} &= \frac{1}{a_0^{(n-1)}} \{ p_n a_2^{(n-2)} - a_2^{(n-1)} - q_{n1} a_1^{(n-1)} \}, \\
 &\quad \vdots \\
 &\quad \vdots \\
 q_{n, v(n)-1} &= \frac{1}{a_0^{(n-1)}} \left\{ p_n a_{v(n)-1}^{(n-2)} - a_{v(n)-1}^{(n-1)} - \sum_{r=1}^{v(n)-2} q_{nr} a_{v(n)-r-1}^{(n-1)} \right\},
 \end{aligned} \tag{3.85}$$

so the algorithm fails if one of the coefficients $\{a_0^{(n)}\}$ is zero.

We have, for $|z|$ small,

$$f_n(z) = a_0^{(n)} z^{\sigma(n)} + O\{z^{\sigma(n)+1}\} \tag{3.86}$$

and comparing (3.86) with the result (1.25) we get

$$a_0^{(n)} = p_1 p_2 \cdots p_{n+1} \tag{3.87}$$

so that $a_0^{(n)}$ is zero only if one of the coefficients $\{p_n\}$ is zero, in which case the fraction (3.83) does not exist.

Essentially, the difference between the two types of algorithm is that, in the CS algorithm, we manipulate a sequence of power series whereas, in the QD algorithm, we manipulate a sequence of continued fractions. In the next chapter we shall devise a more general structure for continued fractions to facilitate the

representation of functions of two variables. In this context the QD approach becomes excessively complicated whereas, to form a CS algorithm, we need only consider a sequence of double series which may be manipulated as easily as single series. Without this corresponding sequence approach the concepts in Chapter 4. would be largely impractical.

PART II

APPLICATIONS IN TWO AND MORE VARIABLES

CHAPTER 4.

A CORRESPONDING FRACTION IN TWO VARIABLES.

Chisholm (1973) has defined a class of rational approximants in two variables. Such approximants correspond to double power series and are chosen so that they have five properties which are natural generalisations of properties of Padé approximants. The possible applications of this technique in theoretical physics and numerical analysis may be very far-reaching and it would be convenient if rational approximants in two variables could be directly related to continued fraction theory, as is the case in one variable. Although there are many feasible ways of defining rational approximants in two variables, it appears there is no clear link with continued fractions of simple form. However, in this chapter we permit a more general structure for continued fractions and define a class of rational approximants which, although more complicated than Chisholm approximants, provide a means for analytic continuation of double power series. Further, these approximants have certain advantages over Chisholm approximants in suitable problems and can be related to well-studied aspects of continued fraction theory.

4.1 The Structure of the S_2 -Fraction.

We shall examine the possibility of constructing a continued fraction which corresponds, in some sense, to the formal double power series

$$f_0(x,y) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_{ij} x^i y^j, \quad (4.1)$$

where x and y are independent complex variables. In Section 1.2 we showed that the partial numerator of a corresponding fraction must be a monomial so the usual structure of a continued fraction is too restrictive to cope with functions of two variables. One approach to the problem is to regard (4.1) as a single series in the variable x and to form a corresponding fraction of the type

$$f_0(x,y) = \frac{\beta_0}{1} + \frac{\beta_1 x}{1} + \frac{\beta_2 x}{1} + \dots + \frac{\beta_n x}{1} + \dots \quad (4.2)$$

where each coefficient β_n is an S-fraction in the variable y .

Similarly, we could form a fraction

$$f_0(x,y) = \frac{\gamma_0}{1} + \frac{\gamma_1 y}{1} + \frac{\gamma_2 y}{1} + \dots + \frac{\gamma_n y}{1} + \dots \quad (4.3)$$

where each γ_n is an S-fraction in x . However, even if the fractions (4.2) and (4.3) both converged to the same function, their convergents would be unsatisfactory approximations because they are not symmetrical in powers of x and y . Clearly, it is desirable that the function is constructed symmetrically.

Accordingly, we shall consider a corresponding fraction in the variable xy , having partial denominators that contain S-fractions

in x and in y . This fraction may be conveniently written in the form

$$f_0(x,y) = \frac{c_{00}}{1+g_0(x)+h_0(y)} + \frac{c_{11}xy}{1+g_1(x)+h_1(y)} + \frac{c_{22}xy}{1+g_2(x)+h_2(y)} + \dots$$

$$\dots + \frac{c_{nn}xy}{1+g_n(x)+h_n(y)} + \dots \quad (4.4)$$

where

$$g_n(x) = \frac{c_{n+1,n}x}{1} + \frac{c_{n+2,n}x}{1} + \dots + \frac{c_{n+r,n}x}{1} + \dots, \quad (4.5)$$

and

$$h_n(y) = \frac{c_{n,n+1}y}{1} + \frac{c_{n,n+2}y}{1} + \dots + \frac{c_{n,n+r}y}{1} + \dots. \quad (4.6)$$

We shall call (4.4) the main-fraction and we call (4.5) and (4.6) the sub-fractions of (4.4). Because the sub-fractions are S -fractions we shall refer to the main-fraction as an S_2 -fraction, i.e. a Stieltjes-type fraction in two variables. The coefficients of the S_2 -fraction are labelled so that c_{ij} corresponds to the coefficient a_{ij} in the series (4.1). In other words, the coefficients of the sub-fraction

$g_n(x)$ "match up" to the terms $(xy)^n \sum_{i=1}^{\infty} a_{n+i,n} x^i$ of the double series

and the $(n+1)$ th partial quotient "matches up" to the terms

$(xy)^n (a_{nn} + \sum_{i=1}^{\infty} a_{n+i,n} x^i + \sum_{j=1}^{\infty} a_{n,n+j} y^j)$. We also note that if we set

$a_{ij} = 0$ for all $i \neq j$ then (4.4) reduces to an S -fraction in

the "single" variable xy .

So far we have merely explained our choice of the structure (4.4) and we must now prove its existence. We discuss existence in the general sense without reference to Hankel determinants, which are very complicated in the case of the S_2 -fraction. However, in Section 4.2 we will show that existence in particular cases may be established by

means of a CS algorithm, as we have shown for corresponding fractions in one variable.

A necessary condition for the existence of an expansion (4.4) of the function $f_0(x,y)$, formally defined by (4.1), is the existence of a sequence $\{T_n(x,y)\}$ of functions, each having an expansion of the form

$$T_n(x,y) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} p_{ij}^{(n)} x^i y^j, \quad (4.7)$$

and satisfying the system of formal identities

$$T_n(x,y) = \frac{1}{1+g_n(x)+h_n(y)+c_{n+1,n+1}xyT_{n+1}(x,y)}, \quad (4.8)$$

for $n = 0,1,2,3, \dots$ and where $f_0(x,y) = c_{00}T_0(x,y)$. We now assume that $T_n(x,y)$, $g_n(x)$ and $h_n(y)$ exist and we express $g_n(x)$ and $h_n(y)$ in series form, writing

$$\left. \begin{aligned} g_n(x) &= \sum_{i=1}^{\infty} u_i^{(n)} x^i, \\ h_n(y) &= \sum_{j=1}^{\infty} v_j^{(n)} y^j, \end{aligned} \right\} \quad (4.9)$$

for $n = 0,1,2,3, \dots$. We also note that $T_n(x,y)$ possesses a reciprocal series expansion

$$\frac{1}{T_n(x,y)} = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} d_{ij}^{(n)} x^i y^j. \quad (4.10)$$

Rearranging (4.8) we get

$$T_{n+1}(x,y) = \frac{1}{c_{n+1,n+1}xy} \left\{ \frac{1}{T_n(x,y)} - 1 - g_n(x) - h_n(y) \right\}, \quad (4.11)$$

or, using (4.9) and (4.10),

$$T_{n+1}(x,y) = \frac{1}{c_{n+1,n+1}xy} \left\{ \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} d_{ij}^{(n)} x^i y^j - 1 - \sum_{i=0}^{\infty} u_i^{(n)} x^i - \sum_{j=0}^{\infty} v_j^{(n)} y^j \right\}. \quad (4.12)$$

Now, choosing

$$d_{00}^{(n)} = 1, \quad d_{i0}^{(n)} = u_i^{(n)}, \quad d_{0j}^{(n)} = v_j^{(n)} \quad (4.13)$$

for $i = 1, 2, 3, \dots$ and $j = 1, 2, 3, \dots$ the identity (4.12) can be simplified to

$$T_{n+1}(x,y) = \frac{1}{c_{n+1,n+1}} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} d_{i+1,j+1}^{(n)} x^i y^j \quad (4.14)$$

so that $T_{n+1}(x,y)$ can be expressed in the form (4.7).

We now let $A_n(x,y)/B_n(x,y)$ denote the n th convergent of the S_2 -fraction (4.4) and we write

$$f_0(x,y) = \frac{c_{00}}{1+g_0+h_0} + \frac{c_{11}xy}{1+g_1+h_1} + \dots + \frac{c_{nn}xy}{1+g_n+h_n+c_{n+1,n+1}xyT_{n+1}(x,y)}. \quad (4.15)$$

Using the result (1.23) we have

$$f_0 - \frac{A_n}{B_n} = \frac{(-1)^n c_{00} c_{11} c_{22} \dots c_{nn} (xy)^n}{B_n (B_{n+1} + c_{n+1,n+1} xy T_{n+1} B_n)}, \quad (4.16)$$

so that

$$f_0 - \frac{A_n}{B_n} = O\{(xy)^n\} \quad (4.17)$$

where $O\{(xy)^n\}$ denotes error terms of order $x^i y^j$ for $i \geq n$ and $j \geq n$.

This is the correspondence property of the fraction (4.4).

Having established existence and correspondence, it is also useful to show that the S_2 -fraction expansion is unique for a given function $f_0(x,y)$. We consider two S_2 -fractions

$$f_0 = \frac{c_{00}}{1+g_0+h_0} + \frac{c_{11}xy}{1+g_1+h_1} + \dots + \frac{c_{nn}xy}{1+g_n+h_n} + \dots \quad (4.18)$$

and

$$f'_0 = \frac{c'_{00}}{1+g'_0+h'_0} + \frac{c'_{11}xy}{1+g'_1+h'_1} + \dots + \frac{c'_{nn}xy}{1+g'_n+h'_n} + \dots \quad (4.19)$$

such that $f_0(x,y) = f'_0(x,y)$. By setting $y = 0$ in (4.18) and (4.19) we see that $c_{00} = c'_{00}$ and $g_0 = g'_0$. Similarly, $h_0 = h'_0$ and so $A_1 = A'_1$ and $B_1 = B'_1$, where A'_n/B'_n is the n th convergent of (4.19). We also have $A_0 = A'_0 = 0$ and $B_0 = B'_0 = 1$ and, for proof by induction, we need to show that if

$$c_{rr} = c'_{rr}, \quad g_r = g'_r, \quad h_r = h'_r, \quad A_{r+1} = A'_{r+1}, \quad B_{r+1} = B'_{r+1} \quad (4.20)$$

for $r = 0, 1, 2, \dots, n-1$, then

$$c_{nn} = c'_{nn}, \quad g_n = g'_n, \quad h_n = h'_n. \quad (4.21)$$

We consider the difference between the $(n+1)$ th convergents

$$\frac{A_{n+1}}{B_{n+1}} - \frac{A'_{n+1}}{B'_{n+1}} = \frac{A_{n+1}B'_{n+1} - A'_{n+1}B_{n+1}}{B_{n+1}B'_{n+1}}. \quad (4.22)$$

Using the recurrence relations (1.8) and the hypothesis (4.20)

we get

$$A_{n+1}B'_{n+1} - A'_{n+1}B_{n+1} = \{(1+g_n+h_n)c'_{nn} - (1+g'_n+h'_n)c_{nn}\} \cdot xy(A_n B_{n-1} - A'_{n-1} B'_n), \quad (4.23)$$

or, using the determinant formula (1.11),

$$A_{n+1} B'_{n+1} - A'_{n+1} B_{n+1} = \{(1+g_n+h_n)c'_{nn} - (1+g'_n+h'_n)c_{nn}\} \cdot O\{(xy)^n\} . \quad (4.24)$$

But, from (4.17) and (4.22), we have

$$A_{n+1} B'_{n+1} - A'_{n+1} B_{n+1} = O\{(xy)^{n+1}\} \quad (4.25)$$

so it follows from (4.24) that

$$(1+g_n+h_n)c'_{nn} - (1+g'_n+h'_n)c_{nn} \equiv 0 . \quad (4.26)$$

This implies that result (4.21) holds and that $f_0(x,y)$ and $f'_0(x,y)$ both have the same coefficients. Hence, S_2 -fraction expansions are unique.

In the above proofs we have used the convergents of the fraction (4.4) in the normal way. However, for practical purposes the use of convergents is not very meaningful as each partial denominator of (4.4) is itself an infinite expression. Therefore we must truncate each sub-fraction after an appropriate number of terms to obtain a sequence of finite approximations. We adopt the notation $O(x,y)^n$ to denote error terms of order $x^r y^{n-r}$ for $r = 0, 1, 2, \dots, n$ and define the sequence $\{K_n(x,y)\}$ of S_2 -approximants by

$$f_0(x,y) - K_n(x,y) = O(x,y)^n . \quad (4.27)$$

Using this definition we find

$$\begin{aligned}
 K_1(x,y) &= c_{00} , \quad K_2(x,y) = \frac{c_{00}}{1+c_{10}x+c_{01}y} , \\
 K_3(x,y) &= \frac{c_{00}}{\frac{1+c_{10}x}{1+c_{20}x} + \frac{c_{01}y}{1+c_{02}y}} + \frac{c_{11}xy}{1} , \\
 K_4(x,y) &= \frac{c_{00}}{\frac{1+c_{10}x}{1+c_{20}x} + \frac{c_{01}y}{1+c_{02}y} + \frac{c_{11}xy}{1+c_{21}x+c_{12}y}} + \frac{c_{11}xy}{1+c_{21}x+c_{12}y} , \\
 K_5(x,y) &= \frac{c_{00}}{\frac{1+c_{10}x}{1+c_{20}x} + \frac{c_{01}y}{1+c_{02}y} + \frac{c_{11}xy}{1+c_{21}x+c_{12}y} + \frac{c_{22}xy}{1}} + \frac{c_{22}xy}{1} , \\
 &\quad \dots \dots \dots \\
 &\quad \dots \dots \dots
 \end{aligned} \tag{4.28}$$

Now, if we let $g_r^{(n)}(x)$ and $h_r^{(n)}(y)$ denote the n th convergents of $g_r(x)$ and $h_r(y)$, respectively, then we can summarise (4.28) by

$$\begin{aligned}
 K_{2n-1}(x,y) &= \frac{c_{00}}{1+g_0^{(2n-2)}+h_0^{(2n-2)}} + \frac{c_{11}xy}{1+g_1^{(2n-4)}+h_1^{(2n-4)}} + \dots \\
 &\quad \dots + \frac{c_{n-1,n-1}xy}{1} , \\
 K_{2n}(x,y) &= \frac{c_{00}}{1+g_0^{(2n-1)}+h_0^{(2n-1)}} + \frac{c_{11}xy}{1+g_1^{(2n-3)}+h_1^{(2n-3)}} + \dots \\
 &\quad \dots + \frac{c_{n-1,n-1}xy}{1+g_{n-1}^{(1)}+h_{n-1}^{(1)}} ,
 \end{aligned} \tag{4.29}$$

for $n = 1, 2, 3, \dots$. Unfortunately, the recurrence relations (1.8) cannot easily be generalised for use with the S_2 -approximants in the form (4.29) and each successive approximant must be completely recalculated. We observe from our definition (4.27) that the S_2 -approximant $K_n(x, y)$ is computed from the triangular array of coefficients

$$\begin{array}{ccccccc}
 c_{00} & c_{01} & c_{02} & \cdots & c_{0,n-1} & & \\
 & c_{10} & c_{11} & \cdots & c_{1,n-2} & & \\
 & & \cdot & & \cdot & & \\
 c_{20} & & \cdot & & \cdot & & \\
 \cdot & & \cdot & & \cdot & & \\
 \cdot & & c_{n-2,1} & & & & \\
 \cdot & & & & & & \\
 c_{n-1,0} & & & & & &
 \end{array} \tag{4.30}$$

so we can compute the value of the n th approximant by a suitable traversal of the tree-structure of the S_2 -fraction, beginning at the bottom of each sub-fraction. There are many possible ways of calculating the approximants but the algorithm (4.31) below requires a minimum of storage space, the value of the approximant K_{2n-1} or K_{2n} being held by the variable F_1 on exit from the algorithm.

$$\begin{array}{l}
 i := n-1, \\
 k := 1; \text{ for } K_{2n-1}, \\
 \quad := 2; \text{ for } K_{2n}, \\
 F_1 := 0, \\
 F_2 := 0; \text{ for } K_{2n-1}, \\
 \quad := c_{i,i+1}^y; \text{ for } K_{2n}, \\
 F_3 := 0; \text{ for } K_{2n-1}, \\
 \quad := c_{i+1,i}^x; \text{ for } K_{2n}, \\
 \\
 F_1 := c_{ii}^{xy} / (1 + F_1 + F_2 + F_3), \\
 j := i+k, \\
 i := i-1, \\
 F_2 := c_{ij}^y, \\
 F_3 := c_{ji}^x, \\
 \\
 \left. \begin{array}{l}
 (n-1) \text{ times} \\
 \\
 k \text{ times} \\
 \\
 \\
 \\
 \\
 \\
 \end{array} \right\} \begin{array}{l}
 j := j-1, \\
 F_2 := c_{ij}^y / (1 + F_2), \\
 F_3 := c_{ji}^x / (1 + F_3), \\
 \\
 k := k+2, \\
 \\
 F_1 := c_{oo} / (1 + F_1 + F_2 + F_3).
 \end{array} \quad (4.31)
 \end{array}$$

In a computer implementation of this algorithm it is necessary to test for division by zero as some approximants may not exist.

Clearly, the notation (4.28) is unwieldy but this presents no problems if we consider the S_2 -fraction as an infinite triangular array of coefficients, to be interpreted in the manner prescribed above.

