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Accelation techniques in numerical analysis, with particular reference to problems in one independent variables

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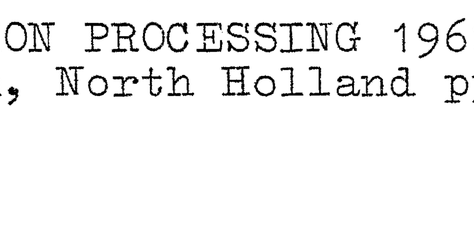

1962

ACCELERATION TECHNIQUES IN NUMERICAL ANALYSIS, WITH PARTICULAR REFERENCE TO PROBLEMS IN ONE INDEPENDENT VARIABLE

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1. Introduction

I propose to discuss certain methods for accelerating the convergence of iterative processes for solving computational problems. In certain respects this paper is an account of work which has recently been carried out, and it is perhaps fair to state at the outset that in order to invest it with some coherence and unity I have borne in mind a remark of Herodotus: In human affairs nothing very much happens at all and certainly the right thing never happens at the right time; the conscientious historian will remedy this.

The problem with which we are concerned is as follows: We are given a sequence $S_0, S_1, S_2, \ldots$, and there is a quantity S which is in some way associated with this sequence. If the sequence converges, S is its limit; if not, the meaning of S is interpreted in some way depending on how the sequence is produced. Our problem is to determine an approximate value of S in terms of the initial members of the sequence. In the first part of the paper we shall assume that the quantities involved are scalar.

2. Procrustean Techniques

One way of solving the problem in hand is by the use of procrustean techniques. The idea behind these techniques is as follows: It is asserted that the numerical behaviour of the S_n is very much like that of some simple function of n, let us call it $\varphi(n)$. $\varphi(n)$ may be a polynomial in $1/(n+1)$, a rational function of n, a linear combination of exponential functions of n, and so on. $\varphi(n)$ will contain certain parameters. For example, if $\varphi(n)$ is a rational function of n, then the parameters are its coefficients.

Let us suppose that these parameters are $2s+1$ in number. We determine their values by letting $\varphi(n)$ take on the values S_n, where $n = m, m+1, \ldots, m+2s$. Having constructed the function $\varphi(n)$ with the help of these parameters we let n tend to infinity; the value of the function is then our estimate of S. We are using the simple function to extrapolate the sequence to infinity.

Clearly, by varying the value of m, we obtain varying estimates of S. Furthermore, by varying the complexity of $\varphi(n)$, we obtain further estimates of S. For example, $\varphi(n)$ may be the quotient of two constants, the quotient of two linear functions of n, the quotient of two quadratic functions of n, and so on.

We may arrange our various estimates of S as shown in fig. 1, the even column φ-array.

The superscript indicates the value of m, and the suffix the number of parameters minus one. In the first column we have the estimates of S which are to be obtained from one member of the sequence alone. In the column with suffix 2 we have estimates derived from

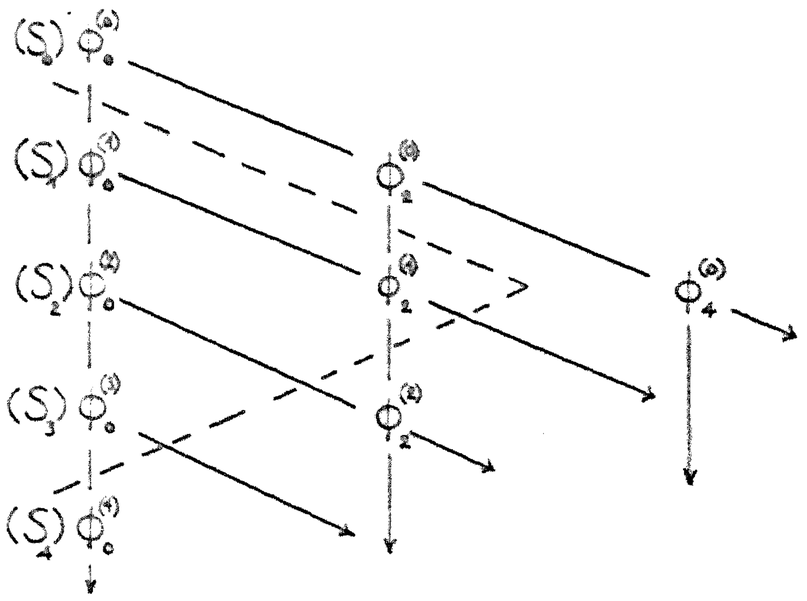

Fig. 1 The even column φ array.

three consecutive members of the sequence; $\varphi_2^{(1)}$ is derived from S_1, S_2 and S_3, for example. In the column with suffix 4 we have estimates derived from five consecutive members of the sequence, and so on.

We now add to the even column φ-array quantities φ with odd suffices (fig. 2).

