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LINEAR MULTISTEP METHODS AND THE CONSTRUCTION
OF QUADRATURE FORMULAE FOR VOLTERRA INTEGRAL
AND INTEGRO-DIFFERENTIAL EQUATIONS

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Linear multistep methods and the construction of quadrature formulae for
Volterra integral and integro-differential equations

by

P.H.M. Wolkenfelt

ABSTRACT

The application of linear multistep methods to differential equations defining quadrature problems yields relations between the multistep coefficients and the quadrature weights. By means of these relations quadrature formulae are constructed and analyzed (in particular, properties of the weights are studied, and an asymptotic expression for the quadrature error is derived). The quadrature rules obtained in this way are used to define a class of step-by-step methods for solving first and second kind Volterra integral equations and integro-differential equations. Convergence and stability results for such methods are unified and extended. In particular, a new result is presented concerning the convergence of these methods for first kind equations. For Volterra integro-differential equations, stability regions are given for quadrature methods which are based on the backward differentiation formulae. The connection between the asymptotic repetition factor and relative stability is discussed.

KEY WORDS & PHRASES: *Numerical analysis, Volterra integral and integro-differential equations, equivalence of linear multistep methods and quadrature formulae, convergence, stability.*

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1. INTRODUCTION

Consider the problem of determining the values of

$$(1.1) \quad I(x) = \int_{x_0}^x \phi(t) dt,$$

on the uniform mesh $\{x_j \mid x_j = x_0 + jh\}$, where ϕ is a sufficiently smooth function. Approximations to $I(x_n)$ can be obtained using quadrature formulae with appropriate weights. On the other hand, the quadrature problem (1.1) can be written as the (rather special) initial value problem

$$(1.2) \quad I'(x) = \phi(x), \quad I(x_0) = 0,$$

and approximations to $I(x_n)$ can be obtained using standard methods for solving ODEs. In this paper, attention is focussed on linear multistep (LMS) methods.

Identification of the approximations to (1.1) and (1.2) yields relations between the weights and the LMS coefficients, and therefore provides a tool for constructing quadrature weights. Such relations are well-known in case of the Adams-Bashforth-Moulton or the Nyström-Milne-Simpson methods, because these methods are derived from interpolatory quadrature rules (see HENRICI [7, p.191]). However, there exist LMS methods which are *not* explicitly derived from quadrature (e.g. the backward differentiation methods) and, therefore, their connection with quadrature rules is less transparent.

The connection between LMS methods and quadrature formulae has been treated before, though in different areas. In the context of Volterra integro-differential equations, MATTHYS [16], generalizing results of BRUNNER & LAMBERT [4], reports on "reducible" quadrature formulae, and exploits them to prove results on A-stability. In most publications, however, only one special class of LMS methods was considered: for first kind Volterra integral equations, TAYLOR [23] "inverts" the backward differentiation formulae, and GLADWIN [6] modifies the Adams-Moulton formulae in order to construct high-order convergent methods. In the field of second kind Volterra integral equations the connection between the Gregory quadrature rules and

the Adams–Moulton formulae has been promulgated in various papers (e.g. [11, 3]). Motivated by these known results, it is our main purpose, in this paper, to give an *unified treatment of convergence and stability results* for reducible quadrature methods for the three classes of Volterra equations mentioned above.

The second purpose is to obtain insight into the connection between the repetition factor of the quadrature weights and the stability properties of the associated method for solving second kind Volterra integral equations. It was conjectured (see LINZ [13], NOBLE [19]) that methods with repetition factor greater than one display unsatisfactory stability properties. For the class of methods we consider, it appears that *stable* quadrature methods can be constructed, which do not have a repetition factor. Investigation of the weights reveals, however, that for such quadrature methods most of the weights *converge to unity*, and therefore their asymptotic values have a repetition factor one. This result suggested the introduction of the notion of *asymptotic repetition factor*. The final result we obtained, at least for the class of methods we have considered, is that there exists a close connection between asymptotic repetition factors and relative stability, but that no such a connection exists with absolute stability.

In section 2 we treat the construction of the quadrature formulae. In section 3 we state some results on linear difference equations, which are used to derive important properties of the quadrature weights. In section 4 an asymptotic expression for the quadrature error is given. As an example, we treat, in section 5, the quadrature formulae generated by the backward differentiation methods. In section 6 the quadrature formulae are used to define step-by-step methods for solving Volterra type equations, and convergence and stability results are treated in a unified way. The connection between repetition factor and numerical stability is discussed in section 7. In section 8 some concluding remarks are given.

2. RELATIONS BETWEEN QUADRATURE RULES AND LMS METHODS

In §2.1 quadrature formulae and LMS methods are presented for the solution of (1.1) and (1.2), respectively and some basic concepts and definitions

are recalled. In §2.2 the construction of the quadrature weights is treated.

2.1. Preliminaries

Numerical approximations I_n to $I(x_n)$ defined by (1.2) are obtained by applying LMS methods (cf. HENRICI [7, p.209], LAMBERT [12, p.11]) of the form

$$(2.1) \quad \sum_{i=0}^k a_i I_{n-i} = h \sum_{i=0}^k b_i \phi(x_{n-i}), \quad n \geq k,$$

where h denotes the stepsize and $x_j = x_0 + jh$, and where the starting values I_0, \dots, I_{k-1} are given. We choose an appropriate normalization (e.g. $\sum b_i = 1$ or $a_0 = 1$), and assume that the first and second characteristic polynomials ρ and σ , associated with (2.1) and defined by

$$\rho(\zeta) := \sum_{i=0}^k a_i \zeta^{k-i}, \quad \sigma(\zeta) := \sum_{i=0}^k b_i \zeta^{k-i},$$

have no common factor. Further we assume that $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$ (condition of consistency).

We also need the following definition:

DEFINITION 2.1. (see MILLER [18, p.398])

- (i) A polynomial is said to be a *simple van Neumann* polynomial if it has no zeros outside the closed unit disk and only simple zeros on the unit circle;
- (ii) A polynomial is said to be a *Schur* polynomial if it has all zeros inside the unit circle;

For the polynomial ρ with $\rho(1) = 0$ we will use:

DEFINITION 2.2.

- (i) The polynomial ρ is said to satisfy the *root condition* if it is a simple van Neumann polynomial;
- (ii) The polynomial ρ is said to satisfy the *strong root condition* if $\rho(\zeta)/(\zeta-1)$ is a Schur polynomial.

Further a LMS method is called zero-stable if the polynomial ρ satisfies the root condition. A LMS method is convergent iff it is both consistent

and zero-stable. A particular LMS method (2.1) is denoted by $\{a_i, b_i\}$ or $\{\rho, \sigma\}$.

For the numerical approximations I_n to $I(x_n)$ defined by the quadrature problem (1.1) we employ quadrature formulae (based on equidistant abscissae $x_j = x_0 + jh$) of the form

$$(2.2a) \quad I_n := h \sum_{j=0}^{k-1} w_{n,j} \phi(x_j), \quad \text{for } n = 0(1)k-1,$$

$$(2.2b) \quad I_n := h \sum_{j=0}^n w_{n,j} \phi(x_j), \quad \text{for } n = k, k+1, \dots$$

The rules (2.2a) use abscissae x_j outside the integration interval in order to obtain sufficiently accurate approximations for small values of n . (In the appendix examples of such quadrature rules are given for $k = 2(1)6$.) As the formulae (2.2a) are used to compute the required starting values for (2.1) we call these the *starting quadrature rules*.