We shall now consider the degree of the rational function representation of $K_n(x,y)$. We denote by $[M/N](x,y)$ a rational function of the form

$$[M/N](x,y) = \frac{\sum_{i=0}^M \sum_{j=0}^M \lambda_{ij} x^i y^j}{\sum_{p=0}^N \sum_{q=0}^N \mu_{pq} x^p y^q} \quad (4.32)$$

and we assume that $\lambda_{00}, \mu_{00}, \lambda_{MM}$ and μ_{NN} are all non-zero. Now, if $[M/N](x,y)$ is some kind of approximant to the function $f_0(x,y)$, defined by the series (4.1), then we may write

$$f_0(x,y) - [M/N](x,y) = O(x,y)^r \quad (4.33)$$

where r depends on M and N . For example, the $[M/N]$ Chisholm approximant satisfies (4.33) with

$$r = M + N + 1 \quad (4.34)$$

We also consider a rational function $[M/N]_0(x,y)$ such that

$$\begin{aligned} [M/N]_0 &= [M/N] ; \text{ with } \lambda_{MM} = 0 \text{ if } M > 0 , & (4.35) \\ &\text{and } \mu_{NN} = 0 \text{ if } N > 0 . \end{aligned}$$

Using this notation we find, from (4.28), that

$$\begin{aligned} K_{4n-3} &= [2n(n-1)/2n(n-1)] , \\ K_{4n-1} &= [2n^2-1/2n^2] , & (4.36) \\ K_{2n} &= [{}^1_2n(n+1)-1/{}^1_2n(n+1)]_0 , \end{aligned}$$

for $n = 1, 2, 3, \dots$. Now, if $[M/N]$ represents K_r then

we have

$$r = 2 \sqrt{M + N + 1} - 1 \quad (4.37)$$

for r odd, and

$$r = 2 \sqrt{M + N + \frac{5}{4}} - 1 \quad (4.38)$$

for r even. Comparing (4.37) and (4.38) with the analogous relation (4.34) we see that Chisholm approximants have greater economy in the sense that they match-up more terms of the power series than do S_2 -approximants of similar degree. However, S_2 -approximants are intended for use in continued fraction form and we shall see in the next section that their coefficients are more easily computed than those of the Chisholm approximants. We will further compare the two methods of approximation in Section 4.4.

To complete this section we now show how S_2 -fraction expansions may be obtained, with coefficients known in closed form, for a certain class of functions. These functions of two variables are somewhat trivial, however, as each is the product of two functions of a single variable. Nevertheless, the formal expansions obtained can be used to measure the usefulness of S_2 -approximants and to test any analytic results that may be developed. We consider two functions $X(x)$ and $Y(y)$ having the S -fraction expansions

$$\left. \begin{aligned} X(x) &= \frac{\lambda_0}{1} + \frac{\lambda_1 x}{1} + \frac{\lambda_2 x}{1} + \dots + \frac{\lambda_n x}{1} + \dots, \\ Y(y) &= \frac{\mu_0}{1} + \frac{\mu_1 y}{1} + \frac{\mu_2 y}{1} + \dots + \frac{\mu_n y}{1} + \dots, \end{aligned} \right\} (4.39)$$

where the coefficients $\{\lambda_n\}$ and $\{\mu_n\}$ are known in closed form, and we will obtain the S_2 -fraction expansion of the function $f_0(x,y)$ where

$$f_0(x,y) = X(x)Y(y) \quad . \quad (4.40)$$

We let the sequence of functions $\{T_n(x,y)\}$ be defined by (4.8)

so that, in particular, $c_{00} = \lambda_0\mu_0$ and

$$T_0(x,y) = \frac{1}{1+g_0(x)+h_0(y)+c_{11}xyT_1(x,y)} \quad . \quad (4.41)$$

Setting $y = 0$ we obtain

$$g_0(x) = \frac{\lambda_0}{X(x)} - 1 \quad (4.42)$$

and, similarly,

$$h_0(y) = \frac{\mu_0}{Y(y)} - 1 \quad . \quad (4.43)$$

In S-fraction form (4.42) and (4.43) may be written

$$\left. \begin{aligned} g_0(x) &= \frac{\lambda_1 x}{1} + \frac{\lambda_2 x}{1} + \frac{\lambda_3 x}{1} + \dots , \\ h_0(y) &= \frac{\mu_1 y}{1} + \frac{\mu_2 y}{1} + \frac{\mu_3 y}{1} + \dots . \end{aligned} \right\} \quad (4.44)$$

Now, rearranging (4.41) and using

$$f_0(x,y) = \lambda_0\mu_0 T_0(x,y) \quad (4.45)$$

together with (4.40), (4.42) and (4.43) we find

$$c_{11}xy T_1(x,y) = g_0(x)h_0(y) \quad . \quad (4.46)$$

From (4.46) it follows that $c_{11} = \lambda_1\mu_1$ and we now show,

in general, that

$$c_{nn}^{xy} T_n(x,y) = g_{n-1}(x)h_{n-1}(y) \quad (4.47)$$

where

$$\left. \begin{aligned} g_{n-1}(x) &= \frac{\lambda_n x}{1} + \frac{\lambda_{n+1} x}{1} + \frac{\lambda_{n+2} x}{1} + \dots, \\ h_{n-1}(y) &= \frac{\mu_n y}{1} + \frac{\mu_{n+1} y}{1} + \frac{\mu_{n+2} y}{1} + \dots, \end{aligned} \right\} \quad (4.48)$$

so that $c_{nn} = \lambda_n \mu_n$. We assume that (4.47) and (4.48) hold and substitute for $T_n(x,y)$ from (4.8) to obtain

$$g_{n-1}(x)h_{n-1}(y) = \frac{\lambda_n \mu_n^{xy}}{1 + g_n(x) + h_n(y) + c_{n+1,n+1}^{xy} T_{n+1}(x,y)}. \quad (4.49)$$

Differentiating with respect to y and setting $y = 0$ we get

$$g_{n-1}(x) = \frac{\lambda_n x}{1 + g_n(x)} \quad (4.50)$$

and, similarly,

$$h_{n-1}(y) = \frac{\mu_n y}{1 + h_n(y)}. \quad (4.51)$$

Using (4.8), (4.50) and (4.51) it follows that results (4.47) and (4.48) hold with n replaced by $(n+1)$. Hence, by induction, the results hold for $n = 1, 2, 3, \dots$. Consequently, the S_2 -fraction expansion of the function $f_0(x,y)$, defined by (4.40), may

be written

$$\begin{aligned}
 f_0(x,y) = & \frac{\lambda_0 \mu_0}{1+\lambda_1 x + \mu_1 y} + \frac{\lambda_1 \mu_1 xy}{\frac{1+\lambda_2 x}{1+\lambda_1 x} + \frac{1+\mu_2 y}{1+\mu_1 y}} + \dots \\
 & + \frac{\lambda_2 \mu_2 xy}{\frac{1+\lambda_3 x}{1+\lambda_2 x} + \frac{1+\mu_3 y}{1+\mu_2 y}} + \dots + \frac{\lambda_n \mu_n xy}{\frac{1+\lambda_{n+1} x}{1+\lambda_n x} + \frac{1+\mu_{n+1} y}{1+\mu_n y}} + \dots
 \end{aligned}
 \tag{4.52}$$

We now consider two examples:

$$\begin{aligned}
 e^{-(x+y)} = & \frac{1}{1+x} + \frac{xy}{1-\frac{1}{2}x - \frac{1}{2}y} + \dots \\
 & + \frac{\frac{1}{4}xy}{1+\frac{1}{6}x + \frac{1}{6}y} + \frac{\frac{1}{36}xy}{1-\frac{1}{6}x - \frac{1}{6}y} + \dots
 \end{aligned}
 \tag{4.53}$$

and

$$\begin{aligned}
 \frac{1}{\sqrt{(1+x)(1+y)}} &= \frac{1}{1+\frac{1}{2}x} + \frac{\frac{1}{2}y}{1+\frac{1}{4}x} + \frac{\frac{1}{4}xy}{1+\frac{1}{4}x} + \frac{\frac{1}{4}y}{1+\frac{1}{4}y} + \\
 &\quad \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} + \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \\
 &\quad \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \\
 &\quad \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \dots \\
 &\quad \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \dots \\
 &\quad \frac{1}{16} xy \frac{1}{16} xy \\
 &+ \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} + \frac{\frac{1}{4}y}{1+\frac{1}{4}y} + \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} + \frac{\frac{1}{4}y}{1+\frac{1}{4}y} + \dots \\
 &\quad \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \dots \\
 &\quad \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \frac{1+\frac{1}{4}x}{1+\frac{1}{4}x} \frac{1+\frac{1}{4}y}{1+\frac{1}{4}y} \dots
 \end{aligned}
 \tag{4.54}$$

In Tables 4.1 and 4.2, below, we compare the convergence of the sequence $\{K_n(x,y)\}$ with that of $\{X_n(x)Y_n(y)\}$, where $X_n(x)$ and $Y_n(y)$ are the n th convergents of the S -fractions for $X(x)$ and $Y(y)$. We note that $K_n(x,y)$ matches $\frac{1}{2}n(n+1)$ terms of the double series for $f_0(x,y)$, whereas the product $X_n(x)Y_n(y)$ matches n^2 terms.

TABLE 4.1

$e^{-(x+y)}$	n	$K_n(x, y)$	$X_n(x)Y_n(y)$	
$x = 0.1, y = 0.1$	3	0.8193	0.81859	
	4	0.81870	0.818729	
	5	0.8187312	0.818730776	
	6	0.818730772	0.81873075330	
	7	0.81873075317	0.81873075308	
	8	0.81873075308	0.81873075308	
	9	0.81873075308	0.81873075308	
	$x = 0.1, y = 0.2$	3	0.7421	0.74026
		4	0.74067	0.740802
5		0.740820	0.74081856	
6		0.74081840	0.7408182272	
7		0.7408182214	0.74081822059	
8		0.74081822058	0.74081822068	
9		0.74081822068	0.74081822068	
10	0.74081822068	0.74081822068		

In the example in Table 4.2 it may be seen that the sequence $\{K_n(x, y)\}$ actually converges slightly faster than $\{X_n(x)Y_n(y)\}$ for the chosen values of x and y . However, the reverse is true for the example in Table 4.1.

TABLE 4.2

$1/\sqrt{(1+x)(1+y)}$	n	$K_n(x,y)$	$X_n(x)Y_n(y)$	
$x = 0.1, y = 0.5$	3	0.7791	0.7801	
	4	0.778405	0.77833	
	5	0.778509	0.77852	
	6	0.7784979	0.7784973	
	7	0.77849904	0.7784991	
	8	0.778498934	0.778498927	
	9	0.7784989452	0.7784989459	
	10	0.77849894406	0.77849894399	
	11	0.77849894417	0.77849894418	
	12	0.77849894416	0.77849894416	
	13	0.77849894416	0.77849894416	
	$x = 1.0, y = 2.0$	4	0.4078	0.4034
		5	0.4094	0.4095
6		0.408200	0.4079	
7		0.408215	0.40833	
8		0.4082452	0.408226	
9		0.4082513	0.408254	
10		0.40824804	0.4082467	
11		0.408248258	0.40824871	
12		0.408248274	0.40824818	
13		0.408248300	0.408248321	
14		0.408248290	0.408248282	
15		0.408248291	0.408248293	
16	0.408248290	0.408248290		

4.2 The Corresponding Sequence Algorithm for the S_2 -Fraction.

In order to obtain S_2 -fraction expansions from double power series we now develop a CS algorithm in a similar way to those described in Chapter 3.

The recurrence relations that give rise to the S_2 -fraction (4.4) are

$$f_{n+1}(x,y) = c_{nn} xy f_{n-1}(x,y) - f_n(x,y) \{1+g_n(x)+h_n(y)\} \quad (4.55)$$

for $n = 0, 1, 2, 3, \dots$ where $\{f_n(x,y)\}$ is the corresponding sequence and we set $f_{-1}(x,y) = 1/xy$. Now, each member of the corresponding sequence has a double series expansion of the form

$$f_n(x,y) = (xy)^n \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_{ij}^{(n)} x^i y^j \quad (4.56)$$

and the sub-fractions correspond to single series expansions of the form

$$\left. \begin{aligned} g_n(x) &= x \sum_{k=0}^{\infty} u_k^{(n)} x^k \\ h_n(y) &= y \sum_{k=0}^{\infty} v_k^{(n)} y^k \end{aligned} \right\} \quad (4.57)$$

Using the series expansions (4.56) and (4.57) we equate

coefficients of $x^i y^j$ in (4.55) to obtain the CS algorithm

$$\begin{aligned}
 c_{oo} &= a_{oo}^{(o)}, \quad c_{nn} = \frac{a_{oo}^{(n)}}{a_{oo}^{(n-1)}}, \quad n = 1, 2, 3, \dots, \\
 u_i^{(n)} &= \frac{1}{a_{oo}^{(n)}} \left\{ c_{nn} a_{i+1,0}^{(n-1)} - a_{i+1,0}^{(n)} - \sum_{k=0}^{i-1} a_{i-k,0}^{(n)} u_k^{(n)} \right\}, \\
 &\quad i = 0, 1, 2, 3, \dots, \quad n = 0, 1, 2, 3, \dots, \\
 v_j^{(n)} &= \frac{1}{a_{oo}^{(n)}} \left\{ c_{nn} a_{0,j+1}^{(n-1)} - a_{0,j+1}^{(n)} - \sum_{k=0}^{j-1} a_{0,j-k}^{(n)} v_k^{(n)} \right\}, \\
 &\quad j = 0, 1, 2, 3, \dots, \quad n = 0, 1, 2, 3, \dots, \\
 a_{ij}^{(n+1)} &= c_{nn} a_{i+1,j+1}^{(n-1)} - a_{i+1,j+1}^{(n)} - \sum_{k=0}^i a_{i-k,j+1}^{(n)} u_k^{(n)} \\
 &\quad - \sum_{k=0}^j a_{i+1,j-k}^{(n)} v_k^{(n)}, \\
 &\quad i = 0, 1, 2, 3, \dots, \quad j = 0, 1, 2, 3, \dots, \\
 &\quad n = 0, 1, 2, 3, \dots,
 \end{aligned} \tag{4.58}$$

where we set $a_{ij}^{(-1)} = 0$ for all i and j . The coefficients $\{c_{ij}\}$ for $i \neq j$ are computed by using the CS algorithm (3.10) for the one-variable S -fraction to convert the series (4.57) to the sub-fractions of the S_2 -fraction.

Clearly, the formation of a QD algorithm in this case presents enormous problems as it would be necessary to find relationships between coefficients of a whole sequence of S_2 -fractions. No attempt is made here to establish such an algorithm as the CS algorithm (4.58) is adequate both as a means for converting a double series to an S_2 -fraction and

for establishing the existence of the fraction. The algorithm (4.58) breaks down only if one of the coefficients $\{a_{oo}^{(n)}\}$ is zero, in which case one of the coefficients $\{c_{nn}\}$ is zero and the S_2 -fraction does not exist. Also, the S_2 -fraction does not exist if any of its sub-fractions does not exist, but this may be determined by the CS algorithm (3.10) for the S-fraction.

The computation of the coefficients of the Chisholm approximants by the "prong" method of Jones and Makinson (1973) requires the solution of sets of simultaneous linear equations. This takes more computing time and requires a much larger program than the algorithm (4.58). However, this disadvantage of Chisholm approximants is compensated by the comparative simplicity of their evaluation, once the coefficients have been computed.

An example of the algorithm (4.58) is given in Table 4.3, below, in which the double series expansion of the function $1/\sqrt{1+x+y}$ is converted to an S_2 -fraction. This function is symmetric in x and y so that $u_i^{(n)} = v_i^{(n)}$ and $c_{io} = c_{oi}$ for all values of i and n .

TABLE 4.3

CS algorithm (4.58) for the S_2 -fraction.

$$\{a_{ij}^{(0)}\} = \begin{bmatrix} 1 & -\frac{1}{2} & \frac{3}{8} & -\frac{5}{16} & \frac{35}{128} & -\frac{63}{256} \\ -\frac{1}{2} & \frac{3}{4} & -\frac{15}{16} & \frac{35}{32} & -\frac{315}{256} & \\ \frac{3}{8} & -\frac{15}{16} & \frac{105}{64} & -\frac{315}{128} & & \\ -\frac{5}{16} & \frac{35}{32} & -\frac{315}{128} & & & \\ \frac{35}{128} & -\frac{315}{256} & & & & \\ -\frac{63}{256} & & & & & \end{bmatrix}$$

$$c_{00} = 1$$

$$\{u_i^{(0)}\} = \left[\frac{1}{2} \quad -\frac{1}{8} \quad \frac{1}{16} \quad -\frac{5}{128} \quad \frac{7}{256} \right]$$

$$\{c_{i0}\} = \left[\frac{1}{2} \quad \frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4} \right], \text{ using algorithm (3.10).}$$

$$\{a_{ij}^{(1)}\} = \begin{bmatrix} -\frac{1}{4} & \frac{5}{16} & -\frac{11}{32} & \frac{93}{256} \\ \frac{5}{16} & -\frac{39}{64} & \frac{117}{128} & \\ -\frac{11}{32} & \frac{117}{128} & & \\ \frac{93}{256} & & & \end{bmatrix}$$

$$c_{11} = -\frac{1}{4}$$

$$\{u_i^{(1)}\} = \left[\frac{3}{4} \quad -\frac{1}{16} \quad \frac{1}{32} \right]$$

$$\{c_{i1}\} = \left[\frac{3}{4} \quad \frac{1}{12} \quad \frac{5}{12} \right], \text{ using (3.10).}$$

TABLE 4.3 (continued)

$$\{a_{ij}^{(2)}\} = \begin{bmatrix} -\frac{3}{64} & \frac{7}{128} \\ \frac{7}{128} & \end{bmatrix}$$

$$c_{22} = \frac{3}{16}, \quad u_0^{(2)} = c_{21} = -\frac{1}{12}.$$

This algorithm indicates the expansion

$$\frac{1}{\sqrt{1+x+y}} = \frac{1}{1+\frac{1}{2}x} + \frac{\frac{1}{2}xy}{1+\frac{1}{4}x} + \frac{\frac{3}{4}y}{1+\frac{1}{2}x} + \frac{\frac{3}{4}y}{1+\frac{1}{2}y} + \dots$$

$$+ \frac{\frac{3}{16}xy}{1-\frac{1}{12}x} - \frac{\frac{1}{12}y}{1+\dots} - \dots$$

4.3 Convergence of S_2 -Fractions.

In this section we will show that the convergence of S_2 -fraction expansions may be established, in many cases, by the application of one of the existing convergence theorems for continued fractions. We first consider a fraction

$$f_0 = \frac{a_1}{b_1} + \frac{a_2}{b_2} + \dots + \frac{a_n}{b_n} + \dots \quad (4.59)$$

where $\{a_n\}$ and $\{b_n\}$ may be finite expressions in one or more variables. We denote the n th convergent of (4.59) by A_n/B_n and we say that f_0 converges if $\lim_{n \rightarrow \infty} A_n/B_n$ exists. If we permit each partial denominator b_n to be an infinite expression then we must be more precise, and we define the convergence of an S_2 -fraction (4.4) as follows:

Definition 4.1: If at all points (x,y) in some region R all the sub-fractions of an S_2 -fraction converge to finite limits, and the main-fraction [with sub-fractions replaced by their limits] converges to a finite limit, then the S_2 -fraction converges everywhere in R . The limit of the main-fraction is the value of the S_2 -fraction at each point $(x,y) \in R$.

This definition provides a basis for studying the convergence of S_2 -fractions in relation to well-known theorems. However, as we explained in Section 4.1 we are interested in the sequence of S_2 -approximants (4.29) for all practical applications, and not the sequence of convergents. Therefore, we must first prove

that, for a convergent S_2 -fraction, the sequence of S_2 -approximants converges to the value of the S_2 -fraction.

Lemma 4.1: In terms of the transformations (1.4), the value of a convergent continued fraction of the form (4.59) may be expressed as

$$f_0 = \lim_{n \rightarrow \infty} t_1 t_2 \dots t_n(w), \quad (4.60)$$

and is independent of the value of w .