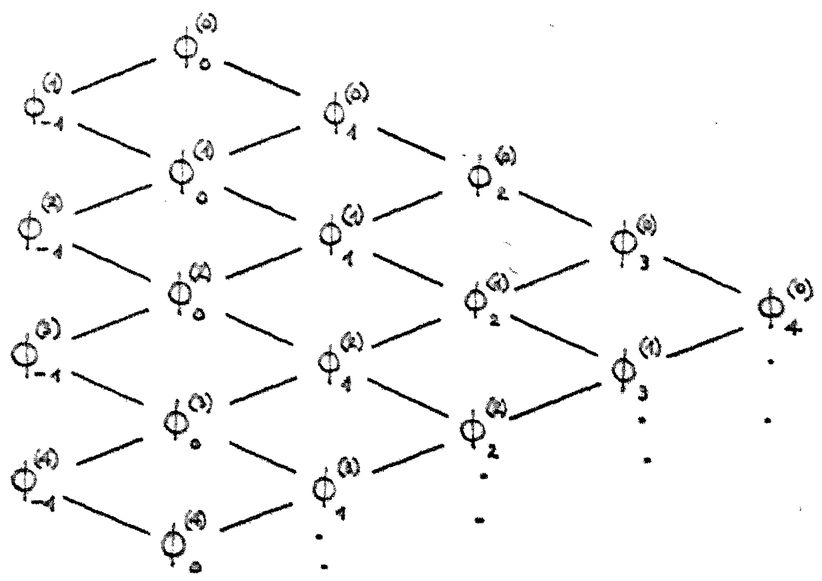

Fig. 2 The complete φ array.

These quantities are auxiliary quantities, of no great interest in themselves. The reason for introducing them is best revealed by considering two transformations in detail.

3. The ϱ-Algorithm [1])

Let us consider the case in which $\varphi(n)$ is a rational function of n, the quotient of two polynomials of the s^{th} degree:

$$\frac{\sum_{r=0}^{s} a_r n^r}{\sum_{r=0}^{s} b_r n^r}.$$

Formally, we can find the coefficients a_r and b_r in this expression by letting it take the values S_n when $n = m, m+1, \ldots, m+2s$. The value of this expression as n tends to infinity is, of course, a_s/b_s. Let us call this quotient $\varrho_{2s}^{(m)}$. These quotients, together with further auxiliary quantities, we may place in the ϱ-array (i.e. the φ-array with the letter φ replaced by ϱ).

I have spoken of letting the rational function take certain values, determining its coefficients, letting n tend to infinity, and so on. This is enormously complicated and totally unnecessary. The quantities of the ϱ-array may be constructed by means of the very simple non-linear recursion:

$$\varrho_{s+1}^{(m)} = \varrho_{s-1}^{(m+1)} + (s+1)\left\{\varrho_s^{(m+1)} - \varrho_s^{(m)}\right\}^{-1}$$

from the initial values

$$\varrho_{-1}^{(m)} = 0 \quad (m = 1, ,2 \ldots), \quad \varrho_0^{(m)} = S_m \ (m = 0, 1, \ldots).$$

4. The ε-Algorithm [2])

This may be considered in the same way. The simple function is a constant plus a linear combination of s exponential terms

$$a + \sum_{r=1}^{s} b_r \lambda_r^n.$$

Except in certain singular cases the parameters of such a function may be determined so that it takes on the values

$$S_m, S_{m+1}, \ldots, S_{m+2s}$$

when

$$n = m, m+1, \ldots, m+2s.$$

If all the λ's are less in modulus than unity the limiting value of this function as n tends to infinity is the constant term. Let us denote by $\varepsilon_{2s}^{(m)}$ the estimate of this constant term derived from the quantities

$$S_m, S_{m+1}, \ldots, S_{m+2s}.$$

Determinantal expressions for the $\varepsilon_{2s}^{(m)}$ in terms of $S_m, S_{m+1}, \ldots, S_{m+2s}$ were given by Shanks [3]).

When $s = 1$, this transformation reduces to the δ^2-process studied by Aitken [4]) and Lubkin [5]). It is not difficult to construct, and certainly there occur in practice, cases in which repeated application of the δ^2-process yields misleading results, whereas application of the more general transformation is successful.

As in the case of the previous algorithm, quantities $\varepsilon_s^{(m)}$ may be placed in an array in which the superscript m indicates a diagonal, and the suffix s a column. The central result of the ε-algorithm is that the quantities $\varepsilon_s^{(m)}$ may be produced by means of the relationship

$$\varepsilon_{s+1}^{(m)} = \varepsilon_{s-1}^{(m+1)} + \left\{\varepsilon_s^{(m+1)} - \varepsilon_s^{(m)}\right\}^{-1}$$

from the initial values

$$\varepsilon_{-1}^{(m)} = 0 \quad (m = 1, 2, \ldots), \quad \varepsilon_0^{(m)} = S_m \quad (m = 0, 1, \ldots).$$

5. A Further Technique

I mention in passing that the same idea can be applied [6,7]) using as a simple function a polynomial in $1/(n+1)$.

6. The ε-Algorithm and the Padé Table

In a series of numerical studies [8,9,10]), it was shown that application of these non-linear algorithms to quantities produced by linear methods, could produce very striking improvement.

Furthermore it appeared that application of the ε-algorithm was successful over a very large range of problems. It is interesting to enquire why this should be so.

Shanks has shown that if $S_0, S_1, S_2, \ldots$ are the successive partial sums of a power series, then the quantities $\varepsilon_{2s}^{(m)}$ are Padé quotients. Indeed the ε-array with odd order columns omitted is half a Padé table. (By inserting the appropriate boundary conditions the ε-algorithm may be used to construct the whole of the Padé table [11]).)

Further research [12]) has shown that the ε-algorithm is very closely related to the theory of continued fractions of a certain type.