The weights $\{w_{n,j}\}$ can be arranged in a matrix W of the form

$$(2.3) \quad W = \left[\begin{array}{ccc|ccc} w_{0,0} & \cdots & w_{0,k-1} & & & \\ \vdots & & \vdots & & & \\ w_{k-1,0} & \cdots & w_{k-1,k-1} & & & \\ \hline w_{k,0} & \cdots & w_{k,k-1} & w_{k,k} & & \\ \vdots & & \vdots & \vdots & \ddots & \\ w_{n,0} & & w_{n,k-1} & w_{n,k} & \cdots & w_{n,n} \\ \vdots & & \vdots & \vdots & & \vdots \\ \vdots & & \vdots & \vdots & & \ddots \end{array} \right] = \left[\begin{array}{c|c} S_k & 0 \\ \hline W_k & \Omega \end{array} \right]$$

where $w_{n,j} = 0$ for $n < j$, $j \geq k$. For subsequent use, we introduce the notion of repetition factor.

DEFINITION 2.3. The weights in the matrix (2.3) are said to have an *exact (rowwise) repetition factor* r if r is the smallest integer such that

$w_{n,j} = w_{n+r,j}$ for $n \geq n_0$ and $n_1 \leq j \leq n-n_2$, where n_i ($i = 0, 1, 2$) are independent of n .

This definition differs slightly from the usual one (see e.g. BAKER [1, p. 823]) in the addition of the adjective "exact". The reason for this is that we will also define (in §3.3) an asymptotic repetition factor. Further, by repetition factor we mean exact repetition factor.

From definition 2.3 it is readily seen that the weights in (2.3) have repetition factor r iff the weights in the submatrix Ω have repetition factor r .

With regard to the accuracy of quadrature rules we give the following definition.

DEFINITION 2.4: A quadrature rule (2.2) is said to be of *precision* q if it is exact for all polynomials of degree $\leq q$.

A particular set of quadrature formulae of the form (2.3) is denoted by $\{W\}$ or by the triple $\{S_k, W_k, \Omega\}$.

2.2. The construction of quadrature rules by means of LMS methods

Assuming that the starting values I_0, \dots, I_{k-1} for (2.1) are computed from (2.2a), the values I_n ($n \geq k$) are uniquely defined by (2.1). Next we require these values to be identical with those obtained with (2.2b). Substitution of I_{n-i} defined by (2.2a-b) into the left-hand side of (2.1) and equating the coefficients of $\phi(x_j)$ for $j = 0(1)n$ yields the following relations between the weights $w_{n,j}$ and the coefficients a_i and b_i

$$(2.4a) \quad \sum_{i=0}^k a_i w_{n-i,j} = b_{n-j}, \quad \text{if } n-k \leq j \leq n, \\ \text{for } n \geq k$$

$$(2.4b) \quad \sum_{i=0}^k a_i w_{n-i,j} = 0, \quad \text{if } 0 \leq j < n-k;$$

or

$$(2.5a) \quad \sum_{i=0}^k a_i w_{n-i,j} = b_{n-j}, \quad \text{for } n = \max(j,k), \dots, j+k,$$

$$(2.5b) \quad \sum_{i=0}^k a_i w_{n-i,j} = 0, \quad \text{for } n = j+k+1, j+k+2, \dots$$

From (2.4a-b) or (2.5a-b) the weights $w_{n,j}$ can be generated provided that the coefficients a_i and b_i , and the weights of the starting quadrature

rules (2.2a) are given. The set of quadrature formulae constructed in this way is called (ρ, σ) -reducible (cf. MATHYS [16, p.86] who gives necessary and sufficient conditions for reducibility).

For j fixed, the j -th column of (2.3) is generated by the recurrence relations (2.5a-b); observe that the element $w_{n,j}$ in the j -th column depends only upon $w_{v,j}$ for $n-k \leq v \leq n-1$. As a consequence, only the weights in the matrix W_k in (2.3) depend upon the choice of the matrix S_k . The remaining weights (the elements of the matrix Ω) are independent of the weights of the starting quadrature rules. Moreover, due to the zero-entries in the upper-triangular part of W , one can derive from (2.5a-b) (taking $j \geq k$) that the matrix Ω has the structure

$$(2.6) \quad \Omega = \begin{bmatrix} \omega_0 & & & & \text{\textcircled{0}} \\ \omega_1 & \omega_0 & & & \\ \omega_2 & \omega_1 & \omega_0 & & \\ \cdot & \omega_2 & \omega_1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} ,$$

where the sequence $\{\omega_n\}_{n=0}^{\infty}$ satisfies

$$(2.7a) \quad \begin{cases} a_0 \omega_0 & = b_0 \\ a_0 \omega_1 + a_1 \omega_0 & = b_1 \\ \cdot & \cdot \\ a_0 \omega_k + a_1 \omega_{k-1} + \dots + a_k \omega_0 & = b_k \end{cases}$$

$$(2.7b) \quad a_0 \omega_n + a_1 \omega_{n-1} + \dots + a_k \omega_{n-k} = 0, \quad n \geq k+1,$$

(Note that $\omega_0 = 0$ iff $b_0 = 0$). From (2.6) we derive that

$$(2.8) \quad w_{n,j} = w_{n+l,j+l} = \omega_{n-j} \quad \text{for } n \geq j \geq k, \quad l \geq 0.$$

Thus, for the construction of the quadrature weights of W , it is sufficient to generate the sequence $\{\omega_n\}$ by means of (2.7) yielding the matrix Ω , and to generate the first k columns by (2.5) yielding W_k . We will denote

a (ρ, σ) -reducible set of quadrature formulae by $\{S_k; \rho, \sigma\}$. In section 5 we give an example in which we have chosen for $\{\rho, \sigma\}$ the *backward differentiation (BD) methods*.

Recall from (2.5b) and (2.7b) that the weights in each column satisfy a linear homogeneous difference equation with constant coefficients a_i ; the starting values for these difference equations are associated with the starting quadrature rules and the coefficients b_i . Therefore, properties of the weights are related directly to the properties of this difference equation and to the structure of the starting values. These properties are studied in the next section.

3. PROPERTIES OF THE WEIGHTS

In §3.1 we state some general results on linear difference equations, which are then used in §3.2 to derive that, under suitable conditions, the elements of each column of W in (2.3) form a convergent sequence. In §3.3 a relationship between the repetition factor of the weights and the location of the zeros of the polynomial ρ is given.

3.1. Results on linear difference equations

Let the sequence $\{y_n\}$ be the solution of the linear, homogeneous difference equation with constant coefficients

$$(3.1) \quad \sum_{i=0}^k a_i y_{n-i} = 0, \quad n \geq k,$$

with given starting values y_0, \dots, y_{k-1} .