Proof: It may be shown by induction that

$$t_1 t_2 \dots t_n(w) = \frac{A_{n-1} w + A_n}{B_{n-1} w + B_n} \quad (4.61)$$

for $n = 1, 2, 3, \dots$ and, by definition,

$$f_0 = \lim_{n \rightarrow \infty} \frac{A_n}{B_n}. \quad (4.62)$$

Clearly, from (4.61) we have

$$f_0 = \lim_{n \rightarrow \infty} t_1 t_2 \dots t_n(0) = \lim_{n \rightarrow \infty} t_1 t_2 \dots t_n(\infty). \quad (4.63)$$

If w is finite and non-zero we write

$$A_n = B_n (f_0 + \epsilon_n) \quad (4.64)$$

so that

$$\lim_{n \rightarrow \infty} \epsilon_n = 0. \quad (4.65)$$

Substituting for A_n in (4.61) and rearranging we get

$$t_1 t_2 \dots t_n(w) = f_0 + \frac{\epsilon_{n-1} w + \epsilon_n (B_n / B_{n-1})}{w + (B_n / B_{n-1})} \quad (4.66)$$

and as $n \rightarrow \infty$ we obtain the result (4.60) even if B_n/B_{n-1} is unbounded.

Consequently, if we can prove a result for the first n terms of a convergent continued fraction then the result will still hold as $n \rightarrow \infty$.

Theorem 4.1: If an S_2 -fraction converges to a finite limit at each point (x,y) of a set E , then the sequence of its S_2 -approximants converges to the same limit at each point of E .

Proof: We let (4.59) represent the main-fraction of an S_2 -fraction f_0 . We consider the first n terms of the m th S_2 -approximant and write

$$\phi_{mn} = \frac{a_1}{b_1 + \eta_{m1}} + \frac{a_2}{b_2 + \eta_{m2}} + \dots + \frac{a_n}{b_n + \eta_{mn}}, \quad (4.67)$$

where η_{mr} represents the truncation error in the r th partial denominator. If all the sub-fractions converge then

$$\lim_{m \rightarrow \infty} \eta_{mr} = 0 \quad (4.68)$$

for $r = 1, 2, \dots, n$ and we have

$$\lim_{m \rightarrow \infty} \phi_{mn} = \frac{a_1}{b_1} + \frac{a_2}{b_2} + \dots + \frac{a_n}{b_n}. \quad (4.69)$$

To complete the proof we let $n \rightarrow \infty$ and apply Lemma 4.1.

The convergence problem for continued fractions in one variable is given a thorough treatment in Wall (1948), and

we can often use existing convergence criteria to establish the convergence of the sub-fractions of an S_2 -fraction expansion.

We must now consider to what extent we can apply existing theorems to the convergence of the main-fraction.

We use a similarity transformation on the fraction (4.4) to obtain

$$\begin{aligned}
 f_0(x,y) = & \frac{\frac{c_{00}}{(1+g_0+h_0)}}{1} + \frac{\frac{c_{11}xy}{(1+g_0+h_0)(1+g_1+h_1)}}{1} + \\
 & + \frac{\frac{c_{22}xy}{(1+g_1+h_1)(1+g_2+h_2)}}{1} + \dots + \frac{\frac{c_{nn}xy}{(1+g_{n-1}+h_{n-1})(1+g_n+h_n)}}{1} + \dots
 \end{aligned}
 \tag{4.70}$$

when none of the partial denominators of (4.4) is zero. We suppose there is a set E_1 of points (x,y) for which there exists N such that $1+g_{n-1}(x)+h_{n-1}(y) \neq 0$ for all $n > N$. Now, for convergence purposes, we consider the function

$$\gamma_n(x,y) = \frac{c_{nn}xy}{\{1+g_{n-1}(x)+h_{n-1}(y)\}\{1+g_n(x)+h_n(y)\}} \tag{4.71}$$

for $n > N$ and $(x,y) \in E_1$.

One of the most useful theorems is one due to Van Vleck (1904) which we now quote.

Theorem 4.2: Let k_1, k_2, k_3, \dots be a sequence of numbers having a finite limit k . If $k \neq 0$, let L denote the rectilinear cut from $-(4k)^{-1}$ to ∞ in the direction of the vector from 0 to $-(4k)^{-1}$. Let G denote an arbitrary closed region whose distance from L is positive or, if $k = 0$, an entirely

arbitrary finite closed region.

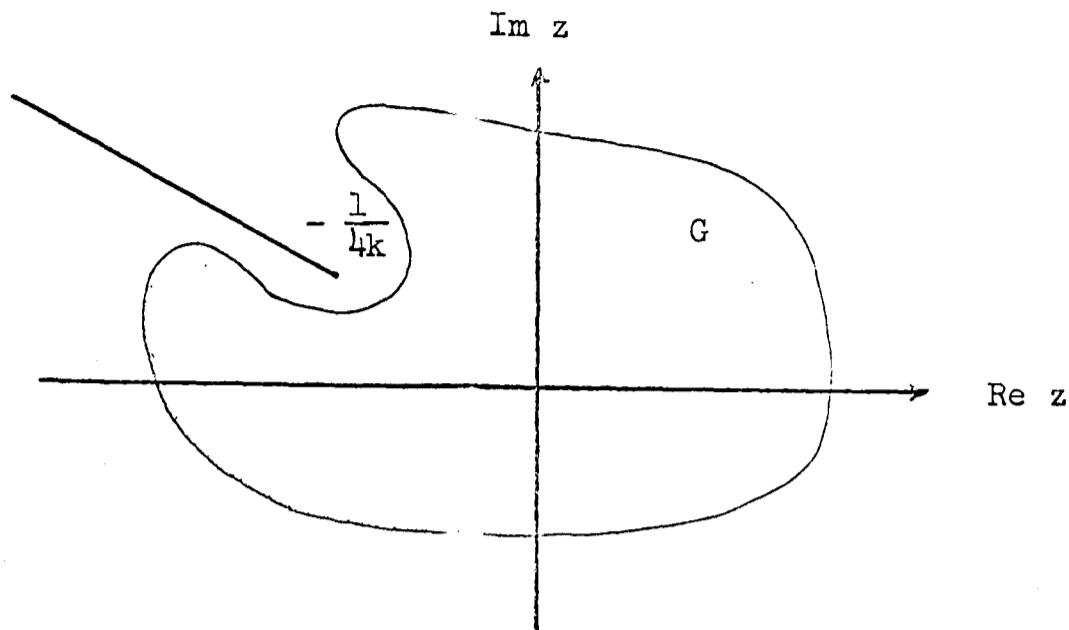


FIG. 4.1

There exists N , depending only on G , such that the S-fraction

$$\frac{1}{1 + \frac{k_n z}{1 + \frac{k_{n+1} z}{1 + \frac{k_{n+2} z}{1 + \dots}}}} \quad (4.72)$$

converges uniformly over G for $n > N$.

The proof is rather long and is not reproduced here but will be found in Wall (1948). It is worth noting that, by a theorem of Pringsheim (1910), uniform convergence of an S-fraction is a sufficient condition for the convergence of the fraction to the function of which it is the S-fraction expansion. Arising from Theorem 4.2 we have the following two theorems for S_2 -fractions:

Theorem 4.3: Let R be a finite closed region in which all the sub-fractions of an S_2 -fraction (4.4) converge uniformly and for which there exists N such that $1 + g_{n-1}(x) + h_{n-1}(y) \neq 0$ for all $n > N$ and $(x, y) \in R$. A sufficient condition

for the S_2 -fraction to converge uniformly over R is that

$$\lim_{n \rightarrow \infty} c_{nn} = 0 . \quad (4.73)$$

Proof: If condition (4.73) holds then, from (4.71),

$$\lim_{n \rightarrow \infty} \gamma_n(x,y) = 0 \quad (4.74)$$

and we can apply Theorem 4.2 .

Theorem 4.4: Let there exist c , $g(x)$ and $h(y)$ such that, in an S_2 -fraction (4.4),

$$\left. \begin{aligned} \lim_{n \rightarrow \infty} c_{nn} &= c , \\ \lim_{n \rightarrow \infty} g_n(x) &= g(x) , \\ \lim_{n \rightarrow \infty} h_n(y) &= h(y) . \end{aligned} \right\} \quad (4.75)$$

Let the region R be defined as in Theorem 4.3 . The S_2 -fraction will converge uniformly in R except when

$$\frac{cxy}{\{1+g(x)+h(y)\}^2} = -\frac{1}{4} - \zeta , \quad (4.76)$$

where ζ is any real positive number.

Proof: Under the conditions (4.75), $\lim_{n \rightarrow \infty} \gamma_n(x,y)$ exists and the restriction (4.76) follows from Theorem 4.2 .

We can apply Theorems 4.3 and 4.4 to the expansions (4.53), for $e^{-(x+y)}$, and (4.54), for $1/\sqrt{(1+x)(1+y)}$. In the case of $e^{-(x+y)}$, all the sub-fractions converge uniformly everywhere in the finite complex plane and condition (4.73) is satisfied so that, by Theorem 4.3,

the expansion (4.53) converges uniformly throughout the finite xy -domain. In the case of $1/\sqrt{(1+x)(1+y)}$, we have $c = 1/16$ and

$$g(x) = \frac{\frac{1}{4}x}{1 + \frac{1}{4}x} + \frac{\frac{1}{4}x}{1 + \frac{1}{4}x} + \dots + \frac{\frac{1}{4}x}{1 + \frac{1}{4}x} + \dots \quad (4.77)$$

which, by Theorem 4.2, converges uniformly except when $x = -1 - \xi$, where ξ is any real positive number. From (4.77) we can write

$$g(x) = \frac{\frac{1}{4}x}{1+g(x)} \quad (4.78)$$

from which we find that $g(x) = \frac{1}{2}(\sqrt{1+x} - 1)$. Similarly, $h(y) = \frac{1}{2}(\sqrt{1+y} - 1)$ except when $y = -1 - \xi$. Now, applying Theorem 4.4 we find that the expansion (4.54) converges uniformly except when any of the following conditions hold:

$$\left. \begin{aligned} x &= -1 - \xi_1, \\ y &= -1 - \xi_2, \\ \frac{xy}{(\sqrt{1+x} + \sqrt{1+y})^2} &= -1 - \xi_3, \end{aligned} \right\} \quad (4.79)$$

where ξ_1 , ξ_2 and ξ_3 are any real positive numbers, and the expression $\sqrt{1+x}$ indicates that branch of the function $(1+x)^{\frac{1}{2}}$ whose real part is positive.

4.4 Comparison of S_2 -Approximants with Chisholm Approximants.

Before comparing the two methods of approximation we define the sequence of diagonal Chisholm approximants to the function $f_0(x,y)$, defined by the double series (4.1). We write $F_{nn}(x,y)$ to denote the $[n/n]$ approximant which is of the form

$$F_{nn}(x,y) = \frac{\sum_{p=0}^n \sum_{q=0}^n b_{pq} x^p y^q}{\sum_{r=0}^n \sum_{s=0}^n d_{rs} x^r y^s} \quad (4.80)$$

Chisholm (1973) normalises the series (4.1) by taking $a_{00} = 1$ so that

$$b_{00} = d_{00} = 1 \quad (4.81)$$

and defines the $[n/n]$ approximant by the relation

$$\left[\sum_{r=0}^n \sum_{s=0}^n d_{rs} x^r y^s \right] \left[\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_{ij} x^i y^j \right] - \sum_{p=0}^n \sum_{q=0}^n b_{pq} x^p y^q = O(x,y)^{2n+1}, \quad (4.82)$$

which leads to $(2n^2+3n)$ linear equations, together with n "symmetrisation" conditions formed by equating to zero the sums of coefficients of the pairs of terms

$$x^k y^{2n+1-k}, \quad x^{2n+1-k} y^k \quad (4.83)$$

for $k = 1, 2, \dots, n$. The $(2n^2+4n)$ coefficients $\{b_{pq}\}$ and $\{d_{rs}\}$ may then be determined. The definition is chosen so that

the approximants have the following five properties:

- (i) Symmetry between x and y .
- (ii) Uniqueness.
- (iii) If $x = 0$ or $y = 0$, they reduce to Padé approximants.
- (iv) Invariance under the group of transformations

$$x = \frac{Au}{1-Bu}, \quad y = \frac{Av}{1-Cv} \quad (4.84)$$

for constants A, B and C such that $A \neq 0$.

- (v) The reciprocal of an approximant is an approximant of the reciprocal series.

Now, S_2 -approximants satisfy property (i), by definition, and property (ii), in the sense that S_2 -fraction expansions are unique. If $x = 0$ or $y = 0$ S_2 -fractions reduce to S -fractions, whose convergents are Padé approximants, so that property (iii) is also satisfied. However, the invariance properties (iv) and (v) are not satisfied by any subsequence of S_2 -approximants, although all S_2 -approximants are invariant under the elementary transformations

$$x = Au, \quad y = Bv \quad (4.85)$$

for constants A and B . This property is not shared by Chisholm approximants.

We now attempt to numerically compare the rates of convergence of the two methods of approximation for a few simple functions of two variables. In Tables 4.4-4.7, below, values of the $[n/n]$ Chisholm approximant are listed alongside values of the S_2 -approximant K_{2n+1} . Strictly, a direct comparison is

slightly biased because the "symmetrisation" of the Chisholm approximants means that the error terms (4.83) become zero when $x = y$. As only a few examples are given the results are inconclusive, but it appears that the rates of convergence of the two methods are generally different and the method to be preferred depends on the function chosen and the values of x and y . The following examples are given in the tables:

$$(i) \quad f(x,y) = 1/\sqrt{1+x+y} ,$$

$$(ii) \quad f(x,y) = e^{-(x+y)} ,$$

$$(iii) \quad f(x,y) = e^{-x}/\sqrt{1+y} ,$$

$$(iv) \quad f(x,y) = 1/\sqrt{(1+x)(1+y)} .$$

The Chisholm approximants were computed using an algorithm given by Graves-Morris, Jones and Makinson (1973).

TABLE 4.4

Example (i).			$f(x,y) = 1/\sqrt{1+x+y}$		
(a) $x = 2, y = 2$.			(b) $x = 1, y = 2$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}
5	0.4455	0.449	5	0.4986	0.5020
7	0.4482	0.452	7	0.5000088	0.5016
9	0.44718	0.44706	9	0.5000055	0.499966
11	0.447200	0.447293	11	0.49999966	0.50014
13	0.447214	0.4472156	13	0.499999980	0.500000088
15	0.4472131	0.4472157	15	0.5000000019	0.5000021
17	0.4472128	0.4472153	17	0.5000046	0.5000015
$f(x,y) = 0.4472136$			$f(x,y) = 0.5$		
(c) $x = 3, y = 3$.			(d) $x = 5, y = 5$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}
5	0.392	0.383	5	0.041	0.312
7	0.391	0.388	7	0.17	0.326
9	0.3740	0.3775	9	-0.27	0.3001
11	0.3778	0.3784	11	9.14	0.3035
13	0.3783	0.377974	13	0.313	0.301518
15	0.3777	0.377978	15	0.373	0.301639
17	0.3783	0.377969	17	0.532	0.301695
$f(x,y) = 0.377964$			$f(x,y) = 0.301511$		

TABLE 4.5

Example (ii).			$f(x,y) = e^{-(x+y)}$		
(a) $x = 0.3, y = 0.3$.			(b) $x = 1, y = 1$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}
5	0.5488154	0.548889	5	0.13573	0.143
7	0.5488116337	0.54881175	7	0.1353325	0.13543
9	0.5488116361	0.5488116364	9	0.135335294	0.1353387
11	0.5488116361	0.5488116361	11	0.1353352832	0.13533530
	$f(x,y) = 0.5488116361$		13	0.1353352832	0.1353352835
			15	0.1353352832	0.1353352832
				$f(x,y) = 0.1353352832$	
(c) $x = 1, y = 2$.			(d) $x = 5, y = 5$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}
5	0.053	0.067	5	0.011	0.042
7	0.049713	0.04984	7	0.000035	-0.0022
9	0.0497882	0.04982	9	0.000060	0.0029
11	0.049787057	0.04978718	11	0.0000446	0.00032
13	0.04978706847	0.049787078	13	0.00004544	0.00037
15	0.04978706838	0.04978706839	15	0.00004541	0.000056
17	0.04978706839	0.04978706837		$f(x,y) = 0.00004540$	
	$f(x,y) = 0.04978706837$				

TABLE 4.6

Example (iii).			$f(x,y) = e^{-x}/\sqrt{1+y}$		
(a) $x = 1, y = 1$.			(b) $x = 1, y = 2$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}
5	0.26059	0.256	5	0.2133	0.201
7	0.2601296	0.260113	7	0.21244	0.21213
9	0.26013013	0.2601318	9	0.2123983	0.2123952
11	0.2601300495	0.260130059	11	0.21239551	0.2123947
13	0.2601300476	0.2601300472	13	0.21239531	0.212395236
15	0.2601300475	0.2601300475	15	0.2123952955	0.2123952906
	$f(x,y) = 0.2601300475$		17	0.2123952942	0.2123952941
				$f(x,y) = 0.2123952944$	
(c) $x = 1, y = 5$.			(d) $x = 5, y = 5$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}
5	0.1544	0.110	5	0.044	0.15
7	0.15088	0.148	7	-0.0024	-0.0073
9	0.15031	0.1499	9	0.0032	0.0069
11	0.15021	0.15012	11	0.002728	0.00280
13	0.1501900	0.150175	13	0.002752	0.00249
15	0.1501868	0.1501842	15	0.002751	0.002748
17	0.1501861	0.1501858	17	0.002753	0.002754
	$f(x,y) = 0.1501862$			$f(x,y) = 0.002751$	

TABLE 4.7

Example (iv).			$f(x,y) = 1/\sqrt{(1+x)(1+y)}$		
(a) $x = 1, y = 1$.			(b) $x = 1, y = 2$.		
$2n+1$	$[n/n]$	K_{2n+1}^*	$2n+1$	$[n/n]$	K_{2n+1}
5	0.50030	0.50037	5	0.4095	0.4094
7	0.5000088	0.499989	7	0.40833	0.408215
9	0.50000026	0.50000032	9	0.408254	0.408251
11	0.5000000076	0.4999999906	11	0.40824871	0.408248258
13	0.5000000002	0.5000000003	13	0.40824832	0.4082482995
15	0.5000000001	0.5000000000	15	0.4082482926	0.4082482906
	$f(x,y) = 0.5$		17	0.4082482904	0.4082482905
				$f(x,y) = 0.4082482905$	
(c) $x = 1, y = 5$.			(d) $x = 5, y = 5$.		
$2n+1$	$[n/n]$	K_{2n+1}	$2n+1$	$[n/n]$	K_{2n+1}^*
5	0.296	0.294	5	0.176	0.183
7	0.290	0.28887	7	0.1682	0.1640
9	0.28891	0.28876	9	0.16694	0.1672
11	0.28872	0.288686	11	0.16672	0.16658
13	0.288682	0.2886774	13	0.166675	0.166682
15	0.2886764	0.2886755	15	0.166680	0.1666640
17	0.2886752	0.2886752	17	0.1666657	0.1666671
	$f(x,y) = 0.2886751$			$f(x,y) = 0.1666667$	

* For this example the even approximants $\{K_{2n}\}$ are exact when $x = y$.