7. Continued Fractions

A continued fraction may be written as

$$C = b_0 + \frac{a_1}{b_1 +}\,\frac{a_2}{b_2 +}\cdots,$$

C is the limit (if it exists) of the sequence of convergents $C_n (n = 0, 1, \ldots)$ given by

$$C_n = b_0 + \frac{a_1}{b_1 +}\,\frac{a_2}{b_2 +}\cdots\frac{a_n}{b_n}.$$

C_n may be evaluated by dividing a_n by b_n and adding the quotient to b_{n-1}; a_{n-1} is divided by this sum and the quotient added to b_{n-2}, and so on. More concisely, we evaluate the sequence D_s given by

$$D_0 = b_n$$
$$D_{s+1} = b_{n-s-1} + D_s^{-1} a_{n-s} \quad (s = 0, 1, \ldots, n-1)$$

when

$$C_n = D_n.$$

More economically, the successive convergents $C_n (n = 0, 1, \ldots)$ may be computed by evaluating the sequences A_n and B_n by means of the recursions

$$A_n = b_n A_{n-1} + a_n A_{n-2}$$
$$B_n = b_n B_{n-1} + a_n B_{n-2}$$

from the initial values

$$A_{-1}=1,\ A_0=b_0,\ B_{-1}=0,\ B_0=1,$$

for then

$$C_n=B_n^{-1}A_n \quad (n=0, 1, \ldots).$$

8. Corresponding and Associated Continued Fractions

We now turn to continued fractions of the form

$$\sum_{s=0}^{m-1} c_s z^{-s-1}+z^{-m}\left\{\frac{c_m}{z-}\,\frac{q_1^{(m)}}{1-}\,\frac{e_1^{(m)}}{z-}\cdots\frac{q_r^{(m)}}{1-}\,\frac{e_r^{(m)}}{z-}\cdots\right\}.$$

The nth convergent of this continued fraction is a rational function of z. If we are given a power series

$$S\sim\sum_{s=0}^{\infty} c_s z^{-s-1},$$

then (except in certain singular cases), the coefficients $q_r^{(m)}$, $e_r^{(m)}$ in this continued fraction may be determined, and determined uniquely, from the condition that the power series expansion of the sth convergent agrees with that of S [13,14]), as far as the term $c_{m+s}z^{-m-s-1}$. For this reason we may speak of such a continued fraction as corresponding to the power series for S. Such expansions have been extensively studied by Chebychev [15]), Stieltjes [16]), Markoff [18,19,20,21,22,23]), and others.

The rth convergent of the continued fraction

$$\sum_{s=0}^{m-1} c_s z^{-s-1}+z^{-m}\cdot\left\{\frac{c_m}{z-\alpha_0^{(m)}-}\cdot\frac{\beta_0^{(m)}}{z-\alpha_1^{(m)}-}\cdots\frac{\beta_{r-1}^{m}}{z-\alpha_r^{(m)}-}\cdots\right\}$$

is a rational function of z. The coefficients $\alpha_r^{(m)}$, $\beta_{r-1}^{(m)}$ in this continued fraction (again excepting certain singular cases) may be uniquely determined from the condition that the power series expansion of the rth convergent agrees with that of S as far as the term $c_{m+2r}z^{-m-2r-1}$. We say that this second continued fraction is associated with the power series for S.

The denominators of the successive convergents of the associated expansion are polynomials in z. Let us write them as

$$p_r^{(m)}(z)=\sum_{s=0}^{r} k_{r,s}^{(m)}\, z^s.$$

These polynomials are orthogonal polynomials: they are orthogonal in the sense that the scalar product

$$\sum_{s=0}^{r} c_{m+h+s}\, k_{r,s}^{(m)}$$

is zero for $h=0, 1\ldots, r-1$ and non-zero for $h=r$.

The successive convergents of the associated continued fraction are identical with the successive convergents of even order of the corresponding expansion.

If

$$\varepsilon_0^{(m)}=\sum_{s=0}^{m-1} c_s z^{-s-1} \quad (m=0, 1, \ldots),$$

the successive convergents of the associated fraction lie on the diagonal $\varepsilon_0^{(m)}$, $\varepsilon_2^{(m)}$, $\varepsilon_4^{(m)}$, ... of the ε-array; the successive convergents of the corresponding expansion lie on the staircase

$$\varepsilon_0^{(m)},\ \varepsilon_0^{(m+1)},\ \varepsilon_2^{(m)},\ \varepsilon_2^{(m+1)},\ \varepsilon_4^{(m)},\ \varepsilon_4^{(m+1)},\ \ldots$$

of the ε-array (fig. 3).