Assuming that the polynomial $\rho(\zeta)$ associated with (3.1) has q *different* zeros ζ_1, \dots, ζ_q with multiplicities m_1, \dots, m_q ($m_1 + \dots + m_q = k$) the solution can be written in the form (see e.g. STOER & BULIRSCH [22, p.132])

$$(3.2) \quad y_n = \sum_{v=1}^q \sum_{i=0}^{m_v-1} c_{v,i} \binom{n}{i} \zeta_v^{n-i}, \quad n = 0, 1, \dots,$$

with the convention

$$\binom{n}{i} \zeta_v^{n-i} := \begin{cases} 0 & \text{for } n = 0(1)i-1, \\ 1 & \text{for } n = i. \end{cases}$$

Given the values y_0, \dots, y_{k-1} , the equations (3.2) for $n = 0(1)k-1$ constitute a non-singular linear system for the k unknown coefficients $c_{v,i}$, and therefore these coefficients depend linearly on the starting values.

It appears that simple explicit expressions for the coefficients c_{j,m_j-1} , $j = 1(1)q$ can be derived. To this end, define (see [7, p.238]) the polynomial $\rho_j(\zeta)$ and the coefficients $\alpha_{j,i}$ by

$$(3.3) \quad \rho_j(\zeta) := \rho(\zeta)/(\zeta - \zeta_j) = \sum_{i=0}^{k-1} \alpha_{j,i} \zeta^i,$$

and Δ_j by

$$(3.4) \quad \Delta_j := \sum_{i=0}^{k-1} \alpha_{j,i} y_i.$$

If we multiply the n -th equation in (3.2) by $\alpha_{j,n}$ for $n = 0(1)k-1$, and add the resulting equations, we obtain after some manipulation

$$(3.5) \quad \sum_{v=1}^q \sum_{i=0}^{m_v-1} c_{v,i} \rho_j^{(i)}(\zeta_v)/i! = \Delta_j.$$

For $v \neq j$, ζ_v is a zero of $\rho(\zeta)$ with multiplicity m_v and thus a zero of $\rho_j(\zeta)$ with the same multiplicity, that is

$$(3.6) \quad \rho_j^{(i)}(\zeta_v) \begin{cases} = 0 & \text{for } i = 0(1)m_v-1 \\ \neq 0 & \text{for } i = m_v \end{cases}, \quad v \neq j$$

Since ζ_j is a zero of $\rho_j(\zeta)$ with multiplicity m_j-1 , we have

$$(3.7) \quad \rho_j^{(i)}(\zeta_j) = 0 \quad \text{for } i = 0(1)m_j-2.$$

Moreover, since $(\zeta - \zeta_j)\rho_j^{(i)}(\zeta) + i\rho_j^{(i-1)}(\zeta) = \rho^{(i)}(\zeta)$ for all i ,

$$(3.8) \quad \rho_j^{(m_j-1)}(\zeta_j) = \rho^{(m_j)}(\zeta_j)/m_j.$$

Substitution of the results (3.6), (3.7) and (3.8) into (3.5) yields the expression

$$(3.9) \quad c_{j, m_j - 1} = m_j! \Delta_j / \rho^{(m_j)}(\zeta_j), \quad j = 1(1)q.$$

(The remaining coefficients can be determined using polynomials of the form $\rho(\zeta)/(\zeta - \zeta_j)^i$, $i = 1, \dots, m_j$ yielding a lower-triangular system of equations for the coefficients $c_{j,i}$, $i = 0(1)m_j - 1$. This will not be pursued here.) In the following remarks some observations are given.

REMARKS.

3.1. If ζ_ν is a simple zero of ρ , we derive from (3.2) and (3.9) that

$$\sum_{i=0}^{m_\nu - 1} c_{\nu, i} \binom{n}{i} \zeta_\nu^{n-i} = \zeta_\nu^n \Delta_\nu / \rho'(\zeta_\nu).$$

3.2. When ρ is a simple van Neumann polynomial with s zeros ζ_1, \dots, ζ_s on the unit circle, then y_n , defined by (3.1), can be written

$$y_n = c_{1,0} \zeta_1^n + \dots + c_{s,0} \zeta_s^n + \text{terms approaching zero as } n \rightarrow \infty,$$

where $|\zeta_i| = 1$, $i = 1(1)s$. In this case the sequence $\{y_n\}$ is *bounded uniformly in n* .

3.3. In particular, if $\zeta_1 = 1$ is a simple zero of ρ and if the remaining zeros are inside the unit circle (that is, if ρ satisfies the strong root condition), then $\lim_{n \rightarrow \infty} y_n = \Delta_1 / \rho'(1)$.

When certain simple zeros of ρ are known, this information can be used to construct the solution of (3.1) in another way, which is, in certain cases, more stable. This construction appears in the following lemma.

LEMMA 3.1. Let the sequence $\{y_n\}_{n=0}^\infty$ satisfy the difference equation (3.1) with starting values y_0, \dots, y_{k-1} . Further, let the polynomial ρ^* , with coefficients a_i^* , be defined by

$$\rho^*(\zeta) = \rho(\zeta) / \prod_{i=1}^s (\zeta - \zeta_i) = \sum_{i=0}^{k-s} a_i^* \zeta^{k-s-i},$$

where ζ_1, \dots, ζ_s are simple zeros of ρ , which are supposed to be known. Then y_n can be split into

$$y_n = u_n + v_n \quad \text{for } n \geq 0,$$

where

$$(3.10) \quad u_n = \frac{\Delta_1}{\rho'(\zeta_1)} \zeta_1^n + \dots + \frac{\Delta_s}{\rho'(\zeta_s)} \zeta_s^n \quad \text{for } n \geq 0,$$

with Δ_j ($j = 1(1)s$) given by (3.4), and where v_n is the solution of

$$(3.11) \quad \sum_{i=0}^{k-s} a_i^* v_{n-i} = 0 \quad \text{for } n \geq k-s,$$

with starting values $v_n = y_n - u_n$, $n = 0(1)k-s-1$.

PROOF. To simplify the presentation of the proof of this lemma we assume that all zeros of ρ are simple (where ζ_1, \dots, ζ_s are known, $\zeta_{s+1}, \dots, \zeta_k$ are unknown). The proof for the general case is along similar lines.

From (3.2), the solution y_n can be written as

$$y_n = c_1 \zeta_1^n + \dots + c_s \zeta_s^n + c_{s+1} \zeta_{s+1}^n + \dots + c_k \zeta_k^n,$$

(here, we have omitted the second subscript of c_{vi}).

The coefficients c_j can be found by solving the non-singular linear system

$$(3.12) \quad \begin{bmatrix} 1 & \dots & 1 & | & 1 & \dots & 1 \\ \zeta_1 & \dots & \zeta_s & | & \zeta_{s+1} & \dots & \zeta_k \\ \vdots & & \vdots & | & \vdots & & \vdots \\ \vdots & & \vdots & | & \vdots & & \vdots \\ \vdots & & \vdots & | & \vdots & & \vdots \\ \zeta_1^{k-1} & \dots & \zeta_s^{k-1} & | & \zeta_{s+1}^{k-1} & \dots & \zeta_k^{k-1} \end{bmatrix} \begin{bmatrix} c_1 \\ \vdots \\ c_s \\ c_{s+1} \\ \vdots \\ c_k \end{bmatrix} = \begin{bmatrix} y_0 \\ \vdots \\ y_{s-1} \\ y_s \\ \vdots \\ y_{k-1} \end{bmatrix}.$$