The results in Tables 4.4 - 4.7, above, show that S_2 -approximants converge more rapidly for the function $1/\sqrt{1+x+y}$, whereas Chisholm approximants converge more rapidly for $e^{-(x+y)}$. There is little to choose between the methods in the other two examples given.

It is also of interest to examine the singularity structure of the two methods of approximation. In Figs. 4.2 - 4.13, below, are sketches of the zeros and poles, near the origin in the real xy -plane, of some approximants with quadratic and cubic numerators and denominators. Both the S_2 -approximants and the Chisholm approximants satisfactorily represent the singularities although, in the examples shown, the Chisholm approximants do so more accurately because they correspond to more terms of the power series. The graphs shown are as follows:

FIG.

4.2	Branch points of $1/\sqrt{1+x+y}$ [left diagram] and $1/\sqrt{(1+x)(1+y)}$ [right diagram].
4.3	Zeros [left] and poles [right] of K_3 for $1/\sqrt{1+x+y}$.
4.4	" " " " " of K_4 " " .
4.5	" " " " " of [2/2] C.A. for $1/\sqrt{1+x+y}$.
4.6	" " " " " of [3/3] " " " .
4.7	" " " " " of K_3 for $e^{-(x+y)}$.
4.8	" " " " " of K_4 " " .
4.9	" " " " " of [3/3] C.A. for $e^{-(x+y)}$.
4.10	" " " " " of K_3 for $1/\sqrt{(1+x)(1+y)}$.
4.11	" " " " " of K_4 " " .
4.12	" " " " " of [2/2] C.A. for $1/\sqrt{(1+x)(1+y)}$.
4.13	" " " " " of [3/3] " " " .

The [2/2] Chisholm approximant (C.A.) for $e^{-(x+y)}$ has no real zeros or poles.