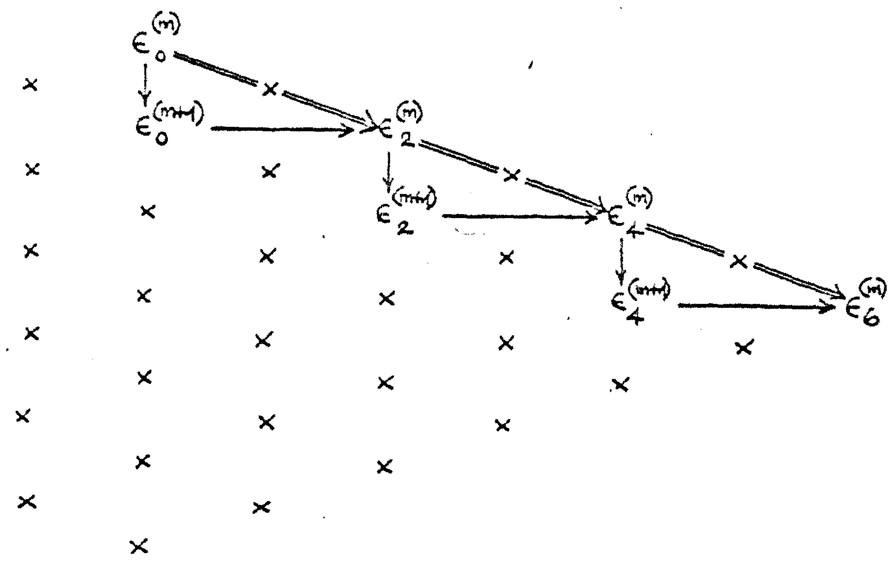

Fig. 3. The sequence of convergents.

9. Some Convergence Criteria

Corresponding continued fractions in which the $q_r^{(m)}$, $e_r^{(m)}$ $(r=1, 2, \ldots)$ are real and negative, are known as S-fractions. A considerable theory of such fractions has been established. It is known, for example, that if the series

$$\sum_{s=0}^{\infty} l_s$$

diverges, where

$$l_0=1,\ l_1=\frac{1}{q_1^{(m)}},\ l_{2s}=\frac{q_s^{(m)}}{e_s^{(m)}}\,l_{2s-2},\ l_{2s+1}=\frac{e_s^{(m)}}{q_{s+1}^{(m)}}\,l_{2s-1},$$

then the S-fraction converges for all z not lying on the negative real axis [16]). This continued fraction also converges for these values of z if the series

$$\sum_{s=0}^{\infty}(c_{m+s})^{1/2s}$$

diverges [24]).

The corresponding continued fraction is a convergent S-fraction if and only if the moment problem

$$\int_0^{\infty} t^s\, \mathrm{d}\,\psi^{(m)}(t)=c_{m+s} \qquad (s=0, 1, \ldots)$$

is determinate [25]). That is to say, if given the real constants c_m, c_{m+1}, c_{m+2}, ..., we can find one and only one function $\psi^{(m)}(t)$ which is finite and non-decreasing in the interval $0\leqslant t\leqslant\infty$. The existence of such Stieltjes integrals has close connections with the existence of solutions to the Dirichlet and Neumann problems [26]).

The S-fraction converges for values of z which are not real and negative, if the bound

$$\lim_{s=\infty}\inf\left(\frac{c_{m+s}}{(2s)\,!}\right)^{1/s}$$

is finite and there exists some function $F_m(z)$ which has the asymptotic expansion

$$\sum_{s=0}^{\infty} c_{m+s}\, z^{-s-1}$$

in the domain $\varepsilon \leqslant a\,rg(z) \leqslant \pi - \varepsilon$, where $0 < \varepsilon < \pi/2$, if $F_m(z)$ is analytic and $I_m\{F_m(z)\} < 0$ for $I(z) > 0$, and furthermore if $F_m(z)$ has the asymptotic representation [27]),

$$F_m(z) = \frac{c_m}{z} + \frac{O(1)}{zI_m(z)}.$$

The behaviour of the quantities in the ε-array may thus be seen to depend on the behaviour of the functions $F_m(z)$ in the large.

It is often true that the corresponding continued fraction converges in domains of the z-plane in which the power series $F(z)$ diverges. The use of continued fractions to transform divergent power series, or the method of Stieltjes summability as this is sometimes called, is well known. As I have said, in the context of Numerical Analysis, application of a non-linear transformation often effects a considerable improvement upon results produced by linear operator methods, but this is hardly surprising since we are catching up with a situation which prevailed in classical analysis eighty years ago. However, let us on this occasion attempt to make some progress.

10. The QD – Algorithm

The coefficients of the corresponding expansion obey the relationships

$$e_r^{(m+1)}\, q_r^{(m+1)} = q_{r+1}^{(m)}\, e_r^{(m)}$$

$$q_r^{(m+1)} + e_{r-1}^{(m+1)} = e_r^{(m)} + q_r^{(m)} \qquad (m = 0, 1, \ldots; r = 1, 2, \ldots)$$

where

$$e_0^{(m)} = 0, \quad q_1^{(m)} = c_{m+1}\, c_m^{-1} \qquad (m = 0, 1, \ldots)$$

These are the QD-algorithm relationships of H. Rutishauser [27]). The quantities q and e may be placed in an array similar to the ϱ-array, the quantities $q_r^{(m)}$ occur in the even order columns, the quantities $e_r^{(m)}$ in the odd order columns.

If

$$\sum_{s=0}^{\infty} c_s z^{-s-1}$$

is the power series expansion of a rational function, the quantities $q_r^{(m)}$ tend, for increasing m, to the roots of its denominator. (This has important applications to the eigenvalue problem [29,30]). F. L. Bauer [31]) has shown that the same information may be deduced from the quantities $\varepsilon_s^{(m)}$ with odd suffix.