Since ζ_1, \dots, ζ_s are known, the coefficients c_j ($j = 1(1)s$) are known and are equal to $\Delta_j/\rho'(\zeta_j)$ in view of (3.9). This yields the expression (3.10) for u_n . Substituting the values of c_1, \dots, c_s and transposing them to the right-hand side of (3.12) yields that the coefficients c_{s+1}, \dots, c_k satisfy the non-singular linear system

$$(3.13) \quad \begin{bmatrix} 1 & \dots & 1 \\ \zeta_{s+1} & \dots & \zeta_k \\ \vdots & & \vdots \\ \zeta_{s+1}^{k-s-1} & \dots & \zeta_k^{k-s-1} \end{bmatrix} \begin{bmatrix} c_{s+1} \\ \vdots \\ c_k \end{bmatrix} = \begin{bmatrix} y_0 \\ \vdots \\ y_{k-s-1} \end{bmatrix} - \begin{bmatrix} c_1 + \dots + c_s \\ \vdots \\ c_1 \zeta_1^{k-s-1} + \dots + c_s \zeta_s^{k-s-1} \end{bmatrix}$$

$$= \begin{bmatrix} y_0 & -u_0 \\ \vdots & \\ y_{k-s-1} & -u_{k-s-1} \end{bmatrix}.$$

We now look at (3.11). Since the polynomial $\rho^*(\zeta)$ associated with (3.11) has the zeros $\zeta_{s+1}, \dots, \zeta_k$, the solution v_n can be written as

$$v_n = d_{s+1} \zeta_{s+1}^n + \dots + d_k \zeta_k^n \quad \text{for } n \geq 0.$$

The coefficients d_{s+1}, \dots, d_k are determined by solving the linear system with the same matrix as in (3.13) and with the right-hand side v_0, \dots, v_{k-s-1} . However, since $v_n = y_n - u_n$ ($n = 0(1)k-s-1$) we find that $d_j = c_j$ for $j = s+1(1)k$, and therefore $y_n = u_n + v_n$ for all $n \geq 0$. \square

The practical importance of this lemma is indicated in the following remarks.

REMARKS.

3.4. If ρ satisfies the strong root condition then $y_n = \Delta_1/\rho'(1) + v_n$ where $v_n \rightarrow 0$ as $n \rightarrow \infty$. If we generate the sequence $\{y_n\}$ by means of (3.1) using finite-precision arithmetic, the influence of round-off error and the presence of the zero $\zeta_1 = 1$ (which may differ slightly from 1 due to rounding errors in the coefficients a_1) may cause that we do not obtain the limit $\Delta_1/\rho'(1)$. However, if we compute first $\Delta_1/\rho'(1)$, and then generate the sequence $\{v_n\}$ by means of (3.11), the limit $\Delta_1/\rho'(1)$ is reached even in the case of finite-precision arithmetic. This procedure is followed in section 5.

3.5. Let ρ be a simple van Neumann polynomial with s zeros ζ_1, \dots, ζ_s on

the unit circle. If these zeros also satisfy $\zeta^r = 1$ then u_n , defined by (3.10), has the property that $u_n = u_{n+r}$. In this case, it follows from lemma 3.1 that we need to compute only the values u_0, \dots, u_{r-1} , and the sequence $\{v_n\}$ from (3.11). Moreover, since $v_n \rightarrow 0$, it is easily seen that the subsequences $\{y_{nr}\}_{n=0}^{\infty}, \dots, \{y_{nr+r-1}\}_{n=0}^{\infty}$ converge to the limits u_0, \dots, u_{r-1} , respectively.

In remark 3.5 we have seen that the values u_n are periodic, if the polynomial ρ fulfils a suitable condition. This condition is formalized in the following definition.

DEFINITION 3.1. A simple von Neumann polynomial ρ is said to be of class r if r is the smallest integer with the property that the set of zeros of ρ lying on the unit circle is contained in the set of zeros of $\zeta^r - 1$.

To illustrate this concept, we give the following statements. A Schur polynomial is of class 0; the polynomial $\zeta^r - 1$ is of class r , and the polynomials $(\zeta - 1)(\zeta^2 + 1)$ and $(\zeta - 1)(\zeta^2 + 1)(\zeta - \frac{1}{2})$ are both of class 4. The polynomial $\zeta^2 - (2 \cos \phi)\zeta + 1$, which has two zeros on the unit circle, is of class ∞ if $\phi/2\pi$ is an irrational number.

Further, this concept will be used in §3.3, where we shall indicate a connection between polynomials of class r and the repetition factor of the associated quadrature weights.

3.2. Limits of the weights

We now return to the recurrence relations (2.5) and (2.7) defining W_k and Ω , respectively. We have the following theorem:

THEOREM 3.1. Let $\{\rho, \sigma\}$ define a convergent LMS method. Then

(i) the weights $\{w_{n,j}\}$ generated by $\{\rho, \sigma\}$ are uniformly bounded.

If, in addition, ρ satisfies the strong root condition, then

(ii) the elements of each column in the matrix W form a convergent sequence; the limits of the first k columns depend upon the choice of the starting quadrature rules,

(iii) the elements of each column of the matrix Ω converge to unity; that is

$$(3.14) \quad \lim_{n \rightarrow \infty} \omega_n = 1.$$

PROOF.

(i) follows from remark 3.2, since ρ is simple von Neumann,

(ii) follows from remark 3.3. In particular, we have in view of (3.4)

$$(3.15) \quad \lim_{n \rightarrow \infty} w_{n,j} = \frac{1}{\rho'(1)} \sum_{i=0}^{k-1} \alpha_{1,i} w_{i,j} \quad \text{for } 0 \leq j \leq k-1,$$

where $w_{i,j}$ ($i, j = 0(1)k-1$) are the entries of S_k .

(iii) In view of (2.6), it suffices to prove that the elements of the first column of Ω converge to unity; that is, we have to prove that

$$\lim_{n \rightarrow \infty} \omega_n = 1.$$

The sequence $\{\omega_n\}$ is defined by the difference equation (2.7b) with starting values $\omega_1, \dots, \omega_k$. From (3.2) the solution ω_n can be written as

$$\omega_{n+1} = \sum_{v=1}^q \sum_{i=0}^{m_v-1} c_{v,i} \binom{n}{i} \zeta_v^{n-i}, \quad n = 0, 1, \dots$$

The coefficients c_{j,m_j-1} are defined by (3.9) where

$$(3.16) \quad \Delta_j = \sum_{i=0}^{k-1} \alpha_{j,i} \omega_{i+1}.$$

From (3.3) we derive that

$$(3.17) \quad \alpha_{j,i} = \sum_{v=0}^{k-1-i} a_v \zeta_j^{k-1-i-v}.$$

Substituting (3.17) into (3.16) and using (2.7a) yields

$$\begin{aligned} \Delta_j &= (a_0 \zeta_j^{k-1} + a_1 \zeta_j^{k-2} + \dots + a_{k-1}) \omega_1 + \dots + (a_0 \zeta_j + a_1) \omega_{k-1} + a_0 \omega_k = \\ &= (a_0 \omega_k + a_1 \omega_{k-1} + \dots + a_{k-1} \omega_1) + \zeta_j (a_0 \omega_{k-1} + a_1 \omega_{k-2} + \dots + a_{k-2} \omega_1) + \\ &+ \dots + \zeta_j^{k-2} (a_0 \omega_2 + a_1 \omega_1) + \zeta_j^{k-1} a_0 \omega_1 = \\ &= (b_k - a_k \omega_0) + \zeta_j (b_{k-1} - a_{k-1} \omega_0) + \dots + \zeta_j^{k-2} (b_2 - a_2 \omega_0) + \zeta_j^{k-1} (b_1 - a_1 \omega_0) \end{aligned}$$

$$\begin{aligned}
&= \sum_{i=1}^k b_i \zeta_j^{k-i} - \omega_0 \sum_{i=1}^k a_i \zeta_j^{k-i} = \sigma(\zeta_j) - b_0 \zeta_j^k - \omega_0 \rho(\zeta_j) + a_0 \omega_0 \zeta_j^k \\
&= \sigma(\zeta_j),
\end{aligned}$$

which is unequal to zero, since $\hat{\rho}$ and σ have no common factor and $\rho(\zeta_j) = 0$. From (3.9) we then derive that

$$(3.18) \quad c_{j, m_j-1} = m_j! \sigma(\zeta_j) / \rho^{(m_j)}(\zeta_j) \neq 0, \quad j = 1(1)q.$$