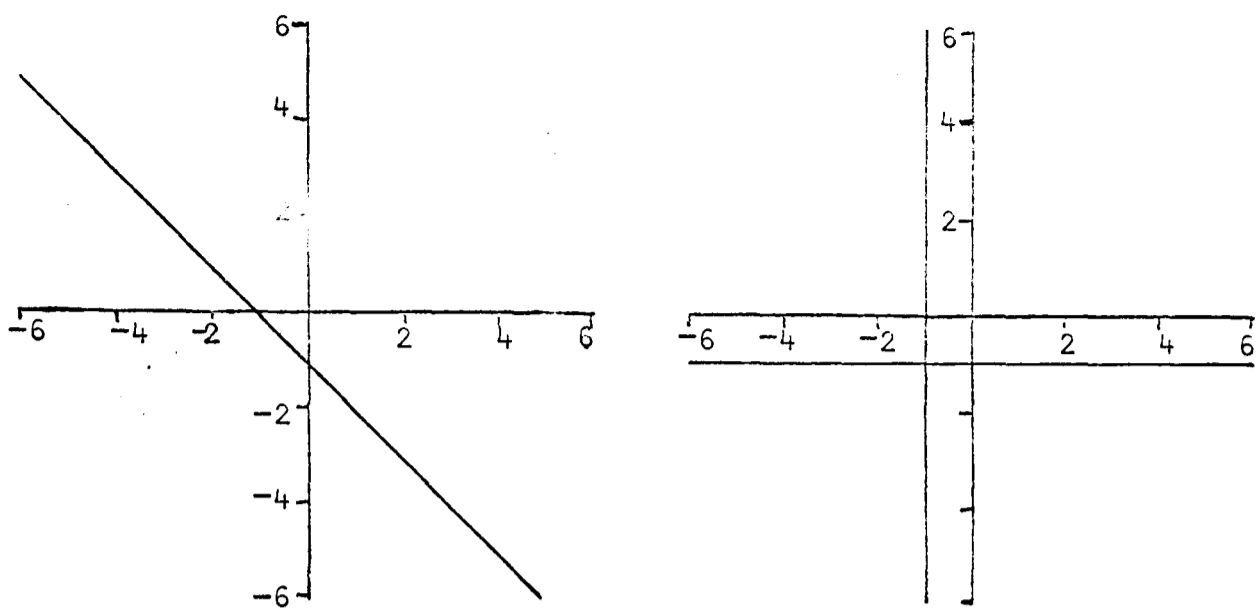


FIG. 4.2

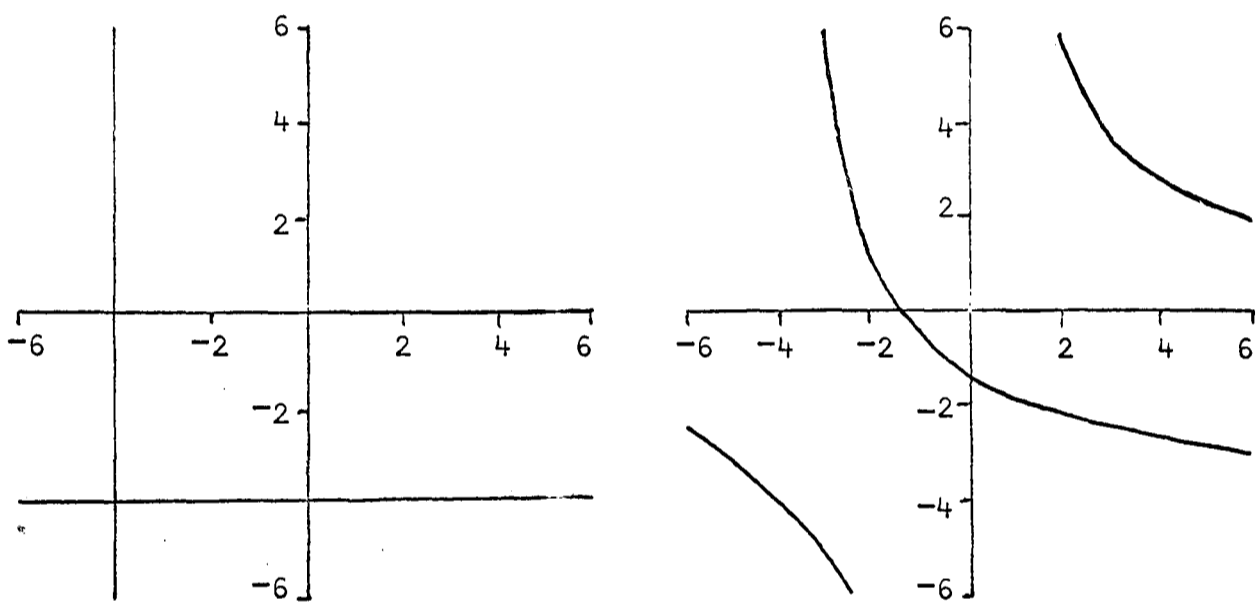


FIG. 4.3

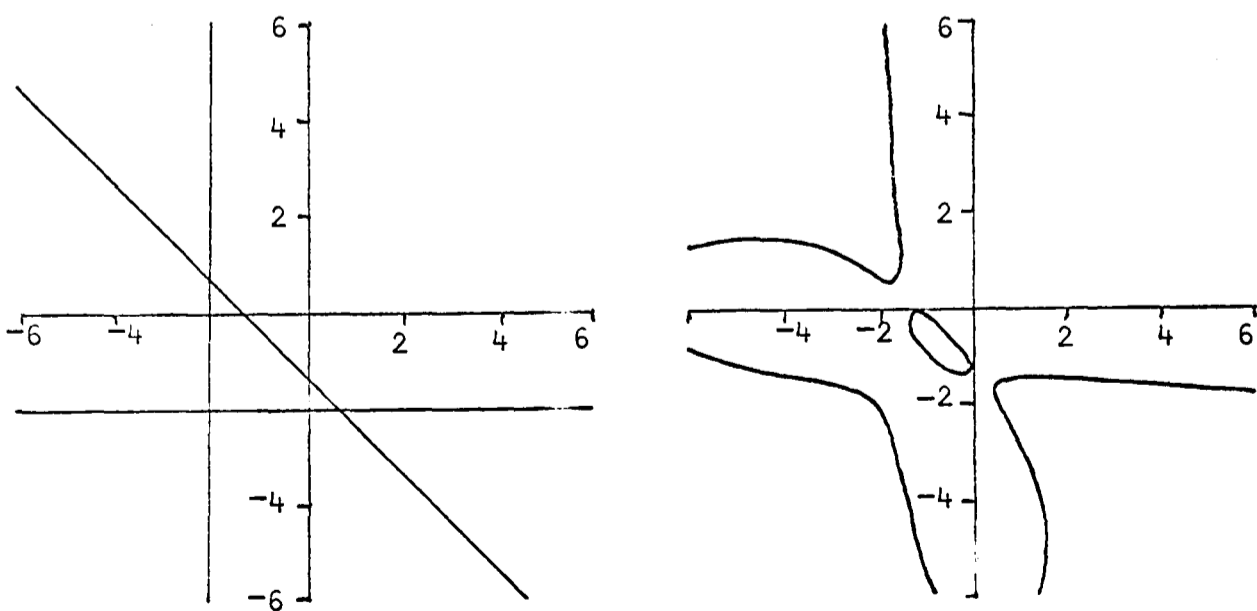


FIG. 4.4

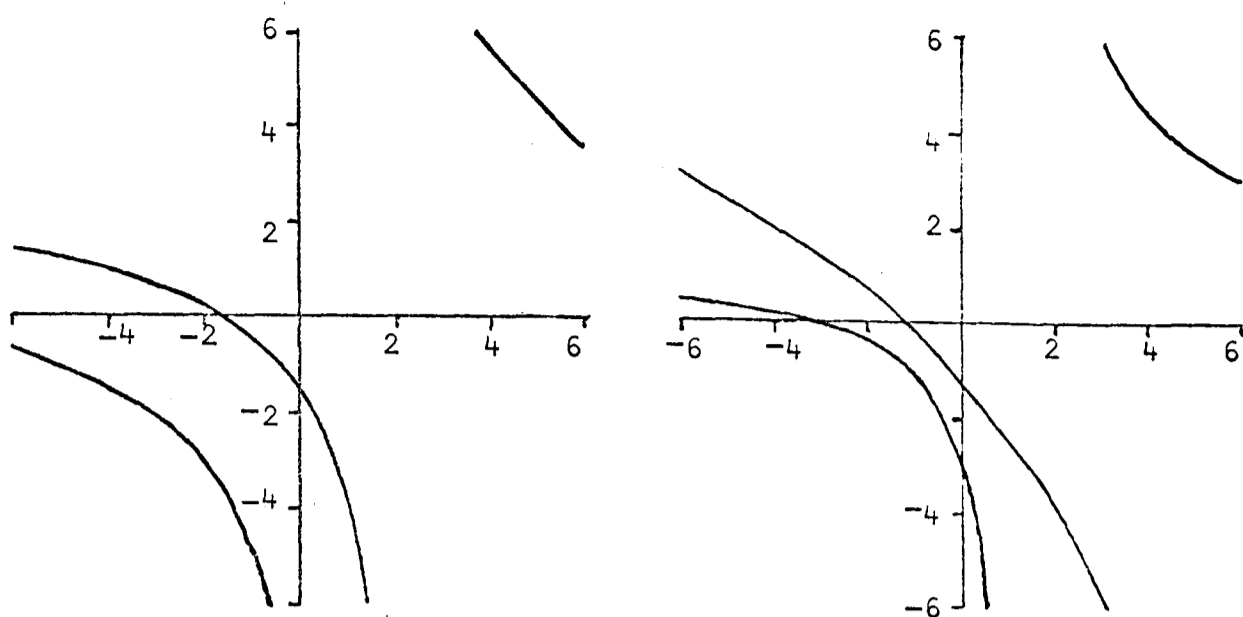


FIG. 4.5

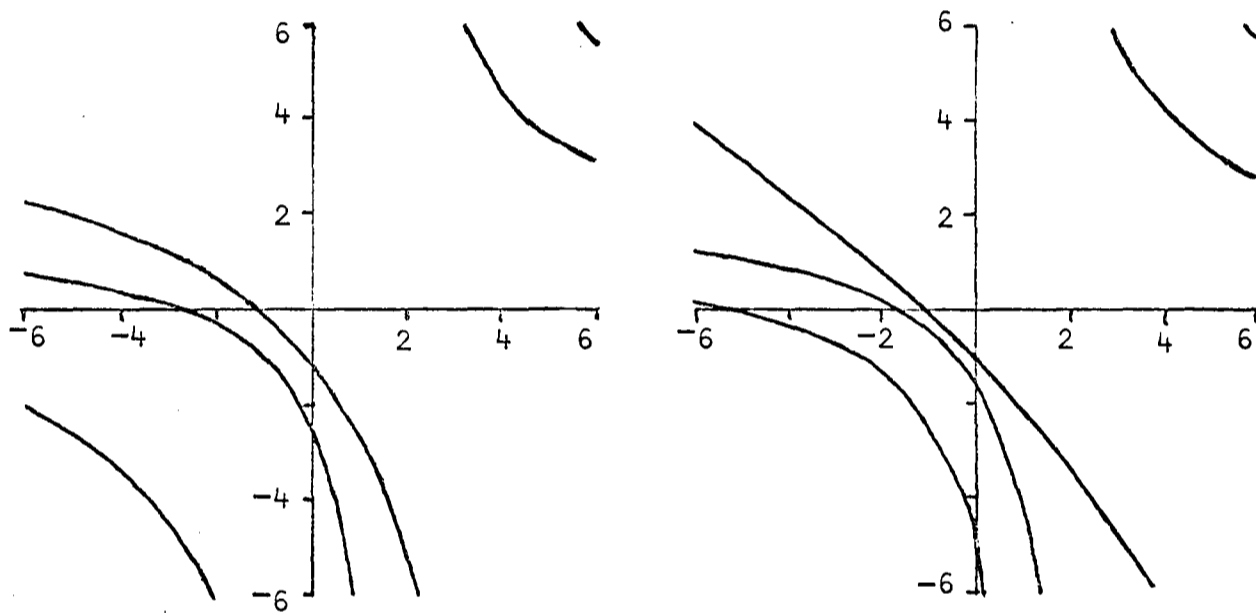


FIG. 4.6

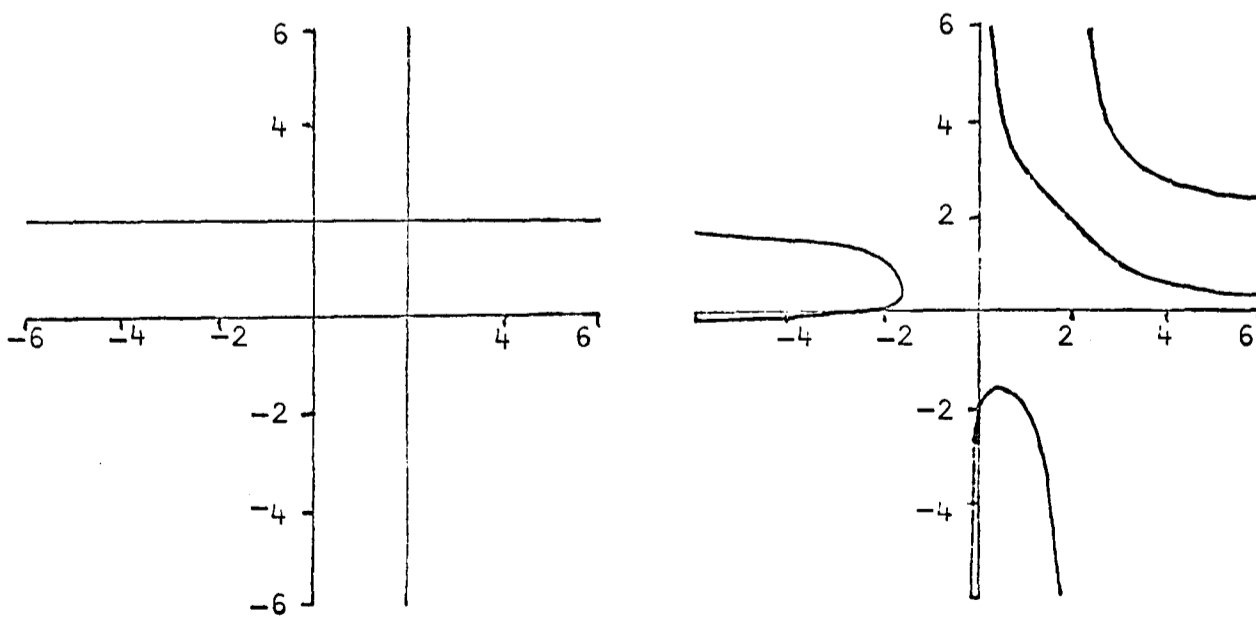


FIG. 4.7

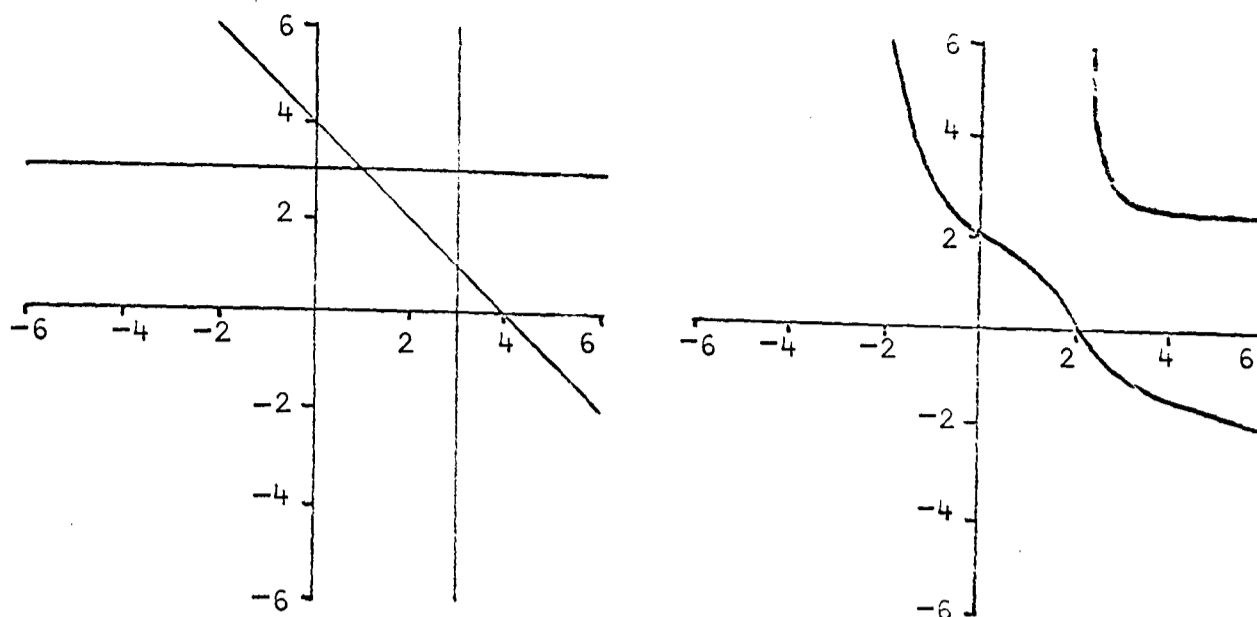


FIG. 4.8

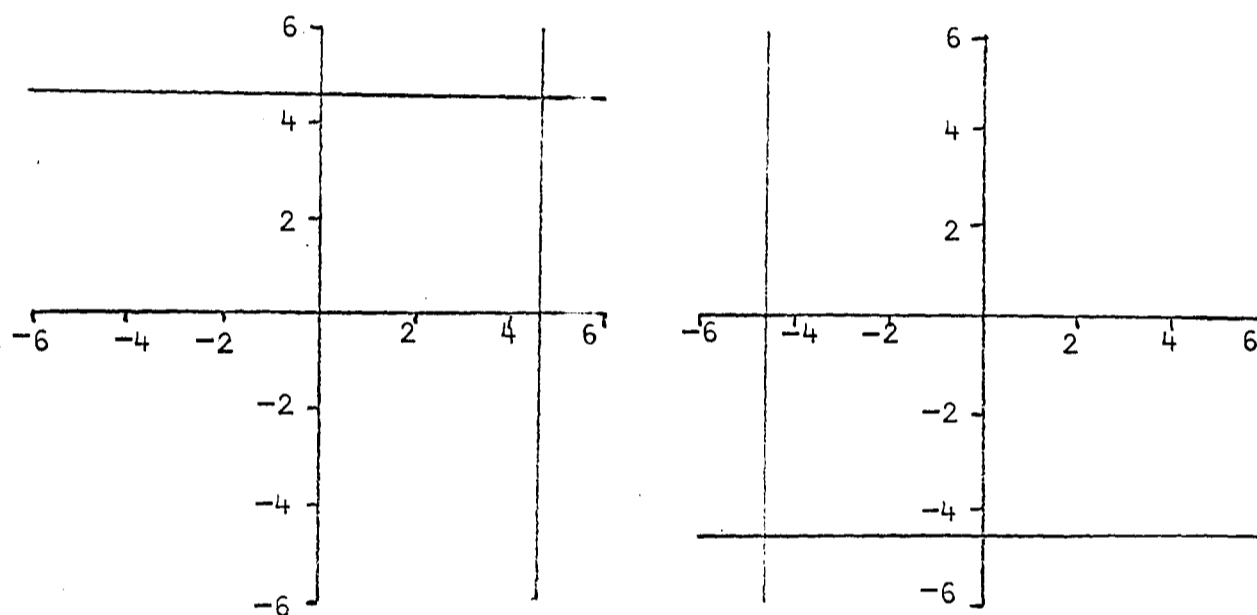


FIG. 4.9

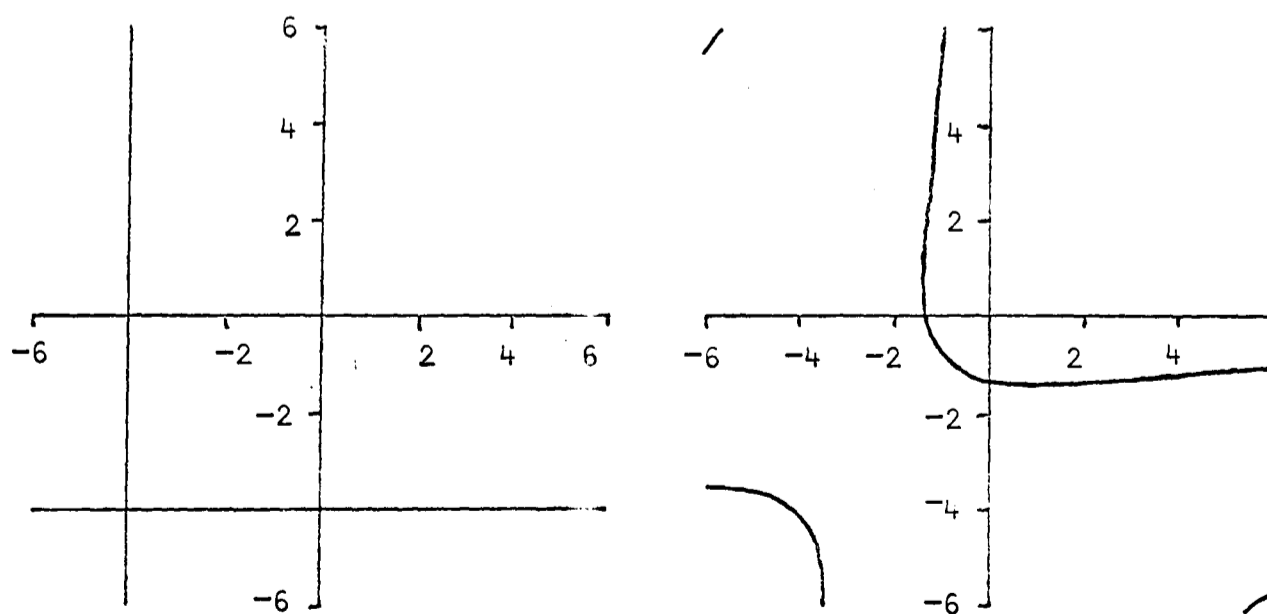


FIG. 4.10

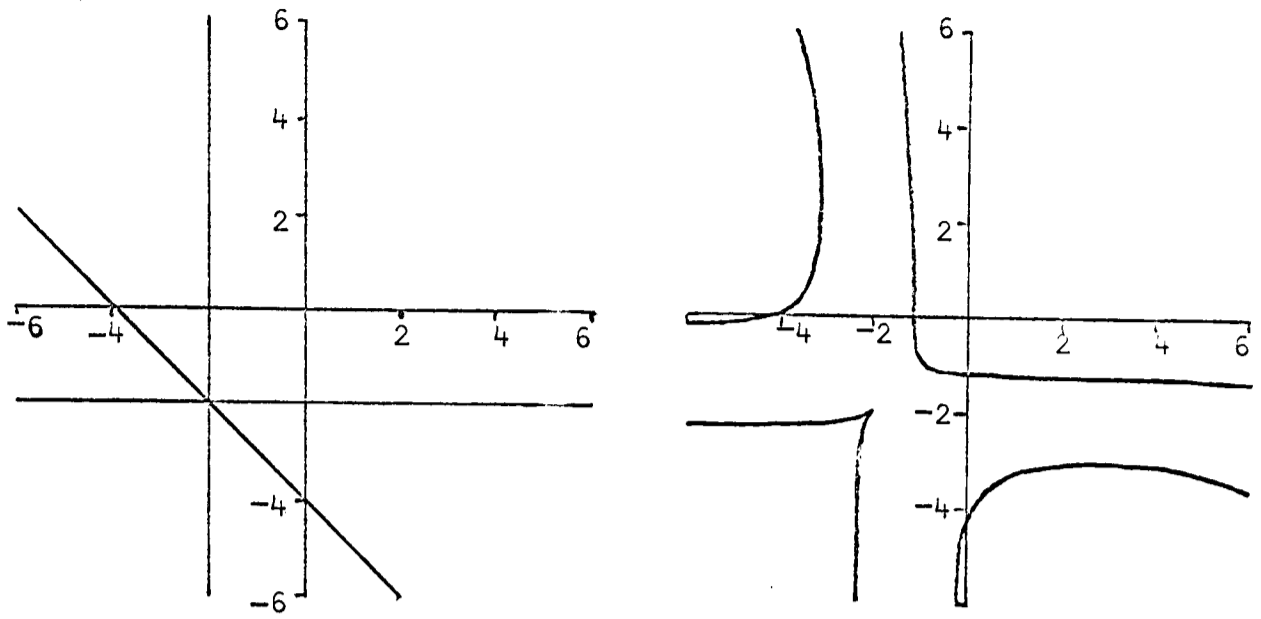


FIG. 4.11

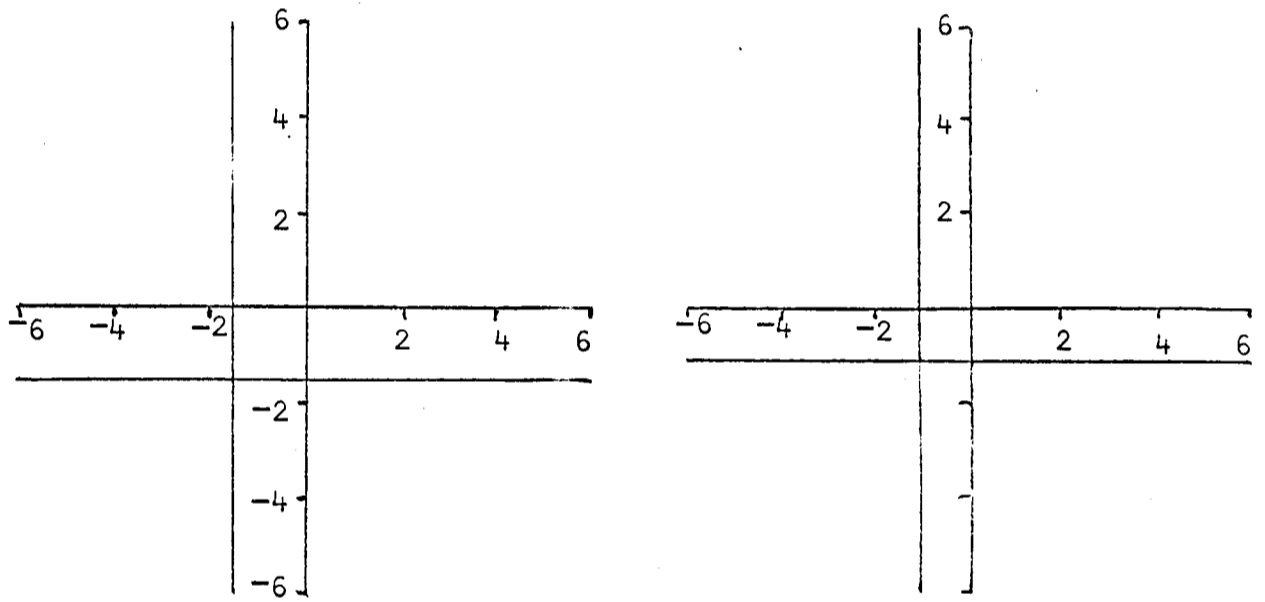


FIG. 4.12

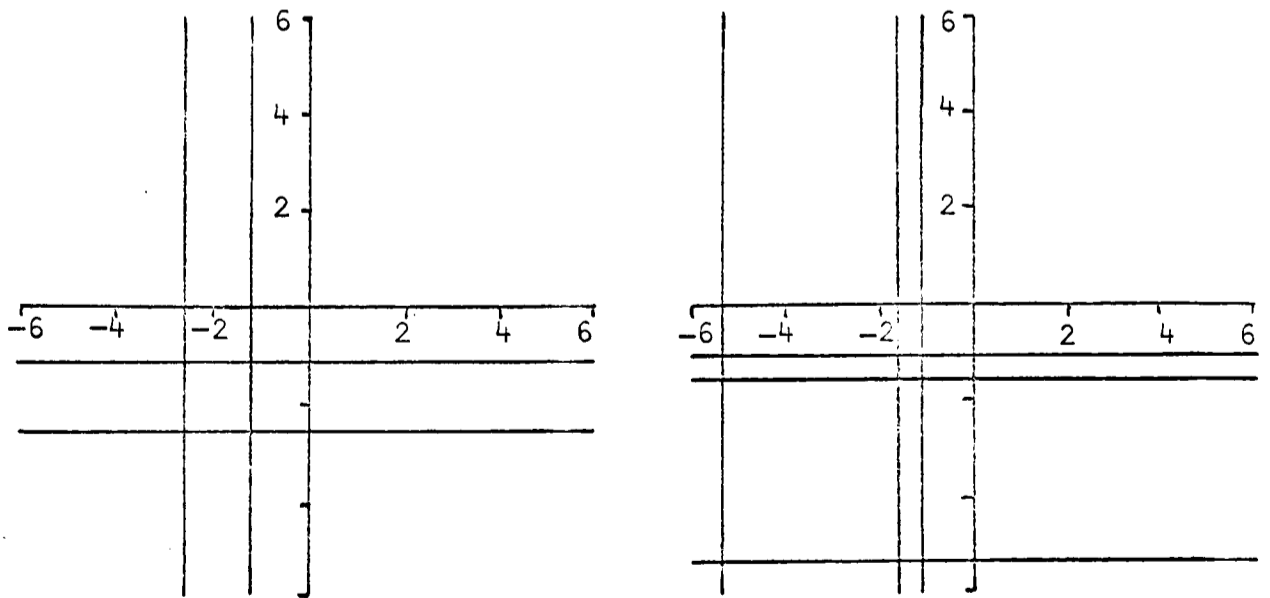


FIG. 4.13

We will now briefly consider functions of two variables that have no S_2 -fraction expansion. As an example, we consider the function $\sinh(x+y)$ for which Chisholm approximants can be obtained. This function has no single S_2 -fraction expansion but may be expressed in the form

$$\sinh(x+y) = x \left\{ \frac{\sinh x \cosh y}{x} \right\} + y \left\{ \frac{\sinh y \cosh x}{y} \right\} \quad (4.86)$$

where the functions $(\sinh x \cosh y)/x$ and $(\sinh y \cosh x)/y$ both have S_2 -fraction expansions in the variables x^2 and y^2 .

We may generalise this idea by defining an odd function of two variables by

$$f(-x,-y) = -f(x,y) , \quad (4.87)$$

and an even function by

$$f(-x,-y) = f(x,y) . \quad (4.88)$$

Neither odd nor even functions have S_2 -fraction expansions but their double series expansions can often be "partitioned" in such a way that an odd function can be expressed in the form

$$f(x,y) = x u(x^2,y^2) + y v(x^2,y^2) , \quad (4.89)$$

and an even function may be written

$$f(x,y) = u(x^2,y^2) + xy v(x^2,y^2) , \quad (4.90)$$

where u and v have S_2 -fraction expansions in each case. Similar "partitioning" may be useful with other types of function. There is a slight risk, however, that additional singularities may be introduced by this process. An alternative method is to

approximate to $f(x,y)$ by forming the S_2 -fraction for $f(x,y)+g(x,y)$ where $g(x,y)$ is any suitable function such that the S_2 -fraction expansion exists. The drawback of this technique is that a poor choice of $g(x,y)$ may lead to difficulties. The fraction may be slowly convergent, or if $|g(x,y)| \gg |f(x,y)|$ in some region of the xy -domain then the value of $f(x,y)$ will be lost in that region.

We will now conclude this chapter with an example of the approximation of a "non-trivial" function of two variables, i.e. a function that cannot be more easily represented in terms of functions of single variables. Such a "non-trivial" function is Appell's hypergeometric function in two variables, defined by

$$F_1(\alpha; \beta, \beta'; \gamma; x, y) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(\beta')} \cdot \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\Gamma(\alpha+m+n)\Gamma(\beta+m)\Gamma(\beta'+n)}{\Gamma(\gamma+m+n)} \frac{x^m y^n}{m!n!} \quad (4.91)$$

and satisfying the pair of partial differential equations

$$x(1-x) \frac{\partial^2 F_1}{\partial x^2} + y(1-x) \frac{\partial^2 F_1}{\partial x \partial y} + \{\gamma - (\alpha + \beta + 1)x\} \frac{\partial F_1}{\partial x} - \beta y \frac{\partial F_1}{\partial y} - \alpha \beta F_1 = \quad (4.92)$$

and

$$y(1-y) \frac{\partial^2 F_1}{\partial y^2} + x(1-y) \frac{\partial^2 F_1}{\partial x \partial y} + \{\gamma - (\alpha + \beta' + 1)y\} \frac{\partial F_1}{\partial y} - \beta' x \frac{\partial F_1}{\partial x} - \alpha \beta' F_1 = \quad (4.93)$$

This is one of four hypergeometric functions defined by Appell.

[See Whittaker and Watson (1927).] In the example in Table 4.8,

below, we make the arbitrary choice of parameters $\alpha = \frac{1}{2}$, $\beta = \frac{1}{4}$,

$\beta' = \frac{1}{2}$ and $\gamma = 1$.

TABLE 4.8

$$f(x,y) = F_1\left(\frac{1}{2}; \frac{1}{4}, \frac{1}{2}; 1; x, y\right) .$$

x	y	n	K_n	x	y	n	K_n
0.1	0.1	2	1.03896	1.0	1.0	4	1.45919
		3	1.038207			5	1.459691
		4	1.03821503			7	1.45962834
		5	1.03821506			9	1.45962805
0.1	0.2	2	1.0526	1.0	2.0	4	1.6568
		3	1.051257			5	1.65846
		4	1.05127653			7	1.6581276
		5	1.05127661			8	1.65812512
0.3	0.3	3	1.1189	2.0	2.0	5	2.1836
		4	1.1191600			8	2.1802394
		5	1.11916265			10	2.18023545
		6	1.11916254			13	2.18023527
0.5	0.5	3	1.2055	1.0	5.0	6	2.5512
		5	1.206689			9	2.550689
		6	1.20668788			12	2.55067838
		7	1.20668783			14	2.55067832
0.5	1.0	4	1.284832	3.0	3.0	9	3.5081
		5	1.284900			12	3.5078654
		7	1.28489343			15	3.50786165
		8	1.28489342			17	3.50786140

CHAPTER 5.

CORRESPONDING FRACTIONS IN MANY VARIABLES.

We will now show how the ideas in Chapter 4. may be generalised to functions of N variables. The investigation does not extend as far as that of the S_2 -fraction but is intended as a foundation for further research.

5.1 The Structure of the S_N -Fraction.

The S_2 -fraction is of the form

$$f_0(x,y) = \frac{c_{00}}{1+g_0(x)+h_0(y)} + \frac{c_{11}xy}{1+g_1(x)+h_1(y)} + \dots$$

$$\dots + \frac{c_{nn}xy}{1+g_n(x)+h_n(y)} + \dots \quad (5.1)$$

where $g_n(x)$ and $h_n(y)$ have both S-fraction and single power series expansions. An analogous continued fraction in three independent variables x, y and z would have the form

$$f_0(x,y,z) = \frac{c_{000}}{1+g_0(x)+h_0(y)+k_0(z)} + \frac{c_{111}xyz}{1+g_1(x)+h_1(y)+k_1(z)}$$

$$+ \frac{u_0(x,y)+v_0(y,z)+w_0(x,z)}{1+g_1(x)+h_1(y)+k_1(z)} + \frac{u_1(x,y)+v_1(y,z)+w_1(x,z)}{1+g_1(x)+h_1(y)+k_1(z)}$$

$$+ \dots + \frac{c_{nnn}xyz}{1+g_n(x)+h_n(y)+k_n(z)} + \dots \quad (5.2)$$

$$+ \frac{u_n(x,y)+v_n(y,z)+w_n(x,z)}{1+g_n(x)+h_n(y)+k_n(z)}$$

where $g_n(x)$, $h_n(y)$ and $k_n(z)$ have both S-fraction and single power series expansions and $u_n(x,y)$, $v_n(y,z)$ and $w_n(x,z)$ have

both S_2 -fraction and double power series expansions. The fraction (5.2), which we call an S_3 -fraction, will correspond to a triple power series. Clearly, the notation of (5.2) is too unwieldy and the formation of an S_N -fraction and its CS algorithm is only feasible if we can use a streamlined notation.