11. Lozenge Algorithms

The ϱ, ε and QD-algorithms are lozenge algorithm relationships. The quantities involved occur in a lozenge in the analogue of the ϱ-array. The quantities of the ε-algorithm, for example, occur as follows in the ε-array:

$$\begin{array}{ccc} & \varepsilon_s^{(m)} & \\ \varepsilon_{s-1}^{(m+1)} & & \varepsilon_{s+1}^{(m)} \\ & \varepsilon_s^{(m+1)}. & \end{array}$$

Such algorithms are not the only lozenge algorithms. F. L. Bauer [32,33]) has shown that the ε and QD-algorithms are members of a class of such algorithms. I shall n give his formulae *in extenso*, but in general terms, l results may be described as follows: there are quantiti $g_s^{(m)}$ which are defined in terms of the polynomi $p_s^{(m)}(z)$, these quantities satisfy a lozenge algorith there are quantities $\pi_s^{(m)}$ defined in terms of the there are quantities $\eta_s^{(m)}$ defined in terms of the $\pi_s^{(m)}$ and finally the quantities $\varepsilon_s^{(m)}$ are defined in terms of t $\eta_s^{(m)}$; all these quantities satisfy lozenge algorithm

The local propagation of error in such algorithms h been studied [34]). Singular rules, which may be appli when the quantities involved become indeterminat have been established [35]). Confluent forms of the algorithms, which result in a sequence of non-linea difference – differential relationships, have been co structed [36,37,38,39,40,41,42,43]). Finally, a class of parti differential equations which may be associated wit these algorithms, has been derived [44]).

The g, π, and η-algorithms are, of course, of interes in their own right, but here we may regard them as bridge between the QD and ε-algorithms.

12. The Computation of Lozenge Algorithms

I wish now to embark upon a tactical digressio concerning the computation of the quantities in th φ-array by means of a lozenge algorithm relationship The fact that we are concerned with a lozenge algorithm means that we are required to store, not a two dimensional array, but a vector of quantities which lie upon what would, in a table of a function and its differences, correspond to a line of backward differences (fig. 4).

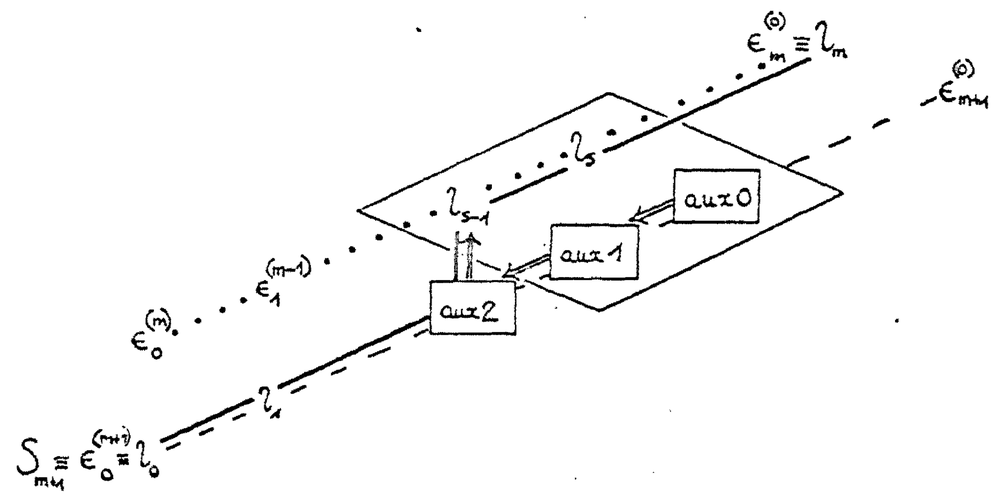

Fig. 4. Programming lozenge algorithms.

With reference to the ε-algorithm this vector, let us call it l, stretches from the ε with a superscript m and suffix nought, to the ε with a superscript nought and suffix m (that is, along the dotted line); we arrive with a new quantity S_{m+1}, and in stages push the backward diagonal l down one place (that is to the dashed line). The process requires two auxiliary storage boxes *aux* 2 and *aux* 1 and a working space *aux* 0. In the diagram, the process has not been completed. The vector l contains quantities lying along the solid line. The contents of l_{s-1}, l_s, *aux* 0 and *aux* 1 form a lozenge. The contents of *aux* 0 are computed from those of l_{s-1}, l_s and *aux* 1; the contents of *aux* 2 are transferred to l_{s-1}, those of *aux* 1 to *aux* 2, and those of *aux* 0 to *aux* 1. The value of s is increased by unity and the process is repeated. If the quantities involved are scalar all this is easily done; if the quantities involved are matrices it is perhaps easier to change the labels on the boxes than to move their contents around.

13. Extension to Non-Scalar Quantities

The relationships of the ε-algorithm involve addition, subtraction and the process of obtaining an inverse. These operations are defined for square matrices. The formal possibility therefore exists of applying the ε-algorithm to a slowly convergent square-matrix sequence. Such sequences arise in the numerical solution of partial differential equations in the following way: We are given a partial differential equation with two independent variables x and y, and boundary values on a square in the (x, y) plane. We wish to obtain the solution to this equation. We replace the square in the (x, y) plane by a square mesh of points and the solution becomes a square matrix of function values. We solve the problem iteratively, and obtain a sequence of square matrices.

14. Continued Fractions whose Elements Obey a Non-Commutative Law of Multiplication

Numerical experiments revealed that in some cases the transformed matrix sequences of the even ε-array converged far more rapidly than the original sequence[45]). Having obtained these promising results we are called upon to explain them: indeed to construct a theory of continued fractions whose elements obey a non-commutative law of multiplication.