Finally, from remark 3.3 it follows that $\lim_{n \rightarrow \infty} \omega_n = \sigma(1) / \rho'(1)$, which equals unity by virtue of consistency. \square

Well-known examples of quadrature rules for which (3.14) holds are the Gregory quadrature rules ([1]). Other examples are the quadrature rules generated by the backward differentiation formulae (see section 5).

3.3. Repetition factor of the weights

In the literature, there has been some emphasis on the connection between the stability properties of direct quadrature methods for solving second kind Volterra integral equations and the repetition factor of the associated quadrature weights. LINZ [13] conjectures that methods with repetition factor greater than one have undesirable stability properties, and NOBLE [19] states that methods with repetition factor one are stable. We will also investigate the relationship between repetition factor and stability. It turns out, that the proper way to do this is to relate the existence of a repetition factor as well as the stability behaviour to the location of the zeros of the polynomial ρ .

With this in mind, the following theorem and its consequences are of importance.

THEOREM 3.2. *Let $\{\rho, \sigma\}$ be a convergent linear k -step method. Then the weights of a (ρ, σ) -reducible set of quadrature formulae have an exact repetition factor r iff $\{\rho(\zeta) = 0 \Rightarrow \zeta = 0 \text{ or } |\zeta| = 1\}$ and ρ is of class r .*

PROOF. It is sufficient to prove (in view of the remark following definition

2.3) that the weights in the matrix Ω in (2.3) given by the sequence $\{\omega_n\}$ have repetition factor r iff the polynomial ρ fulfils the condition of theorem 3.2.

a. Let ρ be of class r and let $\rho(\zeta) = 0$ imply that $\zeta = 0$ or $|\zeta| = 1$. Assume that ζ_1, \dots, ζ_s are the zeros of ρ lying on the unit circle. Then $\omega_{n+1} = c_1 \zeta_1^n + \dots + c_s \zeta_s^n$ ($n = n_0, n_0+1, \dots$), where ζ_i satisfies $\zeta_i^r = 1$ ($i = 1(1)s$) and $c_i = \sigma(\zeta_i)/\rho'(\zeta_i) \neq 0$ in view of (3.18). Therefore $\omega_{n+1} = \omega_{n+1+r}$; that is the weights do repeat. Next we show that r is the smallest integer with this property. Suppose that $\omega_{n+1} = \omega_{n+1+j}$ ($j \geq 1$). Subtracting the expressions for ω_{n+1} and ω_{n+1+j} yields that

$$c_1 \zeta_1^n (\zeta_1^j - 1) + \dots + c_s \zeta_s^n (\zeta_s^j - 1) = 0.$$

Since this expression must be zero for all n , and $c_i \neq 0$, $i = 1(1)s$, the s differing roots ζ_1, \dots, ζ_s have to satisfy $\zeta_i^j = 1$. Since ρ is of class r this implies that $j \geq r$. Hence the weights have an exact repetition factor r .

b. If the weights have an exact repetition factor r , then $\omega_{n+1} = \omega_{n+1+r}$ ($n \geq n_0$). Assume that $\rho(\zeta) = 0$ has j non-zero roots $\zeta_1, \dots, \zeta_{q-1}$ with multiplicities m_1, \dots, m_{q-1} ($m_1 + \dots + m_{q-1} = j$) and one root $\zeta_q = 0$ with multiplicity $m_q = k-j$. (Notice that $j \geq 1$ since $\rho(1) = 0$ by virtue of consistency.) The general expression for ω_{n+1} can be written (cf. (3.2))

$$(3.19) \quad \omega_{n+1} = \sum_{v=1}^{q-1} \sum_{i=0}^{m_v-1} c_{v,i} \zeta_v^{n-i} \binom{n}{i}, \quad n \geq m_q = k-j,$$

since the terms corresponding to $\zeta_q = 0$ in (3.2) vanish for $n \geq m_q$.

From (3.19) we derive that for all $n \geq m_q$

$$\omega_{n+1+r} - \omega_{n+1} = \sum_{v=1}^{q-1} \sum_{i=0}^{m_v-1} c_{v,i} \zeta_v^{n-i} \left\{ \binom{n+r}{i} \zeta_v^r - \binom{n}{i} \right\}.$$

Since this expression must vanish identically for all $n \geq m_q$, all terms must be zero. From (3.18) we recall that $c_{v, m_v-1} \neq 0$; hence a necessary condition is that

$$\binom{n+r}{m_\nu-1} \zeta_\nu^r - \binom{n}{m_\nu-1} = 0 \quad \text{for } \nu = 1(1)q-1, \quad n \geq m_q.$$

These equations can only be satisfied if $m_\nu = 1$ and if $\zeta_\nu^r = 1$ ($\nu = 1(1)q-1$). This means that the j non-zero roots are simple roots lying on the unit circle and satisfy $\zeta^r = 1$. Now suppose that ρ is of class s . Then we obtain from the first part of this theorem (which is proved in part(a)) that the weights have repetition factor s . Hence $s = r$, and thus ρ is of class r . \square

An immediate consequence is the following.

COROLLARY: If $\rho(\zeta) = a_0(\zeta^k - \zeta^{k-r})$ then the weights have an exact repetition factor r .

If ρ does not satisfy the condition of theorem 3.2, then the weights do not have an exact repetition factor in the sense of definition 2.3. In theorem 3.1 we have seen, however, that the weights in each column of the matrix W converge, if ρ satisfies the strong root condition. Therefore, in such a case the weights have repetition factor one as $n \rightarrow \infty$. Likewise, the weights have repetition factor r as $n \rightarrow \infty$ if ρ is of class r (see remark 3.5). In particular, when the weights are computed using finite-precision arithmetic we have the identity $w_{n+r,j} = w_{n,j}$ for n sufficiently large. These observations suggest the following definition:

DEFINITION 3.2. The weights in (2.3) are said to have an *asymptotic (rowwise) repetition factor* r if r is the smallest integer such that for all $\varepsilon > 0$ there exist n_0, n_1 and n_2 independent of n such that $|w_{n+r,j} - w_{n,j}| < \varepsilon$ for $n \geq n_0$ and $n_1 \leq j \leq n-n_2$.

The following theorem is now self-evident.