We consider a set of N independent variables $\{x_k\}$ and write

$$\underline{x} \equiv \{x_1, x_2, \dots, x_N\} \quad (5.3)$$

and we consider the function $f_0(\underline{x})$, formally defined by a Taylor series in N variables. We write the S_N -fraction in the form

$$f_0(\underline{x}) = \frac{c_0}{1+g_0(\underline{x})} + \frac{c_1 \prod_{k=1}^N x_k}{1+g_1(\underline{x})} + \frac{c_2 \prod_{k=1}^N x_k}{1+g_2(\underline{x})} + \dots$$

$$\dots + \frac{c_n \prod_{k=1}^N x_k}{1+g_n(\underline{x})} + \dots \quad (5.4)$$

where we abbreviate $c_{nn\dots n}$ to c_n and $g_n(\underline{x})$ denotes the sum of all the sub-fractions in the $(n+1)$ th partial denominator.

Now, the formal power series expansion of $g_n(\underline{x})$ can be written

$$g_n(\underline{x}) = \sum_{j_1=0}^{\infty} \sum_{j_2=0}^{\infty} \dots \sum_{j_N=0}^{\infty} b_{j_1 j_2 \dots j_N}^{(n)} \prod_{k=1}^N x_k^{j_k} \quad (5.5)$$

where $\prod_{k=1}^N j_k = 0$ and $b_{00\dots 0}^{(n)} = 0$. As this expression is

complicated we introduce an abbreviated notation using vector suffices. Writing

$$\underline{j} \equiv \{j_1, j_2, \dots, j_N\} \quad (5.6)$$

we can write (5.5) more succinctly as

$$g_n(\underline{x}) = \sum_{\underline{j}=0}^{\infty} b_{\underline{j}}^{(n)} \prod_{k=1}^N x_k^{j_k} \quad (5.7)$$

where $\prod_{k=1}^N j_k = 0$ and $b_0^{(n)} = 0$. The summation over the vector \underline{j} denotes N summations. The recurrence relations that give rise to the fraction (5.4) are

$$f_{n+1}(\underline{x}) = c_n \left(\prod_{k=1}^N x_k \right) f_{n-1}(\underline{x}) - \{1+g_n(\underline{x})\} f_n(\underline{x}) \quad (5.8)$$

for $n = 0, 1, 2, 3, \dots$ and where we set $f_{-1}(\underline{x}) = 1 / \left(\prod_{k=1}^N x_k \right)$.

Using notation similar to (5.7) we can write $f_n(\underline{x})$ in the series form

$$f_n(\underline{x}) = \prod_{m=1}^N x_m^n \sum_{\underline{i}=0}^{\infty} a_{\underline{i}}^{(n)} \prod_{k=1}^N x_k^{i_k} \quad (5.9)$$

for $n = 0, 1, 2, 3, \dots$.

We will now generalise the results in Section 4.1 to prove the existence, correspondence and uniqueness of S_N -fraction expansions. A necessary condition for the existence of the fraction (5.4) is the existence of a sequence $\{T_n(\underline{x})\}$ of functions, each having an expansion of the form

$$T_n(\underline{x}) = \sum_{\underline{i}=0}^{\infty} p_{\underline{i}}^{(n)} \prod_{k=1}^N x_k^{i_k}, \quad (5.10)$$

and satisfying the system of formal identities

$$T_n(\underline{x}) = \frac{1}{1+g_n(\underline{x})+c_{n+1} \prod_{k=1}^N x_k \cdot T_{n+1}(\underline{x})}, \quad (5.11)$$

for $n = 0, 1, 2, 3, \dots$ and where $f_0(\underline{x}) = c_0 T_0(\underline{x})$. We now assume the existence of $T_n(\underline{x})$ and $g_n(\underline{x})$ and note that $T_n(\underline{x})$ has a reciprocal series expansion

$$\frac{1}{T_n(\underline{x})} = \sum_{\underline{i}=0}^{\infty} d_{\underline{i}}^{(n)} \prod_{k=1}^N x_k^{i_k} \quad (5.12)$$

Rearranging (5.11) we get

$$T_{n+1}(\underline{x}) = \frac{1}{c_{n+1} \prod_{k=1}^N x_k} \left\{ \frac{1}{T_n(\underline{x})} - 1 - g_n(\underline{x}) \right\} \quad (5.13)$$

or, using (5.7) and (5.12),

$$T_{n+1}(\underline{x}) = \frac{1}{c_{n+1} \prod_{k=1}^N x_k} \left\{ \sum_{\underline{i}=0}^{\infty} d_{\underline{i}}^{(n)} \prod_{m=1}^N x_m^{i_m} - 1 - \sum_{\underline{j}=0}^{\infty} b_{\underline{j}}^{(n)} \prod_{m=1}^N x_m^{j_m} \right\} \quad (5.14)$$

where $\prod_{m=1}^N j_m = 0$ and $b_0^{(n)} = 0$. Now, choosing

$$d_0^{(n)} = 1, \quad d_{\underline{j}}^{(n)} = b_{\underline{j}}^{(n)}, \quad (5.15)$$

for $\underline{j} \neq 0$ and $\prod_{m=1}^N j_m = 0$, the identity (5.14) can be

simplified to

$$T_{n+1}(\underline{x}) = \frac{1}{c_{n+1}} \sum_{\underline{i}=0}^{\infty} d_{\underline{i}+1}^{(n)} \prod_{m=1}^N x_m^{i_m} \quad (5.16)$$

where the suffix $\underline{i}+1$ denotes the vector of elements $\{i_k+1\}$.

Thus, $T_{n+1}(\underline{x})$ can be expressed in the form (5.10).

Now, letting $A_n(\underline{x})/B_n(\underline{x})$ denote the n th convergent of the S_N -fraction (5.4) and using the result (1.23)

we have

$$f_0 - \frac{A_n}{B_n} = \frac{(-1)^n c_0 c_1 c_2 \dots c_n \prod_{k=1}^N x_k^n}{B_n (B_{n+1} + c_{n+1} \prod_{k=1}^N x_k \cdot T_{n+1} B_n)} \quad (5.17)$$

so that

$$f_0 - \frac{A_n}{B_n} = 0 \left\{ \left(\prod_{k=1}^N x_k \right)^n \right\} \quad (5.18)$$

Hence we have established existence and correspondence.

To establish uniqueness we consider the two S_N -fractions

$$f_0 = \frac{c_0}{1+g_0} + \frac{c_1 \prod_{k=1}^N x_k}{1+g_1} + \dots + \frac{c_n \prod_{k=1}^N x_k}{1+g_n} + \dots \quad (5.19)$$

and

$$f'_0 = \frac{c'_0}{1+g'_0} + \frac{c'_1 \prod_{k=1}^N x_k}{1+g'_1} + \dots + \frac{c'_n \prod_{k=1}^N x_k}{1+g'_n} + \dots \quad (5.20)$$

such that $f_0(\underline{x}) = f'_0(\underline{x})$. By setting each variable to zero in turn it is easily verified that $c_0 = c'_0$ and $g_0 = g'_0$, so that $A_1 = A'_1$ and $B_1 = B'_1$, where A'_n/B'_n is the n th convergent of (5.20). We also have $A_0 = A'_0 = 0$ and $B_0 = B'_0 = 1$ and we need to show that if

$$c_r = c'_r, \quad g_r = g'_r, \quad A_{r+1} = A'_{r+1}, \quad B_{r+1} = B'_{r+1} \quad (5.21)$$

for $r = 0, 1, 2, \dots, n-1$, then

$$c_n = c'_n, \quad g_n = g'_n \quad (5.22)$$

We consider the difference between the $(n+1)$ th convergents

$$\frac{A_{n+1}}{B_{n+1}} - \frac{A'_{n+1}}{B'_{n+1}} = \frac{A_{n+1}B'_{n+1} - A'_{n+1}B_{n+1}}{B_{n+1}B'_{n+1}} \quad (5.23)$$

Using the recurrence relations (1.8) and the hypothesis (5.21) we get

$$\begin{aligned} A_{n+1}B'_{n+1} - A'_{n+1}B_{n+1} &= \{(1+g_n)c'_n - (1+g'_n)c_n\} \\ &\quad \cdot (A_n B_{n-1} - A'_{n-1} B'_n) \prod_{k=1}^N x_k, \end{aligned} \quad (5.24)$$

or, using the determinant formula (1.11),

$$\begin{aligned} A_{n+1}B'_{n+1} - A'_{n+1}B_{n+1} &= \{(1+g_n)c'_n - (1+g'_n)c_n\} \\ &\quad \cdot O \left\{ \binom{N}{\prod_{k=1} x_k}^n \right\}. \end{aligned} \quad (5.25)$$

But, from (5.18) and (5.23), we have

$$A_{n+1}B'_{n+1} - A'_{n+1}B_{n+1} = O \left\{ \binom{N}{\prod_{k=1} x_k}^{n+1} \right\} \quad (5.26)$$

so it follows from (5.25) that

$$(1+g_n)c'_n - (1+g'_n)c_n \equiv 0 \quad (5.27)$$

This implies that result (5.22) holds and that $f_0(\underline{x})$ and $f'_0(\underline{x})$ both have the same coefficients. Hence we have proved the uniqueness of S_N -fraction expansions.

To define the approximants of the S_N -fraction we shall adopt the notation $O(\underline{x})^n$ to denote error terms of order

$$\prod_{k=1}^N x_k^{r_k} \quad \text{such that} \quad \sum_{k=1}^N r_k = n \quad \text{where} \quad r_k \geq 0 \quad \text{for} \quad k = 1, 2, \dots, N.$$

Then we define the sequence $\{K_n(\underline{x})\}$ of S_N -approximants by

$$f_0(\underline{x}) - K_n(\underline{x}) = O(\underline{x})^n . \quad (5.28)$$

The coefficients of S_N -fractions may be stored on a computer as an N -dimensional array and the values of the S_N -approximants evaluated by a generalisation of the algorithm (4.31). Ideally such an algorithm would be recursive, using the fact that each partial denominator of an S_N -fraction has $(2^{N-1}-2)$ sub-fractions. These sub-fractions are made up of

$$\left\{ \begin{array}{l} N \text{ } S\text{-fractions,} \\ \binom{N}{2} \text{ } S_2\text{-fractions,} \\ \dots \\ \binom{N}{r} \text{ } S_r\text{-fractions,} \\ \dots \\ N \text{ } S_{N-1}\text{-fractions.} \end{array} \right.$$

5.2 The Corresponding Sequence Algorithm for the S_N -Fraction.

We can most easily obtain the CS algorithm for the S_N -fraction by substituting the series expressions (5.7) and (5.9) in the recurrence relations (5.8). We have

$$\left(\prod_{m=1}^N x_m \right) \sum_{\underline{i}=0}^{\infty} a_{\underline{i}}^{(n+1)} \prod_{k=1}^N x_k^{i_k} = c_n \sum_{\underline{i}=0}^{\infty} a_{\underline{i}}^{(n-1)} \prod_{k=1}^N x_k^{i_k} - \left(1 + \sum_{\underline{j}=0}^{\infty} b_{\underline{j}}^{(n)} \prod_{m=1}^N x_m^{j_m} \right) \left(\sum_{\underline{i}=0}^{\infty} a_{\underline{i}}^{(n)} \prod_{k=1}^N x_k^{i_k} \right). \quad (5.29)$$

Equating coefficients of $\prod_{k=1}^N x_k^{i_k+1}$ in (5.29) we obtain the

summarised form of the CS algorithm

$$a_{\underline{i}}^{(n+1)} = c_n a_{\underline{i}+1}^{(n-1)} - a_{\underline{i}+1}^{(n)} - \sum_{\underline{j}=0}^{\underline{i}+1} b_{\underline{j}}^{(n)} a_{\underline{i}-\underline{j}+1}^{(n)} \quad (5.30)$$

where $\prod_{m=1}^N j_m = 0$ and $b_{\underline{0}}^{(n)} = 0$. We require that relation (5.30)

holds for $n = 0, 1, 2, 3, \dots$ and $i_k = -1, 0, 1, 2, 3, \dots$ so we

choose $a_{\underline{i}}^{(n)} = 0$ if any $i_k = -1$, $a_{\underline{0}}^{(-1)} = 1$ and $a_{\underline{i}}^{(-1)} = 0$

for $\underline{i} \neq \underline{0}$. In particular, if we choose $i_k = -1$ for $k = 1, 2, \dots, N$

we get from (5.30) that

$$c_n = \frac{a_{\underline{0}}^{(n)}}{a_{\underline{0}}^{(n-1)}} \quad (5.31)$$

for $n = 0, 1, 2, 3, \dots$ so it may easily be shown that the

CS algorithm breaks down only if the S_N -fraction does not exist.

Using the algorithm (5.30) the coefficients $\{c_{ijk}\}$ of the S_3 -fraction expansion of the function $1/\sqrt{(1+x)(1+y)(1+z)}$ were

found for $i+j+k \leq 6$. These coefficients are given in Table 5.1, below, and a selection of values of the S_3 -approximants are given in Table 5.2.

TABLE 5.1

Coefficients of S_3 -fraction
expansion of $1/\sqrt{(1+x)(1+y)(1+z)}$.

$$\{c_{ij0}\} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{16} & \frac{1}{4} & \frac{1}{4} & & \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{16} & & & \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & & & & \\ \frac{1}{4} & \frac{1}{4} & & & & & \\ \frac{1}{4} & & & & & & \end{bmatrix}$$

$$\{c_{ij1}\} = \begin{bmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{8} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{16} & \frac{1}{4} & & \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & & & \\ \frac{1}{4} & \frac{1}{4} & & & & \\ \frac{1}{4} & & & & & \end{bmatrix}$$

$$\{c_{ij2}\} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{16} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{16} & \frac{1}{4} & \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{64} & & \\ \frac{1}{4} & \frac{1}{4} & & & \\ \frac{1}{4} & & & & \end{bmatrix}$$

$$\{c_{ij3}\} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{16} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \\ \frac{1}{4} & \frac{1}{4} & & \\ \frac{1}{16} & & & \end{bmatrix}$$

$$\{c_{ij4}\} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \\ \frac{1}{4} & & \end{bmatrix}$$

$$\{c_{ij5}\} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{bmatrix}$$

$$c_{006} = \frac{1}{4}$$

TABLE 5.2

S_3 -approximants for $f(x,y,z) = 1/\sqrt{(1+x)(1+y)(1+z)}$.

x	y	z	n	$K_n(x,y,z)$	x	y	z	n	$K_n(x,y,z)$
1	1	1	4	0.320	1	2	2	4	0.18
			5	0.35390				5	0.2372
			6	0.35372				6	0.2364
			7	0.35387				7	0.2369
			8	0.353549				8	0.23566
			9	0.3535530				9	0.235702
			10	0.3535519				10	0.235690
			11	0.3535533				11	0.235699
			12	0.3535534				12	0.235701
			f	0.3535534				f	0.235702
1	1	2	4	0.245	2	2	2	4	0.138
			5	0.2895				5	0.1943
			6	0.2890				6	0.1937
			7	0.2893				7	0.1944
			8	0.288659				8	0.19236
			9	0.288675				9	0.192441
			10	0.288670				10	0.192416
			11	0.288674				11	0.192444
			12	0.288675				12	0.192446
			f	0.288675				f	0.192450

CHAPTER 6.

INTERPOLATORY FRACTIONS IN TWO AND MORE VARIABLES.

An important problem in applied mathematics is the interpolation to a function whose values are known at the intersection-points of a rectangular mesh. Such an array of function values may arise from a finite-difference solution of a P.D.E. problem. In this chapter we will show how the method outlined in Section 1.3 may be generalised to form continued fractions which interpolate on rectangular, cuboid or hypercuboid meshes.

6.1 Bivariate Interpolation on a Rectangular Mesh.

We consider first a set of function values F_0, F_1, \dots, F_n given at $(n+1)$ points $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ which lie on some monotonic curve in the real xy -plane.

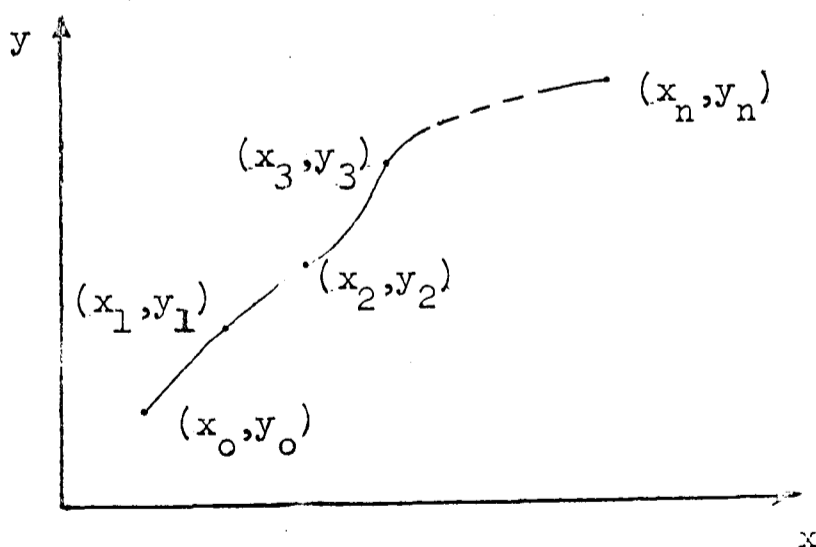


FIG. 6.1

A possible approach to the problem of interpolation is to construct a continued fraction, analogous to the fraction (1.74),

having the form

$$f(x,y) = c_0 + \frac{(x-x_0)(y-y_0)}{c_1} + \frac{(x-x_1)(y-y_1)}{c_2} + \dots$$

$$\dots + \frac{(x-x_{n-1})(y-y_{n-1})}{c_n} \quad (6.1)$$

Provided none of the points were unattainable this fraction would provide a means of interpolation in some region of the xy -plane. However, we shall not discuss such continued fractions except to observe that the formula (6.1) does not exist if any two of the points $\{(x_r, y_r)\}$ lie on a line $x = a$ or on a line $y = b$, where a and b are constants. Consequently, we cannot interpolate on a rectangular mesh using a continued fraction of the form (6.1) so we must consider a more general structure as we have done for corresponding fractions.

In fact, a continued fraction similar in structure to the S_2 -fraction is useful for rectangular mesh interpolation although special continued fractions may be constructed to cope with more general sets of points. We consider a double array of points $\{(x_i, y_j)\}$ which are the nodal points of a rectangular mesh in a quarter-plane, as shown below.