You will recall that the n-th convergent of a continued fraction could be defined by a recursive process of division and addition. In the new theory[46]), division must be replaced by multiplication by the inverse. There is a theory of two types of continued fraction: those for which premultiplication is consistently used and those for which postmultiplication takes place. The fundamental formulae relating to continued fractions which have been given so far (the definition of C_n, the recursions for A_n and B_n, the orthogonality condition for $p_r^{(m)}(z)$, the QD-algorithm, and so on) relate to the pre-system. The corresponding formulae for the post-system may be obtained by reversing the order of the products which occur in these formulae. The relationships of the ε-algorithm do not involve multiplication; they are the same in both cases.

15. Degenerate Theory

With regard to all the algorithms which have been mentioned so far, there exists what might be called a degenerate theory. If the ϱ-algorithm is applied to a sequence of values of a rational function the quantities $\varrho_{2s}^{(m)}$ in a certain column will all be the same; if the QD-algorithm is applied to the power series development of a rational function, the quantities $e_s^{(m)}$ of a certain order are all zero; and so on. In these cases, we are not dealing with infinite continued fractions, merely with finite sequences of rational operations. Such a degenerate theory has been established for the new continued fractions.

In the theory of continued fractions of scalar quantities, many of the results just quoted were proved by an appeal to the theory of determinants. Regrettably, the theory of determinants whose elements obey a non-commutative law of multiplication (in so far as this has been established) cannot be used for such a purpose in the theory of the new continued fractions. However, the results relating to the QD-algorithm may be established by induction, adapting Rutishauser's addition theorem for continued fractions. The results relating to the other algorithms may be derived by adapting Bauer's work.

The result relating to the ε-algorithm may be stated as follows: If the quantities $\mathbf{S}_m$ $(m = 0, 1, \ldots)$ satisfy a non-cummutative law of multiplication, and a recursion of the form

$$\sum_{s=0}^{n} b_s \mathbf{S}_{m+s} = \mathbf{S}\left(\sum_{s=0}^{n} b_s\right) \qquad (m=0, 1, \ldots)$$

exists, in which the $b_s (s = 0, 1, \ldots, n)$ are scalar, and the ε-algorithm relationships are applied to the initial values

$$\varepsilon_{-1}^{(m)}=0, \ (m=1,2,\ldots), \ \varepsilon_0^{(m)}=\mathbf{S}_m \qquad (m=0,1,\ldots),$$

then

$$\varepsilon_{2n}^{(m)}=\mathbf{S} \qquad (m=0, 1, \ldots).$$

16. Iterated Vector Sequences: The Samelson Inverse

We come now to the point of application of the theory of this talk: the application of acceleration techniques to sequences of vectors.

Before, we may apply the ε-algorithm to such sequences, it is first necessary to define the inverse of a vector. Use has been made of a suggestion due to Samelson. He defines the inverse of a vector by the relationship

$$(y_1, y_2, \ldots, y_n)^{-1} = \left(\sum_{r=1}^{n} y_r \bar{y}_r\right)^{-1} (\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_n),$$

where the bars indicate a complex conjugate. When $n = 1$ this definition reduces to the conventional reciprocal of a complex number. $\mathbf{y}^{-1}$ is of course the inverse point of $\mathbf{y}$ with respect to the unit sphere in n-space.

17. Some Applications

Iterated vector sequences occur, of course, in computational problems of linear algebra. It is a simple consequence of the theorem just stated, that application of the ε-algorithm to the iterated vectors produced by the Gauss-Seidel relaxation process, results in an n-step procedure for the exact solution of a set of n linear equations.

Iterated vector sequences also occur in a number of optimisation problems: here again application of the ε-algorithm has been shown to be useful[47]).

18. Problems in One Independent Variable

Iterated vector sequences occur most naturally in Numerical Analysis in the following way: We are concerned with the function $f(x)$ which is defined for $a < x < b$, and satisfies a functional equation of some sort (an integral equation, for example). This equation is solved numerically using finite difference approximations; we are concerned with a vector of solution values. The equation is solved iteratively and we obtain a sequence of vectors.

19. The Lichtenstein-Gershgorin Integral Equation

In order to illustrate the acceleration of such vector sequences, I have chosen a problem from the theory of conformal mapping. The theory of conformal mapping has direct application to a number of problems and is of indirect application in many others [48]). The problem which I have chosen has been treated by various authors [49,50,51,52]) and is eminently suitable for numerical experiments in the solution of integral equations.

Suppose that we are given a curve C which encloses a domain D. C has a continuously turning tangent. We wish to find that function $w = f(z)$ which maps D conformally on the circle $|w| < 1$, such that a given point z_0 in D becomes the origin, and a second given point z_1 on C becomes the point $1 + i0$.

Suppose that the length of the arc of C from some point ξ on C to a point of reference on C, is s; so that the points on C may be represented by $\xi \equiv \xi(s)$. Now $f(z)$ has, of course, the Cauchy integral representation

$$f(z) = \frac{1}{2\pi i}\int_0 \frac{f(\xi)}{\xi - z}\,d\xi. \qquad z \in D$$

But on C, the modulus of $f(z)$, which is the modulus o $f(z)$ on the unit circle, is unity. Thus, if we write

$$\theta(s) = \arg\,[f\{\xi(s)\}]$$

we have

$$f(z) = \frac{1}{2\pi i}\int_0^L \frac{e^{i\theta(s)}}{\xi(s) - z}\,\frac{d\xi(s)}{ds}\,ds,$$

where L is the length of C. This is the integral with respect to a real variable s, of a complex-valued function. $\xi(s)$ will of course be given. If $\theta(s)$ can be found, the problem of constructing $f(z)$ is solved.