THEOREM 3.3. Let $\{\rho, \sigma\}$ be a convergent linear k -step method. Then the weights of a (ρ, σ) -reducible set of quadrature formulae have an asymptotic repetition factor r iff the polynomial ρ is of class r .

The relationship between the location of the zeros of the polynomial ρ and the stability behaviour of the associated quadrature method for

second kind Volterra integral equations is treated in section 7.

4. ASYMPTOTIC EXPRESSION AND ORDER OF THE QUADRATURE ERROR

In this section we will give an expression for the quadrature error $Q_n[\phi]$ defined by

$$(4.1) \quad Q_n[\phi] := I_n - I(x_n) = h \sum_{j=0}^n w_{n,j} \phi(x_j) - \int_{x_0}^{x_n} \phi(t) dt$$

under the assumption that the quadrature weights are reducible to a convergent LMS method of order p . This expression is valid for $h \rightarrow 0$, $n \rightarrow \infty$ while $nh = x_n - x_0$ remains fixed and is, in this sense, asymptotic.

Recall from §2.2 that the value I_n obtained with the quadrature formula $h \sum_{j=0}^n w_{n,j} \phi(x_j)$ is identical to the value of I_n resulting from the application of the LMS method $\{\rho, \sigma\}$ to the ODE (1.2) with starting values I_0, \dots, I_{k-1} defined by (2.2a). As a consequence, we can apply the convergence theorems of LMS methods for ODEs. Assuming that the starting errors Q_0, \dots, Q_{k-1} are $O(h^S)$, we apply theorem 5.11 from HENRICI [7, p.248] yielding $Q_n = O(h^S) + O(h^P)$ as $h \rightarrow 0$, $n \rightarrow \infty$.

An expression for Q_n including the coefficients of h^P and h^S can be derived along the lines indicated in [7, p.249-255], but due to the special form of the differential equation (1.2) (i.e. the right-hand side does not depend on $I(x)$) the derivation is less complicated in this case. Assuming sufficient smoothness of ϕ , the errors Q_n satisfy the inhomogeneous difference equation

$$(4.2) \quad \sum_{i=0}^k a_i Q_{n-i} = -C_{p+1} h^{p+1} \phi^{(p)}(x_n) + O(h^{p+2}), \quad \text{as } h \rightarrow 0,$$

where C_{p+1} is the error constant of the LMS method. If we split Q_n into $Q_n^{(1)} + Q_n^{(2)}$, where $Q_n^{(1)}$ represents the solution of (4.2) with zero starting values, and $Q_n^{(2)}$ represents the solution of the homogeneous version of (4.2) with starting values Q_0, \dots, Q_{k-1} , then we can derive that

$$(4.3) \quad Q_n^{(1)} = -\frac{C_{p+1}}{\sigma(1)} h^p \{\phi^{(p-1)}(x_n) - \phi^{(p-1)}(x_0)\} + O(h^{p+1}).$$

For the determination of $Q_n^{(2)}$ we proceed as follows. For each of the starting quadrature rules considered in (2.2a) the quadrature error assumes the form

$$Q_j = d_j h_j^{s_j} \phi^{(s_j-1)}(x_0) + O(h_j^{s_j+1}), \quad j = 0(1)k-1.$$

Let $s = \min\{s_0, \dots, s_{k-1}\}$ then $Q_j = d_j^* h_j^s \phi^{(s-1)}(x_0) + O(h_j^{s+1})$ where $d_j^* = d_j$ if $s_j = s$ and $d_j^* = 0$ if $s_j > s$ ($j = 0(1)k-1$). Since $Q_n^{(2)}$ satisfies the homogeneous version of (4.2) with starting values Q_0, \dots, Q_{k-1} , $Q_n^{(2)}$ can be written

$$(4.4) \quad Q_n^{(2)} = d_n^* h_n^s \phi^{(s-1)}(x_0) + O(h_n^{s+1}),$$

where d_n^* satisfies $\sum_{i=0}^k a_i d_{n-i}^* = 0$ with starting values d_0^*, \dots, d_{k-1}^* .

From (4.4) we see that $Q_n^{(2)} = 0$ if ϕ is a polynomial of degree $\leq s-2$, and from (4.3) $Q_n^{(1)} = 0$ if ϕ is a polynomial of degree $\leq p-1$. Therefore the total error $Q_n = 0$ if ϕ is a polynomial of degree $\leq p-1$ and if $s = p+1$. In this case the quadrature formulae $\{S_k; \rho, \sigma\}$ are of precision $p-1$ (see definition 2.4). In order to have this convenient property we will always tacitly assume that the *starting quadrature rules are of order h^{p+1}* . This choice has also the advantage that the starting errors do not influence the h^p -term, in the total error Q_n , so that we finally arrive at

$$(4.5) \quad Q_n = -\frac{C}{\sigma(1)} h^{p+1} \{\phi^{(p-1)}(x_n) - \phi^{(p-1)}(x_0)\} + O(h^{p+1}),$$

as $h \rightarrow 0$, $n \rightarrow \infty$ while $nh = x_n - x_0$ fixed.

The foregoing suggests the following definition.

DEFINITION 4.1. (ρ, σ) -reducible quadrature formulae are said to be (*convergent*) of order p if the LMS method $\{\rho, \sigma\}$ is convergent of order p and if the starting quadrature rules are of order $p+1$.

5. AN EXAMPLE: THE BACKWARD DIFFERENTIATION FORMULAE

We pause for a moment to give an illustration of the results derived

in the previous sections. We consider the k -step backward differentiation (BD) formulae for $k = 2(1)6$. The coefficients a_i and b_0 ($b_1 = \dots = b_k = 0$) can be found in LAMBERT [12, p.242] and are reproduced in table 5.1 (here, we have chosen the normalization $a_0 = 1$).

k	c_k	$b_0 \times c_k$	$a_1 \times c_k$	$a_2 \times c_k$	$a_3 \times c_k$	$a_4 \times c_k$	$a_5 \times c_k$	$a_6 \times c_k$
2	3	2	-4	1				
3	11	6	-18	9	-2			
4	25	12	-48	36	-16	3		
5	137	60	-300	300	-200	75	-12	
6	147	60	-360	450	-400	225	-72	10

Table 5.1. Coefficients of the BD formulae ($a_0 = 1$)

Since the coefficients b_1, \dots, b_k vanish the recurrence relations (2.7a-b) defining the sequence $\{\omega_n\}$ can be simplified to

$$(5.1) \quad \sum_{i=0}^k a_i \omega_{n-i} = 0, \quad n \geq 1, \quad \omega_{-k+1} = 0, \dots, \omega_{-1} = 0, \quad \omega_0 = b_0.$$

Explicit values of ω_n can be computed from (5.1). Since ρ satisfies the strong root condition, we know from theorem 3.1 that $\omega_n \rightarrow 1$ as $n \rightarrow \infty$. However, if we compute the weights using finite-precision arithmetic, the influence of rounding errors may cause that we do not obtain this limit exactly. This undesirable behaviour can be avoided using the construction given in lemma 3.1 (see also remark 3.4): we have computed the sequence $\{v_n\}$ from the recurrence relation $\sum_{i=0}^{k-1} a_i^* v_{n-i} = 0$ for $n \geq 0$ with starting values $v_{-k+1} = -1, \dots, v_{-1} = -1$, where the a_i^* -s are the coefficients of the reduced polynomial $\rho^*(\zeta) = \rho(\zeta)/(\zeta-1)$ (see table 5.2), and finally we put $\omega_n = 1 + v_n$.