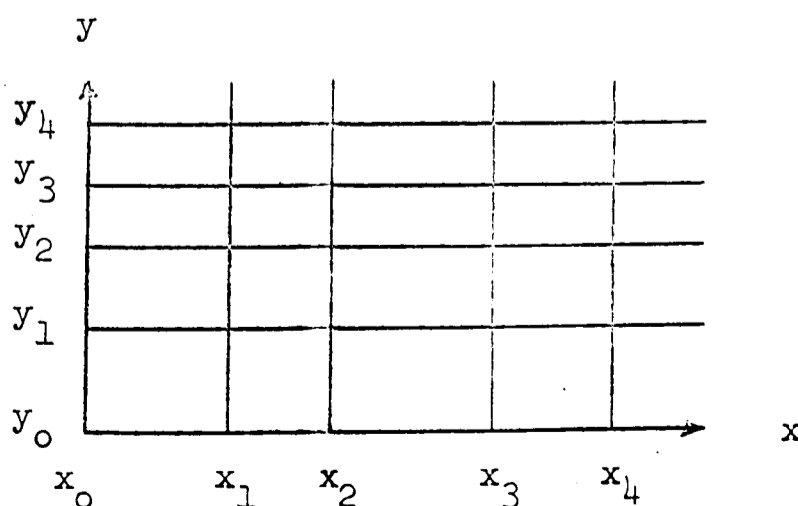


FIG. 6.2

We let $\{c_{ij}\}$ be a double array of coefficients to be determined and define the sequence of functions $\{w_n(x,y)\}$ by

$$w_n(x,y) = c_{nn} + g_n(x) + h_n(y) + \frac{(x-x_n)(y-y_n)}{w_{n+1}(x,y)} \quad (6.2)$$

for $n = 0, 1, 2, 3, \dots$ where

$$\left. \begin{aligned} c_{nn} + g_n(x) &= u_0^{(n)}(x) \\ c_{nn} + h_n(y) &= v_0^{(n)}(y) \end{aligned} \right\} \quad (6.3)$$

such that $g_n(x_n) = h_n(y_n) = 0$ and

$$\left. \begin{aligned} u_r^{(n)}(x) &= u_r^{(n)}(x_{n+r}) + \frac{x-x_{n+r}}{u_{r+1}^{(n)}(x)} \\ v_r^{(n)}(y) &= v_r^{(n)}(y_{n+r}) + \frac{y-y_{n+r}}{v_{r+1}^{(n)}(y)} \end{aligned} \right\} \quad (6.4)$$

for $n = 0, 1, 2, 3, \dots$ and $r = 0, 1, 2, 3, \dots$. The recurrence formulae (6.2), (6.3) and (6.4) lead to the continued fraction

$$\begin{aligned} f(x,y) &= c_{00} + g_0(x) + h_0(y) + \frac{(x-x_0)(y-y_0)}{c_{11} + g_1(x) + h_1(y)} + \\ &+ \frac{(x-x_1)(y-y_1)}{c_{22} + g_2(x) + h_2(y)} + \dots + \frac{(x-x_{n-1})(y-y_{n-1})}{c_{nn} + g_n(x) + h_n(y)} + \dots, \end{aligned} \quad (6.5)$$

where $f(x,y) = w_0(x,y)$ and the sub-fractions may be written

$$\left. \begin{aligned} g_n(x) &= \frac{x-x_n}{c_{n+1,n}} + \frac{x-x_{n+1}}{c_{n+2,n}} + \dots + \frac{x-x_{n+r-1}}{c_{n+r,n}} + \dots \\ h_n(y) &= \frac{y-y_n}{c_{n,n+1}} + \frac{y-y_{n+1}}{c_{n,n+2}} + \dots + \frac{y-y_{n+r-1}}{c_{n,n+r}} + \dots \end{aligned} \right\} \quad (6.6)$$

From (6.2) we have

$$c_{nn} = w_n(x_n, y_n) \quad , \quad (6.7)$$

and comparing (6.4) and (6.6) we get

$$\left. \begin{aligned} c_{n+r,n} &= u_r^{(n)}(x_{n+r}) \quad , \\ c_{n,n+r} &= v_r^{(n)}(y_{n+r}) \quad , \end{aligned} \right\} \quad (6.8)$$

for $n = 0, 1, 2, 3, \dots$ and $r = 0, 1, 2, 3, \dots$. Also,

rearranging (6.2) we have

$$w_{n+1}(x, y) = \frac{(x-x_n)(y-y_n)}{w_n(x, y) - w_n(x_n, y_n) - g_n(x) - h_n(y)} \quad , \quad (6.9)$$

which leads to a two-variable inverse difference scheme.

For the nodal values of the functions $\{w_n(x, y)\}$ we now use the abbreviated notation

$$f_{ij}^{(n)} = w_n(x_i, y_j) \quad (6.10)$$

and we describe how to proceed systematically to calculate the coefficients $\{c_{ij}\}$.

Beginning with the double array of function values $\{f_{ij}^{(0)}\}$, we have $c_{00} = f_{00}^{(0)}$ and we compute the coefficients $c_{10}, c_{20}, c_{30}, \dots$ from the function values $f_{00}^{(0)}, f_{10}^{(0)}, f_{20}^{(0)}, f_{30}^{(0)}, \dots$ using the one-variable algorithm defined by (1.78) and (1.79). Similarly, we compute $c_{01}, c_{02}, c_{03}, \dots$ from the values $f_{00}^{(0)}, f_{01}^{(0)}, f_{02}^{(0)}, f_{03}^{(0)}, \dots$. Discarding the first row and column of mesh points we use (6.9) to form the new array $\{f_{ij}^{(1)}\}$ for $i = 1, 2, 3, \dots$ and $j = 1, 2, 3, \dots$. We then compute the coefficients $c_{11}, c_{21}, c_{31}, c_{41}, \dots$

and $c_{12}, c_{13}, c_{14}, \dots$. In general we proceed to the array $\{f_{ij}^{(n)}\}$ for $i = n, n+1, n+2, \dots$ and $j = n, n+1, n+2, \dots$ and we note that

$$\left. \begin{aligned} g_n(x_i) &= f_{in}^{(n)} - f_{nn}^{(n)}, \\ h_n(y_j) &= f_{nj}^{(n)} - f_{nn}^{(n)}. \end{aligned} \right\} \quad (6.11)$$

so we may write (6.9) in the form

$$f_{ij}^{(n+1)} = \frac{(x_i - x_n)(y_j - y_n)}{f_{ij}^{(n)} + f_{nn}^{(n)} - f_{in}^{(n)} - f_{nj}^{(n)}} \quad (6.12)$$

when x and y have nodal values.

So far we have considered a rectangular mesh in a quarter-plane. However, in a practical problem we are generally concerned with some finite region R covered by a rectangular mesh over which we wish to interpolate to some function. We must now investigate the class of finite regions R over which we can interpolate using only one continued fraction expression of the form (6.5). Firstly, it is implied by formula (6.12) that if a point $(x_i, y_j) \in R$ then all points $(x_p, y_q) \in R$ for $p = 0, 1, 2, \dots, i$ and $q = 0, 1, 2, \dots, j$. Clearly, this is too restrictive in practical applications so we must form alternative expressions to (6.12) to cover the cases when the computations break down.

If we wish to compute $f_{ij}^{(n+1)}$ and the point $(x_i, y_n) \notin R$ then we use the formula

$$f_{ij}^{(n+1)} = \frac{(x_i - x_n)(y_j - y_n)}{f_{ij}^{(n)} - f_{nj}^{(n)}} \quad (6.13)$$

Similarly, if the point $(x_n, y_j) \notin R$ then we use

$$f_{ij}^{(n+1)} = \frac{(x_i - x_n)(y_j - y_n)}{f_{ij}^{(n)} - f_{in}^{(n)}} \quad (6.14)$$

However, if both $(x_i, y_n) \notin R$ and $(x_n, y_j) \notin R$ then we use

$$f_{ij}^{(n+1)} = \frac{(x_i - x_n)(y_j - y_n)}{f_{ij}^{(n)} - f_{nn}^{(n)}} \quad (6.15)$$

in which we require that $(x_n, y_n) \in R$.

By considering the form of the interpolatory fraction (6.5) and the conditions under which the formulae (6.12) - (6.15) are valid we can describe the most general form that the region R may take.

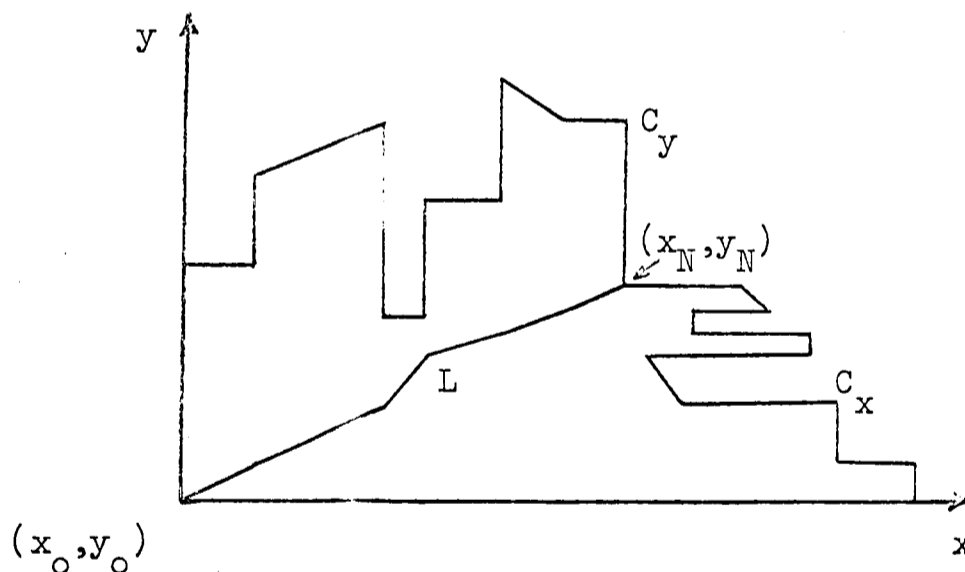


FIG. 6.3

In Fig. 6.3 the finite closed region R is bounded by the contours C_x and C_y which form the perimeter of a rectangular mesh, possibly triangular at the boundary. These contours meet at the points (x_0, y_0) and (x_N, y_N) and the contour L joins the points $\{(x_r, y_r)\}$ for $r = 0, 1, 2, \dots, N$. Necessary

conditions for interpolation over R using only one continued fraction of the form (6.5) are:

- (i) The contour L lies entirely inside R , or on its boundary.
- (ii) The contour C_y is single-valued with respect to x , except when its gradient is infinite.
- (iii) The contour C_x is single-valued with respect to y , except when its gradient is zero.

More general regions of interpolation may also be dealt with by modifying the structure of the fraction (6.5). It has been found empirically that the accuracy of the interpolation formula is largely unaffected by the choice of the point (x_0, y_0) although some choices are inadmissible, as we shall see. However, points may be reordered as in the one-variable case and (x_0, y_0) may be an internal point of the region R . If large problems are attempted with very many mesh points it may be advisable to use more than one interpolatory fraction to save rounding error. Also, as in the one-variable case, we expect that some problems will have unattainable points or give rise to fractions with unwanted singularities.

We now give a selection of examples. Except where otherwise stated, the values of the function $F(x, y)$ are specified accurate to approximately 20 significant figures at the mesh points, and square regions of interpolation are sub-divided into smaller squares of side h . The numerical results, in Tables 6.1 - 6.6 below, include some unsuccessful examples to illustrate the

limitations of the method. The functions chosen are:

- (i) $F(x,y) = \cos x \sin y$, interpolated over the unit square $0 \leq x \leq 1$, $0 \leq y \leq 1$ with h successively equal to $1/4$, $1/8$ and $1/16$. Results are evaluated at points which are at various distances from mesh points.
- (ii) Two functions interpolated over the L-shaped region shown in Fig. 6.4. The region is divided into squares with $h = 0.1$.

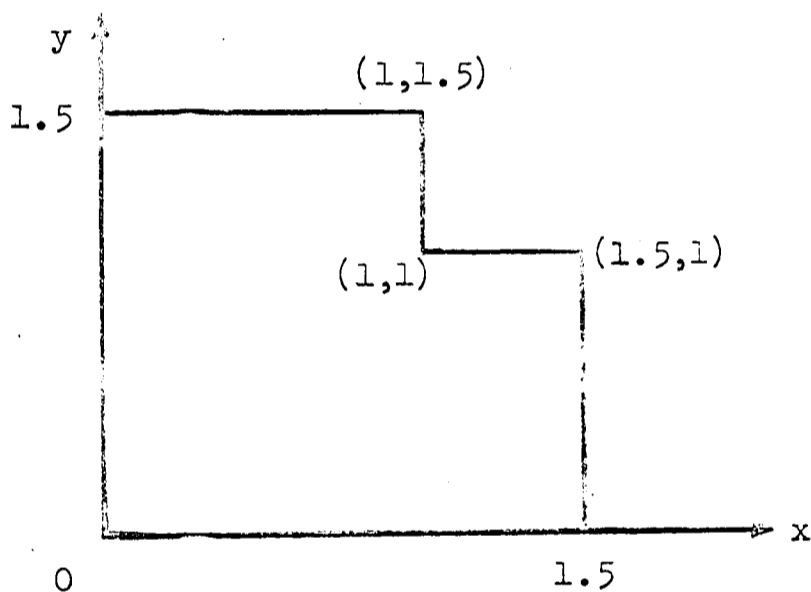


FIG. 6.4

The functions are:

- (a) $F(x,y) = e^{-x} \cos y$, which is regular over the whole region.
- (b) $F(x,y) = \{(1-x)^2 + (1-y)^2\}^{\frac{1}{3}} \cos\left\{\frac{2}{3} \tan^{-1}\left(\frac{1-y}{1-x}\right)\right\}$,

which is harmonic, finite and continuous over the whole region but with singularities in its derivatives at the re-entrant corner $(1,1)$.

Results are evaluated near to the point $(1,1)$ in both cases.

(iii) Four functions with point singularities on or outside the boundary of a rectangular region of interpolation. These are:

(a) $F(x,y) = e^{-x} \cos y / \sqrt{(x-0.1)^2 + (y-0.045)^2}$,
interpolated over the square $0 \leq x \leq 0.1$,
 $0 \leq y \leq 0.1$ with $h = 0.01$. Results are
evaluated at a selection of points, including
the singularity at $(0.1, 0.045)$.

(b) $F(x,y) = e^{-x} \cos y / \{(x-0.1)^2 + (y-0.045)^2\}$,
interpolated over the same region as (a).

(c) $F(x,y) = e^{-x} \cos y / \{(x-0.105)^2 + (y-0.045)^2\}$,
interpolated over the same region as (a).

The singularity lies just outside the region.

(d) The same function as (c), interpolated over the
rectangle $0 \leq x \leq 0.1$, $0 \leq y \leq 0.05$ which is
sub-divided into smaller rectangles with $h = 0.01$
and $k = 0.005$. The singularity lies outside
the region and near to a corner.

(iv) Two functions with line singularities just outside the
boundary of a square region of interpolation. These are:

(a) $F(x,y) = e^{-x} \cos y / (0.105-x)$, interpolated over
the square $0 \leq x \leq 0.1$, $0 \leq y \leq 0.1$ with $h = 0.01$.

(b) $F(x,y) = e^{-x} \cos y / \{(0.105-x)(0.105-y)\}$, interpolated
over the same region as (a).

(v) $F(x,y) = \log(x+2) e^{-y}$, interpolated over the square $0 \leq x \leq 0.5$, $0 \leq y \leq 0.5$ with $h = 0.05$.

The values of $F(x,y)$ are specified to

(a) 4 decimal places, and

(b) 6 decimal places,

as might arise from a finite-difference solution of a boundary-value problem.

(vi) $F(x,y) = e^{-x} \cos y$, interpolated over the unit square $0 \leq x \leq 1$, $0 \leq y \leq 1$ with $h = 0.1$. Results are evaluated both inside and outside the region of interpolation.

TABLE 6.1

Example (i).				$F(x,y) = \cos x \sin y$			
x	y	h	Interpolant	x	y	h	Interpolant
0.1	0.1	1/4	0.09976	0.3	0.5	1/4	0.4978245
		1/8	0.099666333412			1/8	0.497821359652
		1/16	0.0996663334924674			1/16	0.49782135964978353
		F	0.0996663334924677			F	0.49782135964978354
0.4	0.1	1/4	0.09235	0.9	0.5	1/4	0.323931
		1/8	0.09225968626			1/8	0.323918036302
		1/16	0.09225968633959600			1/16	0.3239180363133665073
		F	0.09225968633959604			F	0.3239180363133665076
0.5	0.1	1/4	0.087986	0.4	0.7	1/4	0.698729
		1/8	0.087904593026			1/8	0.698701858471
		1/16	0.0879045930989681222			1/16	0.6987018584553260455
		F	0.0879045930989681226			F	0.6987018584553260462
0.7	0.1	1/4	0.076682	0.7	0.7	1/4	0.58021
		1/8	0.076611756115			1/8	0.580196817766
		1/16	0.07661175617835403			1/16	0.580196817755370565
		F	0.07661175617835401			F	0.580196817755370564
0.9	0.1	1/4	0.06233	0.2	0.9	1/4	1.00596
		1/8	0.06226465025			1/8	1.00605473453
		1/16	0.06226465030172394			1/16	1.00605473446350329
		F	0.06226465030172392			F	1.00605473446350331
0.3	0.3	1/4	0.290898	0.5	0.9	1/4	0.90078
		1/8	0.29091934799			1/8	0.90085317804
		1/16	0.2909193480119365			1/16	0.9008531779721276056
		F	0.2909193480119371			F	0.9008531779721276064
0.6	0.3	1/4	0.251309	0.6	0.9	1/4	0.84714
		1/8	0.251331443631			1/8	0.847220813094
		1/16	0.2513314436461836			1/16	0.8472208130257737771
		F	0.2513314436461832			F	0.8472208130257737776
0.9	0.3	1/4	0.189286	0.9	0.9	1/4	0.638064
		1/8	0.189292849931			1/8	0.63809302933
		1/16	0.1892928499489957787			1/16	0.63809302929689140021
		F	0.1892928499489957790			F	0.63809302929689140029

TABLE 6.2

Example (ii).

(a) $F(x,y) = e^{-x} \cos y$

(b) $F(x,y) = \{(1-x)^2 + (1-y)^2\}^{\frac{1}{2}} \cdot \cos \left\{ \frac{2}{3} \tan^{-1} \left(\frac{1-y}{1-x} \right) \right\}$

x	y			x	y		
0.8	0.875	Int	0.288018454280064	0.8	0.875	Int	0.355518
		F	0.288018454280082			F	0.355565
0.8	1.125	Int	0.193740097615	0.8	1.125	Int	0.3569
		F	0.193740097644			F	0.3556
0.8	1.25	Int	0.14168346999	0.8	1.25	Int	0.386933
		F	0.14168347046			F	0.386947
0.8	1.375	Int	0.087415916	0.8	1.375	Int	0.4247600
		F	0.087415920			F	0.4247680
0.9	0.875	Int	0.260609874517860	0.9	0.875	Int	0.2485
		F	0.260609874517877			F	0.2438
0.9	1.125	Int	0.175303289696	0.9	1.125	Int	0.203
		F	0.175303289723			F	0.244
0.9	1.25	Int	0.12820050516	0.9	1.25	Int	0.29237
		F	0.12820050559			F	0.29244
0.9	1.375	Int	0.0790971921	0.9	1.375	Int	0.341664
		F	0.0790971954			F	0.341680
0.95	0.875	Int	0.247899780957910	0.95	0.875	Int	0.196
		F	0.247899780957926			F	0.184
0.95	1.0	Int	0.2089570667468796	0.95	1.0	Int	0.142
		F	0.2089570667468795			F	0.136
0.95	1.125	Int	0.166753647371	0.95	1.125	Int	0.23
		F	0.166753647397			F	0.18
0.95	1.25	Int	0.1219480927	0.95	1.25	Int	0.2493
		F	0.1219480932			F	0.2450
0.95	1.375	Int	0.0752395765	0.95	1.375	Int	0.3023
		F	0.0752395797			F	0.3005
0.95	1.5	Int	0.027356960	0.95	1.5	Int	0.3529
		F	0.027356978			F	0.3517

Int = Interpolant

TABLE 6.3

Example (iii).