$\theta(s)$ satisfies the Lichtenstein-Gershgorin [53,54]) integral equation

$$\theta(s) = \int_0^L K(s,t)\,\theta(t)\,dt - 2\beta(s)$$

where

$$K(s,t) = \frac{1}{\pi}\,\frac{\sin\{\tau(t) - \varphi(s,t)\}}{r(s,t)},$$

s and t being the arc distances of two points; β, τ, φ and r s shown in fig. 5.

' is given, then β, τ, φ and r are, of course, all . I mention in passing that it may be convenient ess θ as a function of t', where t' is a function of length s, but this is not an essential complication.

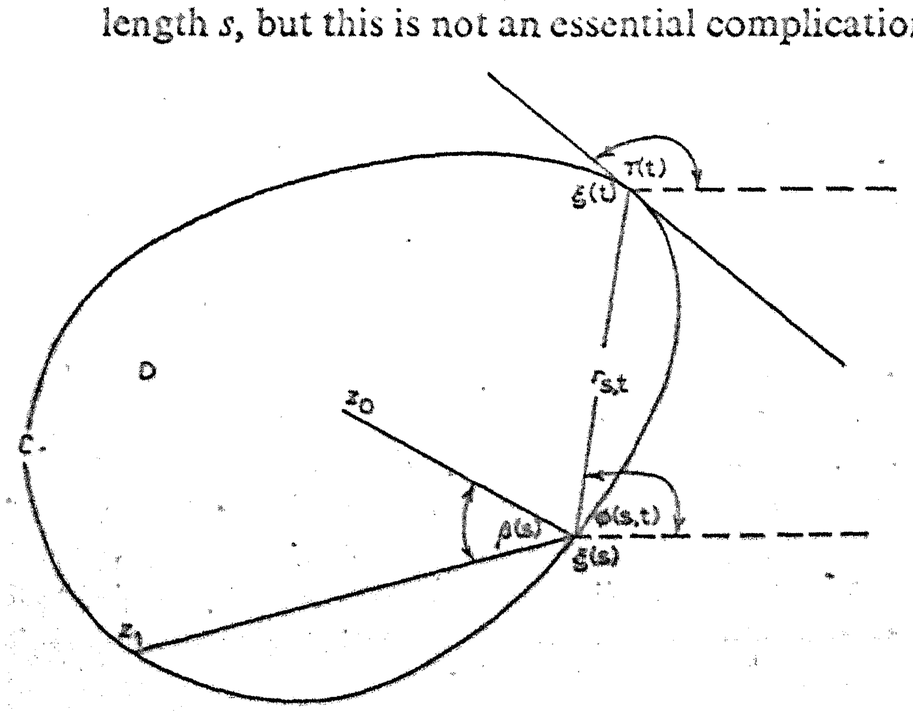

Fig. 5. Conformal mapping problem.

20. A Numerical Example

If C is the ellipse $x = a\cos t, y = b\sin t$, where $z = x + iy$, z_0 is the origin and z_1 the point $a + i0$, then, from considerations of symmetry the above integral equation reduces to

$$\theta(s) = \frac{k}{\pi}\int_0^\pi \left[\frac{k_1\theta(t)}{1 - k_2\cos(t+s)} - \frac{k_1\theta(\pi - t)}{1 + k_2\cos(t+s)}\right]dt + 2\arctan\left\{\frac{k^{-1}\sin(s)}{(1-\cos(s))\,[k_3\cos(s) - k^{-2}]}\right\},$$

where k, k_1, k_2 and k_3 are defined by

$$k = a/b,\ k_1 = (k^2+1)^{-1},\ k_2 = k_1(k^2-1),\ k_3 = 1 - k^{-2}.$$

Let us, for the moment, discuss how this integral equation would be solved normally by iterative methods.

Firstly, the integrals involved are replaced by a finite difference approximation. In the production of the numerical results to be given I have used the operational formula of Stone Age Numerical Analysis:

$$\int_a^{a+nh} f(t)\,dt = h\{\tfrac{1}{2}f_0 + f_1 + \ldots + f_{n-1} + \tfrac{1}{2}f_n + C\},$$

where

$$C = \tfrac{1}{2}(\Delta f_0 - \nabla f_n) - \tfrac{1}{24}(\Delta^2 f_0 + \nabla^2 f_n) + \tfrac{19}{720}(\Delta^3 f_0 - \nabla^3 f_n) - \tfrac{3}{160}(\Delta^4 f_0 - \nabla^4 f_n).$$

This is certainly not the best, and the iteration should wisely be prefaced by some skirmishing to find the best integration scheme, and the concomitant largest possible interval.

However, this scheme has been adopted for simplicity in presentation.