k	c_k	$a_1^* \times c_k$	$a_2^* \times c_k$	$a_3^* \times c_k$	$a_4^* \times c_k$	$a_5^* \times c_k$
2	3	-1				
3	11	-7	2			
4	25	-23	13	-3		
5	137	-163	137	-63	12	
6	147	-213	237	-163	62	-10

Table 5.2. Coefficients of the reduced polynomial
($a_0^* = 1$)

In order to get an impression of the rate of convergence, we give in the following table the value n_0 such that for $n \geq n_0$ $|\omega_n - 1| \geq 10^{-15}$ (which is approximately the precision of our computer).

k	2	3	4	5	6
n_0	31	40	57	97	227

Only in the case that the zeros of ρ are known explicitly the closed form (3.2) can be used. For $k = 2$ these zeros are $\zeta_1 = 1$ and $\zeta_2 = 1/3$ so that

$$\omega_n^{(k=2)} = 1 - (1/3)^{n+1} \quad \text{for } n \geq 0,$$

and, in view of (2.8),

$$w_{n,j}^{(k=2)} = 1 - (1/3)^{n+1-j} \quad \text{for } n \geq j \geq k.$$

So the weights are completely determined, except for the first k columns. As already pointed out in section 2, these columns depend upon the weights of the starting quadrature rules. Choosing the formulae given in Appendix I, the first k columns can be computed explicitly using the recurrence relations (2.5a-b) (or its modification indicated in lemma 3.1). Again in the case $k = 2$ explicit expressions can be obtained using (3.2) and remark


3.1. We obtain

$$w_{n,j} = \frac{1}{\rho'(1)} (\alpha_{1,0} w_{0,j} + \alpha_{1,1} w_{1,j}) + \frac{1}{\rho'(1/3)} (\alpha_{2,0} w_{0,j} + \alpha_{2,1} w_{1,j}) (1/3)^n, \\ j = 0, 1,$$

where the coefficients $\alpha_{j,i}$ are defined in (3.3) (note that $\alpha_{1,i} = a_{k-1-i}^*$ for $i = 0(1)k-1$). For these values we find $\alpha_{1,0} = -1/3$, $\alpha_{1,1} = 1$, $\rho'(1) = 2/3$ and $\alpha_{2,0} = -1$, $\alpha_{2,1} = 1$, $\rho'(1/3) = -2/3$. Using the starting formulae $w_{0,0} = w_{0,1} = 0$ and $w_{1,0} = w_{1,1} = 1/2$ one then derives that

$$w_{n,j}^{(k=2)} = \frac{3}{4} (1 - (1/3)^n) \quad \text{for } n \geq 0, j = 0, 1.$$

From this expression it is seen that $\lim w_{n,0} = \lim w_{n,1} = 3/4$. In summary, the matrix of quadrature weights for $k = 2$ is

0	0	
1/2	1/2	
2/3		2/3
13/18	13/18	8/9 2/3
↓	↓	↓ . . .
3/4	3/4	1 8/9 2/3

For $k > 2$, the limiting values of the elements in each column can be obtained without explicit knowledge of the weights. Recall from (3.15) that

$$\lim_{n \rightarrow \infty} w_{n,j} = \frac{\Delta_1}{\rho'(1)} = \frac{1}{\rho'(1)} \sum_{i=0}^{k-1} a_i^* w_{k-1-i,j}, \quad j = 0(1)k-1.$$

We illustrate this for the case $k = 3$. From table 5.1 we obtain $\rho'(1) = \sigma(1) = b_0 = 6/11$ and from table 5.2 $(a_0^*, a_1^*, a_2^*) = (1, -7/11, 2/11)$. Taking the first column of weights in the starting quadrature rules (cf. Appendix I) $(w_{0,0}, w_{1,0}, w_{2,0}) = (0, 5/12, 4/12)$, we obtain

$$w_{n,0}^{(k=3)} \rightarrow 1/8, \quad \text{as } n \rightarrow \infty.$$

Likewise, we obtain for the remaining two columns

$$w_{n,1}^{(k=3)} \rightarrow 5/3, \quad w_{n,2}^{(k=3)} \rightarrow 17/24 \quad \text{as } n \rightarrow \infty.$$

Finally we treat the quadrature error of the BD formulae. We recall that a k -step BD formula for the solution of ODEs has order k with error constant $C_{k+1}/\sigma(1) = -1/(k+1)$ (cf. [7, p.224]). Therefore, if we employ starting quadrature rules of order $k+1$ (e.g. the rules given in Appendix I), we derive from (4.5) the following asymptotic expression for the quadrature error

$$Q_n[\phi] = \frac{h^k}{k+1} \{ \phi^{(k-1)}(x_n) - \phi^{(k-1)}(x_0) \} + O(h^{k+1}), \quad \text{as } h \rightarrow 0.$$

6. APPLICATIONS

In this section we employ the quadrature formulae derived in §2.2 for the construction of methods for solving problems involving a Volterra integral operator. We restrict our considerations to Volterra integral equations of the first and second kind and to integro-differential equations. In this order, these equations have the form

$$(6.1) \quad \int_{x_0}^x K(x,y)f(y)dy = g(x), \quad x_0 \leq x \leq X,$$

$$(6.2) \quad f(x) = g(x) + \int_{x_0}^x K_*(x,y,f(y))dy, \quad x_0 \leq x \leq X,$$

$$(6.3) \quad \begin{cases} f'(x) = F(x, f(x), z(x)), f(x_0) = f_0, & x_0 \leq x \leq X, \\ z(x) = \int_{x_0}^x K_*(x,y,f(y))dy. \end{cases}$$

We make the assumption that the functions g, K, K_* and F are continuously differentiable to sufficiently high order with respect to each of their arguments. Further we assume in the case of (6.1) that $g(x_0) = 0$ and that $K(x,x) \neq 0$ for all $x \in [x_0, X]$. These assumptions guarantee the existence of a unique solution $f(x)$ which is continuously differentiable to suf-

ficiently high order on $[x_0, X]$.

The numerical methods are simple to derive: in each equation the integral is discretized by numerical quadrature using the weights of (ρ, σ) -reducible quadrature formulae, that is

$$\int_{x_0}^{x_n} K_*(x_n, y, f(y)) dy \simeq h \sum_{j=0}^n w_{n,j} K_*(x_n, x_j, f_j), \quad n \geq k.$$

The resulting schemes can be applied in a step-by-step fashion. The required starting values f_0, \dots, f_{k-1} are assumed to result from some adequate starting procedure (e.g. Runge-Kutta methods or low order one-step methods combined with Richardson extrapolation). If $w_{n,n} \neq 0$ (i.e. $b_0 \neq 0$) then the methods are implicit and the solution of a linear or non-linear equation is needed. This can be achieved by predictor-corrector techniques or Newton-Raphson type iteration. The schemes are also applicable to systems of equations.