(a) $F(x,y) = e^{-x} \cos y / \sqrt{(x-0.1)^2 + (y-0.045)^2}$

(b) $F(x,y) = e^{-x} \cos y / \{(x-0.1)^2 + (y-0.045)^2\}$

x	y		(a)	x	y		(b)
0.055	0.005	Int	15.72016	0.055	0.005	Int	261.0982
		F	15.72007			F	261.0961
0.075	0.005	Int	19.6698	0.075	0.005	Int	416.983
		F	19.6679			F	416.958
0.095	0.005	Int	22.576	0.095	0.005	Int	559.599
		F	22.558			F	559.607
0.085	0.035	Int	50.896	0.085	0.035	Int	2824.409
		F	50.919			F	2824.461
0.095	0.035	Int	89.0	0.095	0.035	Int	7274.4
		F	81.3			F	7270.5
0.1	0.035	Int	85.5	0.1	0.035	Int	9042.18
		F	90.4			F	9042.83
0.075	0.045	Int	36.97	0.075	0.045	Int	1482.93
		F	37.07			F	1482.89
0.085	0.045	Int	59.6	0.085	0.045	Int	4078.127
		F	61.2			F	4078.144
0.09	0.045	Int	93.1	0.09	0.045	Int	9130.73
		F	91.3			F	9130.06
0.095	0.045	Int	221.5	0.095	0.045	Int	35610.3
		F	181.7			F	36338.1
0.1	0.045	Int	547.3	0.1	0.045	Int	-1.2×10^8
		F	∞			F	∞
0.085	0.055	Int	54.8	0.085	0.055	Int	2821.31
		F	50.9			F	2821.92
0.095	0.055	Int	-178.4	0.095	0.055	Int	7002.3
		F	81.2			F	7264.0
0.1	0.055	Int	42.4	0.1	0.055	Int	9033.6
		F	90.3			F	9034.7
0.055	0.095	Int	13.90	0.055	0.095	Int	208.09
		F	14.01			F	208.22
0.075	0.095	Int	16.577	0.075	0.095	Int	297.2
		F	16.521			F	295.5
0.095	0.095	Int	18.90	0.095	0.095	Int	359.4
		F	18.02			F	358.5

TABLE 6.3 (continued)

Example (iii).			$F(x,y) = e^{-x} \cos y / \{(x-0.105)^2 + (y-0.045)^2\}$			
x	y	(c)	x	y	(d)	
0.055	0.005	Int 230.853 F 230.847	0.055	0.0025	Int 219.792671139 F 219.792671161	
0.075	0.005	Int 371.104 F 371.093	0.095	0.0025	Int 477.0471 F 477.0466	
0.095	0.005	Int 534.970 F 534.919	0.055	0.0275	Int 337.7150045 F 337.7150033	
0.085	0.035	Int 1835.88 F 1835.90	0.085	0.0375	Int 2011.80 F 2011.76	
0.095	0.035	Int 4543.78 F 4544.08	0.09	0.0375	Int 3247.2492 F 3247.2485	
0.1	0.035	Int 7233.9 F 7234.3	0.095	0.0375	Int 5807.7 F 5815.9	
0.075	0.045	Int 1029.7859 F 1029.7826	0.1	0.0375	Int 11128.684 F 11128.631	
0.085	0.045	Int 2293.976 F 2293.956	0.085	0.0425	Int 2258.991 F 2258.912	
0.09	0.045	Int 4057.90 F 4057.80	0.09	0.0425	Int 3948.5651 F 3948.5661	
0.095	0.045	Int 9090.9 F 9084.5	0.095	0.0425	Int 8523.3 F 8551.1	
0.1	0.045	Int 36166.0 F 36156.9	0.1	0.0425	Int 28928.22 F 28928.65	
0.085	0.055	Int 1834.199 F 1834.247	0.055	0.0475	Int 377.22404 F 377.22398	
0.095	0.055	Int 4552.3 F 4540.0	0.08	0.0475	Int 1460.713143 F 1460.713111	
0.1	0.055	Int 7227.17 F 7227.75	0.085	0.0475	Int 2258.53 F 2258.40	
0.055	0.095	Int 188.39 F 188.44	0.09	0.0475	Int 3947.680 F 3947.677	
0.075	0.095	Int 280.3 F 271.6	0.095	0.0475	Int 8507.9 F 8549.2	
0.095	0.095	Int 540.9 F 348.2	0.1	0.0475	Int 28923.3 F 28922.1	

TABLE 6.4

Example (iv).			(a) $F(x,y) = e^{-x} \cos y / (0.105-x)$		(b) $F(x,y) = e^{-x} \cos y / \{(0.105-x)(0.105-y)\}$	
x	y		(a)	(b)		
0.055	0.005	Int	18.92946633827564961792	189.29466338275649607		
		F	18.92946633827564961771	189.29466338275649618		
0.095	0.005	Int	90.9361567330232116	909.361567330232102		
		F	90.9361567330232134	909.361567330232134		
0.1	0.005	Int	180.965221518359505	1809.65221518359499		
		F	180.965221518359516	1809.65221518359516		
0.095	0.025	Int	90.908877022689345	1136.360962783616887		
		F	90.908877022689352	1136.360962783616899		
0.055	0.045	Int	18.91053986892252780	315.1756644820421249		
		F	18.91053986892252734	315.1756644820421223		
0.095	0.045	Int	90.845234973648630	1514.0872495608120		
		F	90.845234973648614	1514.0872495608102		
0.1	0.045	Int	180.78428494794383	3013.071415799072		
		F	180.78428494794375	3013.071415799063		
0.075	0.065	Int	30.85947727166297978	771.4869317915744997		
		F	30.85947727166297995	771.4869317915744988		
0.095	0.065	Int	90.745256041872059	2268.63140104680178		
		F	90.745256041872065	2268.63140104680163		
0.055	0.085	Int	18.8613605698124824	943.068028490624025		
		F	18.8613605698124806	943.068028490624031		
0.075	0.085	Int	30.81313434548423293	1540.656717274211652		
		F	30.81313434548423288	1540.656717274211644		
0.095	0.085	Int	90.608980217599392	4530.449010879972		
		F	90.608980217599383	4530.449010879969		
0.1	0.085	Int	180.314132086868577	9015.7066043434278		
		F	180.314132086868539	9015.7066043434269		
0.055	0.095	Int	18.8443468983158829	1884.434689831587999		
		F	18.8443468983158805	1884.434689831588050		
0.075	0.095	Int	30.7853397151024916	3078.53397151024912		
		F	30.7853397151024922	3078.53397151024922		
0.095	0.095	Int	90.527247438123670	9052.7247438123682		
		F	90.527247438123681	9052.7247438123688		
0.1	0.095	Int	180.151481815793603	18015.148181579352		
		F	180.151481815793685	18015.148181579369		

TABLE 6.5

Example (v).		$F(x,y) = \log(x+2) e^{-y}$					
x	y		x	y			
0.025	0.025	(a)	0.6881	0.225	0.275	(a)	0.6073
		(b)	0.688148			(b)	0.607487
		F	0.688149			F	0.607473
0.175	0.025	(a)	0.7579	0.275	0.275	(a)	0.6234
		(b)	0.757847			(b)	0.624376
		F	0.757844			F	0.624353
0.325	0.025	(a)	0.8230	0.025	0.325	(a)	0.5097
		(b)	0.822905			(b)	0.509793
		F	0.822889			F	0.509793
0.475	0.025	(a)	0.8835	0.175	0.325	(a)	0.5613
		(b)	0.883903			(b)	0.561421
		F	0.883865			F	0.561424
0.075	0.075	(a)	0.6772	0.325	0.325	(a)	0.6087
		(b)	0.677217			(b)	0.609621
		F	0.677217			F	0.609611
0.025	0.175	(a)	0.5922	0.475	0.325	(a)	0.6489
		(b)	0.592295			(b)	0.654755
		F	0.592295			F	0.654783
0.175	0.175	(a)	0.6523	0.425	0.425	(a)	0.5765
		(b)	0.652281			(b)	0.576961
		F	0.652282			F	0.579130
0.325	0.175	(a)	0.7080	0.025	0.475	(a)	0.4385
		(b)	0.708260			(b)	0.438783
		F	0.708267			F	0.438783
0.475	0.175	(a)	0.7577	0.175	0.475	(a)	0.4827
		(b)	0.760738			(b)	0.483220
		F	0.760750			F	0.483223
0.225	0.225	(a)	0.6385	0.325	0.475	(a)	0.5231
		(b)	0.638616			(b)	0.524834
		F	0.638619			F	0.524697
0.275	0.225	(a)	0.6556	0.475	0.475	(a)	0.5556
		(b)	0.656359			(b)	0.563596
		F	0.656364			F	0.563577

TABLE 6.6

Example (vi).		$F(x,y) = e^{-x} \cos y$					
Points inside the region:				Points outside the region:			
x	y			x	y		
0.05	0.05	Int	0.95004063541524	-0.35	-0.35	Int	1.3330333390
		F	0.95004063541544			F	1.3330333328
0.45	0.05	Int	0.63683128246727	1.45	-0.35	Int	0.2203489289
		F	0.63683128246741			F	0.2203489279
0.85	0.05	Int	0.42688077458039	-0.15	-0.15	Int	1.14878809668
		F	0.42688077458049			F	1.14878809657
0.05	0.45	Int	0.856531778964269	1.25	-0.15	Int	0.283287656853
		F	0.856531778964272			F	0.283287656825
0.45	0.45	Int	0.574150421506317	1.05	0.05	Int	0.349500418046716
		F	0.574150421506319			F	0.349500418046795
0.85	0.45	Int	0.38486453697496	-0.35	0.45	Int	1.277795262182
		F	0.38486453697498			F	1.277795262174
0.05	0.85	Int	0.62779538804031	1.45	0.45	Int	0.211218136206
		F	0.62779538804034			F	0.211218136212
0.45	0.85	Int	0.42082383341214	0.05	1.05	Int	0.473304221529
		F	0.42082383341216			F	0.473304221534
0.85	0.85	Int	0.28208665138572	1.05	1.05	Int	0.1741188925202
		F	0.28208665138574			F	0.1741188925221
				-0.15	1.25	Int	0.3663523169
						F	0.3663523181
				1.25	1.25	Int	0.09034136908
						F	0.09034136938
				-0.35	1.45	Int	0.171001536
						F	0.171001570
				1.45	1.45	Int	0.0282663637
						F	0.0282663693

In example (i) the origin [for interpolation purposes] was taken at the point (1,1) because the function $\cos x \sinh y$ is zero along the mesh line $y = 0$. In fact, the interpolatory fraction (6.5) does not exist if any of its sub-fractions is required to interpolate to a sequence of identical values. Results of similar accuracy to those in Table 6.1 were also obtained for the function $\cos x \sinh y$ by using (0,0) as origin and modifying the form of the interpolatory fraction. This device may be used for interpolation over a circular mesh in polar coordinates (r,θ) in which $r = 0$ is a single point.

In examples (iii)(b) and (iii)(c) the interpolation is unexpectedly inaccurate near the corner (0.1,0.1). This is presumably due to an unwanted singularity inside the region.

In example (v) the method is shown to be of great value when the data is known only to low accuracy. A single interpolatory fraction may thus be used as a global approximation to the solution of a partial differential equation.

In example (vi) the function $e^{-x} \cos y$ is successfully extrapolated outside the region of interpolation. This illustrates the main advantage of rational interpolation, namely, that the fraction approximates closely to the analytic structure of the function and not merely to its values at a few points.

From these examples it may be seen that the method works well for suitable smooth functions which are regular inside and near the interpolation region. The method is unsatisfactory near point

singularities or singularities in derivatives of the interpolated function although, in example (iv), the formula is good near line singularities outside the region of interpolation. In the successful examples results are generally best near the origin but are still good at more distant points.

6.2 Interpolation on Cuboid and Hypercuboid Meshes.

We will now generalise the method described in the previous section for interpolation in Euclidean N -space on a hypercuboid mesh. We adopt a similar notation to that used in Chapter 5. and consider N independent variables $\{x^{(k)}\}$ and write

$$\underline{x} = \{x^{(1)}, x^{(2)}, \dots, x^{(N)}\}. \quad (6.16)$$

We let the hypercuboid mesh occupy the region in which $x^{(k)} \geq x_0^{(k)}$ for $k = 1, 2, \dots, N$ and be defined by the abscissae $\{x_n^{(k)}\}$ for $n = 0, 1, 2, 3, \dots$. Again using a vector suffix notation, we let $\{c_{\underline{1}}\}$ be the array of coefficients to be determined and define the sequence of functions $\{w_n(\underline{x})\}$ by

$$w_n(\underline{x}) = c_n + g_n(\underline{x}) + \frac{\prod_{k=1}^N \{x^{(k)} - x_n^{(k)}\}}{w_{n+1}(\underline{x})} \quad (6.17)$$

where c_n denotes $c_{nn\dots n}$ and $g_n(\underline{x})$ is the sum of all sub-fractions in the n th partial denominator.

The definition (6.17) leads to the interpolatory fraction in N variables

$$f(\underline{x}) = c_0 + g_0(\underline{x}) + \frac{\prod_{k=1}^N \{x^{(k)} - x_0^{(k)}\}}{c_1 + g_1(\underline{x})} + \frac{\prod_{k=1}^N \{x^{(k)} - x_1^{(k)}\}}{c_2 + g_2(\underline{x})} + \dots + \frac{\prod_{k=1}^N \{x^{(k)} - x_{n-1}^{(k)}\}}{c_n + g_n(\underline{x})} + \dots \quad (6.18)$$

Also from (6.17) we have

$$c_n = w_n\left(\frac{x}{x_n}\right) \quad (6.19)$$

where

$$\underline{x}_n = \{x_n^{(1)}, x_n^{(2)}, \dots, x_n^{(N)}\}, \quad (6.20)$$

and if we adopt the notation

$$\underline{x}_j = \{x_{j_1}^{(1)}, x_{j_2}^{(2)}, \dots, x_{j_N}^{(N)}\} \quad (6.21)$$

then we have

$$g_n(\underline{x}_j) = w_n(\underline{x}_j) - w_n(\underline{x}_n) \quad (6.22)$$

for $n = 0, 1, 2, 3, \dots$ provided $\prod_{k=1}^N (j_k - n) = 0$. Rearranging

(6.17) and using (6.19) and (6.22) we obtain the generalised inverse difference scheme

$$w_{n+1}(\underline{x}_i) = \frac{\prod_{k=1}^N \{x_{i_k}^{(k)} - x_n^{(k)}\}}{w_n(\underline{x}_i) + (-1)^N w_n(\underline{x}_n) - \sum_{m=1}^{N-1} \sum_j (-1)^{N-m-1} w_n(\underline{x}_j)}, \quad (6.23)$$

where $\sum_j (-1)^{N-m-1} w_n(\underline{x}_j)$ denotes the sum over the $\binom{N}{m}$ values $w_n(\underline{x}_j)$ associated with the sub-fractions of order m , such that

(i) $j_k = i_k$ or $j_k = n$ for each k ,

(ii) $j \neq i$ and $j \neq n$.

In Table 6.7, below, is an example of continued fraction interpolation in three variables over a mesh of cubes. The function $F(x, y, z) = \cos x \sin(1-y) e^{-z}$ is interpolated over the cube $0 \leq x \leq \alpha$, $0 \leq y \leq \alpha$, $0 \leq z \leq \alpha$ with $h = 0.1$ and α successively equal to 0.4 and 0.6. The fraction was evaluated at the same points for each value of α . The increased accuracy illustrates the value of using a global, as opposed to a local, interpolation formula.

TABLE 6.7

$$F(x,y,z) = \cos x \sin(1-y) e^{-z} .$$

x	y	z	α	Interpolant
0.05	0.05	0.05	0.4	0.77277744
			0.6	0.772777792
			F	0.772777783
0.15	0.15	0.15	0.4	0.63937218
			0.6	0.6393720431
			F	0.6393720453
0.25	0.25	0.25	0.4	0.51435750
			0.6	0.5143576244
			F	0.5143576234
0.35	0.35	0.35	0.4	0.40061232
			0.6	0.4006120745
			F	0.4006120754
0.05	0.05	0.15	0.4	0.6992379
			0.6	0.699238262
			F	0.699238254
0.05	0.15	0.15	0.4	0.645824982
			0.6	0.6458249189
			F	0.6458249143
0.05	0.35	0.35	0.4	0.42593488
			0.6	0.425934682
			F	0.425934679
0.15	0.25	0.35	0.4	0.47494887
			0.6	0.4749489839
			F	0.4749489848
0.35	0.25	0.15	0.4	0.551122300
			0.6	0.5511223779
			F	0.5511223784

CONCLUSION.

The work presented in Part II is intended as a starting-point for further research into several possible applications. Notably, in numerical mathematics there is room for new methods for the solution of boundary-value partial differential equation problems and it is hoped that some of the ideas in this thesis may be useful in this field.

Within the scope of Chapter 4. we could use S_2 -fractions to analytically continue a double series solution of a hyperbolic equation with analytic Cauchy initial conditions. For example, the one-dimensional wave equation

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u(x,t)}{\partial t^2}$$

may be solved in double series form given single power series $\lambda(x)$ and $\mu(x)$ for the initial conditions

$$u(x,0) = \lambda(x) ,$$

$$\left. \frac{\partial u}{\partial t} \right|_{t=0} = \mu(x) .$$

The solution obtained in this case may be expressed as a single integral [d'Alembert's solution] for which univariate methods can be used, although there may be hyperbolic problems for which S_2 -fractions are advantageous.

In harmonic problems that can be solved using Green's functions it is sometimes possible to obtain a double series for the solution although, when the series coefficients are easily

obtained, simpler methods are usually available.

Clearly, if any real progress is to be made with difficult boundary-value problems then more research is needed. It would be premature to consider the advantages of continued fraction solutions of P.D.E. problems but the field holds much promise, although the difficulties to be overcome are large. One plausible line of research would be to develop continued fractions that are part-interpolating and part-corresponding to a power series. There is little doubt that such fractions could be formed, but the details of their structure and their method of application require further study. The method of solution in series for partial differential equations has been largely ignored by mathematicians because of the practical problems involved but, now that means of analytic continuation of such series are available, it is possible to consider the idea more seriously.

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