Thus we are concerned with the scheme

$$\bar{\theta}^{(m+1)} = K\bar{\theta}^{(m)} + \beta$$

where $\bar{\theta}^{(m)}$ is the vector whose components

$$\theta_i (i = 0, 1, \ldots, N)$$

should approximate to the vector of values

$$\theta(i\pi/N)\ (i = 0, 1, \ldots, N)$$

of the solution of the integral equation; K is an matrix depending on the kernel $K(s,t)$ and the above integration formula, and β is a vector of values $-2\beta(i\pi/N)$ $(i = 0, 1, \ldots, N)$

The distance between two iterates $\bar{\theta}^{(m+1)}$ and $\bar{\theta}^{(m)}$ may be defined by introducing a suitable norm; here we can say that this distance is

$$\max_i |\,\theta_i^{(m+1)} - \theta_i^{(m)}\,|.$$

If the finite difference scheme converges, then this distance may, merely by persisting in the iteration, be made less than δ, some stipulated agreement which we care to impose.

Having achieved this agreement there is another factor to be considered. We must obtain an estimate of the truncation error

$$\max_i |\,\theta_i^{(m)} - \theta(i\pi/N)\,|$$

and see if this is also less than δ. (In the numerical results to be given it is assumed that the magnitude of the truncation error is indicated by the last terms in the operational formulae for the integral).

The acceleration technique is only a device for dispensing with a million or so iteration steps; we must decide whether or not to accept a transformed iterate in the same way as before: we must go through one cycle of the original integral equation, examine the distance between the transformed iterate and its successor, examine our estimate of the truncation error, and then, and only then, decide whether to accept the transformed iterate.

In order to illustrate the application of the ε-algorithm to the iterated vectors produced in the above example, I have performed the following computation: with $k = 7.5$, $N = 72$ and $\bar{\theta}^{(0)} = 0$, the vector sequence $\bar{\theta}^{(m)}$ $(m = 0, 1, \ldots)$ has been produced. The ε-algorithm has been applied to these vectors. To each of the vectors in the even columns of the resultant ε-array, one cycle of the original integral equation has been applied. The corresponding distances and estimates of the truncation errors are given in tables 1 and 2.

Table 1

m s	0	2	4	6
0	— 5.41101			
1	+ 3.85450	— 0.50711		
2	— 2.69179	+ 0.04957	— 0.01263	
3	+ 1.89641	— 0.01810	+ 0.00203	— 0.00031
4	— 1.36144	+ 0.00912	— 0.00042	
5	+ 0.99621	— 0.00508		
6	— 0.73976			

Table 2

m s	0	2	4	6
0	0.0			
0	0.0			
1	0.00007	0.00005		
2	0.00004	0.00005	0.00005	
3	0.00005	0.00004	0.00005	0.00005
4	0.00004	0.00005	0.00005	
5	0.00005	0.00005		
6	0.00004			

It must be emphasised that the application of the integral equation to each of the entries in the even order ε-array is, in usual circumstances, unnecessary; it is done here merely for the purpose of display, and should in general be carried out, with a small value of N and for a few steps only, in a provisional investigation into the effect that the acceleration technique might have. Here we can see that the convergence of the original scheme (represented by the distances in the first column) is slow, whilst that of the sequence $\varepsilon_{2s}^{(0)}$ of the transformed vectors is relatively rapid.

In a final programme, the strategy adopted is as follows: the iteration of the integral equation is continued, and the ε-algorithm applied until the distance between $\varepsilon_m^{(0)}$ and $\varepsilon_{m-2}^{(2)}$ if m is even, or between $\varepsilon_{m-1}^{(1)}$ and $\varepsilon_{m-3}^{(3)}$ if m is odd, is less than a stipulated quantity. The vector $\varepsilon_m^{(0)}$ (or $\varepsilon_{m-1}^{(1)}$) is then submitted to the original integral equation cycle; if the distance between the two successive estimates is sufficiently small, then the iteration process is regarded as finished. The estimate of the truncation error is then examined, and if this is sufficiently small then the iterate resulting from $\varepsilon_m^{(0)}$ (or $\varepsilon_{m-1}^{(1)}$) is accepted as the final answer. (If the truncation error is too large, then the whole process may of course be repeated with a smaller finite difference interval.)

Using this programme, with $k = 7.5$, $N = 72$ and a stipulated agreement of the order of $\frac{1}{2} \times 10^{-3}$, it was found that 6 iterations of the integral equation were necessary.

The approach of the $\bar{\theta}^{(m)}$ to a limit is like that of a geometric series of ratio $-(k-1)/(k+1)$, thus approximately 54 iterations of the original equation are necessary to produce an agreement of $\frac{1}{2} \times 10^{-3}$.

When $N = 72$, one iteration of the integral equation on the X 1 computer (using an ALGOL compiler) takes of the order of 7 minutes, agreement to within $\frac{1}{2} \times 10^{-3}$ may be produced in about 50 minutes with acceleration, and six and a quarter hours without acceleration (this last figures is an estimate).*

21. Conclusion

We have seen the active interplay of ideas from Classical Analysis, Numerical Analysis, and Digital Computer Usage. As so often in the past, fundamental progress has been made, following the confrontation of alien disciplines. On the one hand, the numerical experiments which I have described hint that there exist a comprehensive theory of continued fractions in n-space; on the other, acceleration techniques will play an increasingly important role in enlightened computational practice, and their use increases the range of problems which may feasibly be solved on a digital computer.

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* Due to restrictions upon space, the ALGOL programs which were to have been included at this point will appear in the Communications of the ACM. (Editor)

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