In the following paragraphs the three different classes of equations are treated separately. The numerical approximation to $f(x_n)$ is denoted by f_n and the global error e_n is defined by $e_n = f_n - f(x_n)$. A method is said to be convergent if $e_n \rightarrow 0$ as $h \rightarrow 0$, $n \rightarrow \infty$ ($n = (x - x_0)/h$) for any $x \in [x_0, X]$. The method is convergent of order p if $e_n = O(h^p)$. Conditions for the convergence of the methods are stated and convergence-theorems are proved. In addition, the stability behaviour for fixed $h \neq 0$ is treated. The definition of absolute (block) stability to be used is the one given by BAKER and KEECH [3].

6.1. First kind Volterra integral equations

Numerical methods for solving the equation (6.1) have the form

$$(6.4) \quad h \sum_{j=0}^n w_{n,j} K(x_n, x_j) f_j = g(x_n), \quad n \geq k.$$

The starting values f_0, \dots, f_{k-1} must be available. With respect to the convergence of this scheme we have the following theorem.

THEOREM 6.1. *In addition to the conditions for existence and uniqueness of a smooth solution $f(x)$ of (6.1), assume that*

- (i) *the weight $(w_{n,j})$ in (6.4) are the weights of (ρ, σ) -reducible quadrature formulae of order p ,*
- (ii) *σ is a simple von Neumann polynomial,*
- (iii) *the starting errors e_j ($j = 0(1)k-1$) are of order s .*

Let $r = \min(p, s)$, then

$$e_n = O(h^r), \quad \text{as } h \rightarrow 0, n \rightarrow \infty, nh = x_n - x_0.$$

PROOF. The proof of this theorem is involved and lengthy, and can be found in Appendix II. \square

This theorem generalizes the theorems derived by GLADWIN [6] and TAYLOR [23]. The former treats methods of Adams type ($\rho(\zeta) = \zeta^k - \zeta^{k-1}$) whilst the latter considers backward differentiation type methods ($\sigma(\zeta) = b_0 \zeta^k$). It also includes the methods treated by LINZ [14].

The stability behaviour for fixed $h \neq 0$ is analyzed by applying (6.4) to the test equation

$$(6.5) \quad \int_0^x f(y) dy = g(x), \quad g(0) = 0,$$

with solution $f(x) = g'(x)$, to obtain the equations

$$(6.6) \quad h \sum_{j=0}^n w_{n,j} f_j = g(x_n).$$

As in the proof of theorem 6.1, we take linear combinations with the coefficients a_i of successive equations in (6.6). This yields

$$(6.7) \quad h \sum_{j=0}^n \sum_{i=0}^k a_i w_{n-i,j} f_j = \sum_{i=0}^k a_i g(x_{n-i}).$$

Using (2.4a-b) we arrive at

$$(6.8) \quad \sum_{i=0}^k b_i f_{n-i} = \frac{1}{h} \sum_{i=0}^k a_i g(x_{n-i}).$$

which is a k -term recurrence relation for f_n . This device of taking linear combinations of successive rows in order to get a recurrence relation with a fixed number of terms is easily seen to be a generalization of the differencing operation as is done in the case of quadrature methods having a repetition factor.

From (6.8) it is verified that the scheme (6.4) is *stable iff* $\sigma(\zeta)$ *simple von Neumann*. Since this condition is independent of the stepsize h , stability regions cannot be defined. The largest (in modulus) zero of σ is of practical importance and gives an indication of the damping properties of the scheme. If this value exceeds one then the scheme is unstable and divergent. In this connection, GLADWIN & JELTSCH [5] have shown that (in our notation) a q -th order LMS method $\{\rho, \sigma\}$ with $\rho(\zeta) = \zeta^k - \zeta^{k-r}$, $b_0 \neq 0$ and $q > k \geq 2$ generates an unstable (and thus divergent) method for solving first kind equations (cf. the Adams-Moulton formulae).

In some cases the methods applied to (6.5) yield "local differentiation formulae" (see KEECH [9] for a definition). A necessary condition for this property is that $\zeta = 0$ is the only zero of σ . For our class of methods this is also sufficient and can be shown as follows. Let b_j be the only non-zero coefficient in σ , $0 \leq j \leq k-1$, then, from (6.8) we have

$$b_j f_{n-j} = \frac{1}{h} \sum_{i=0}^k a_i g(x_{n-i}) = \rho'(1)g'(x_{n-j}) + O(h),$$

so that $f_{n-j} = \rho'(1)/\sigma(1)g'(x_{n-j}) + O(h) = g'(x_{n-j}) + O(h)$. Examples of such methods are the mid-point rule ($\sigma(\zeta) = 2\zeta$) and the BD formulae ($\sigma(\zeta) = b_0 \zeta^k$).

6.2. Second kind Volterra integral equations

For solving (6.2) the schemes have the form

$$(6.9) \quad f_n = g(x_n) + h \sum_{j=0}^n w_{n,j} K_*(x_n, x_j, f_j), \quad n \geq k$$

with $f_0 = g(x_0)$, f_1, \dots, f_{k-1} given. The following convergence theorem holds.

THEOREM 6.2. *In addition to the conditions for existence and uniqueness of a sufficiently smooth solution $f(x)$ of (6.2) assume that*

- (i) the weights $(w_{n,j})$ in (6.9) are the weights of (ρ, σ) -reducible quadrature formulae of order p ,
- (ii) the starting errors e_j ($j = 0(1)k-1$) are of order s .

Let $r = \min(p, s+1)$, then

$$e_n = O(h^r) \quad \text{as } h \rightarrow 0, n \rightarrow \infty, nh = x_n - x_0.$$

PROOF. We check the conditions given in a general convergence theorem (see BAKER [1, p.836]), that is, we have to show that the weights are uniformly bounded and that the quadrature error is of order p . This has been shown, however, in theorem 3.1 and section 4, respectively. \square

The stability behaviour for fixed $h \neq 0$ is analyzed by applying the scheme (6.9) to the test equation

$$(6.10) \quad f(x) = g(x) + \lambda \int_0^x f(y) dy, \quad \lambda \in \mathbb{C},$$

yielding

$$(6.11) \quad f_n = g_n + h\lambda \sum_{j=0}^n w_{n,j} f_j, \quad n \geq k.$$

Application of the same differencing technique as in §6.1 results in the relations

$$(6.12) \quad \sum_{i=0}^k (a_i - h\lambda b_i) f_{n-i} = \sum_{i=0}^k a_i g(x_{n-i}), \quad n \geq 2k,$$

and therefore the scheme (6.9) is *stable iff* $\rho(\zeta) - h\lambda\sigma(\zeta)$ is a simple von Neumann polynomial. Stability regions can be defined in the usual way. We emphasize that the stability regions are exactly the same as the stability regions of the LMS method $\{\rho, \sigma\}$ for ODEs. This, of course, is not surprising and a consequence of the construction of the weights. Thus, highly stable methods for solving ODEs can be used to generate highly stable methods for solving second kind Volterra integral equation. In particular, the use of BD methods is advocated when the kernel K_* has a large Lipschitz constant.

4.3. Volterra integro-differential equations

Let us apply a linear \tilde{k} -step method $\{\tilde{\rho}, \tilde{\sigma}\}$ to the differential part of (6.3) and (ρ, σ) -reducible quadrature formulae to the integral term in (6.3) (here, $\{\rho, \sigma\}$ has stepnumber k). Then we obtain a large class of methods which take the form

$$(6.13) \quad \sum_{i=0}^k \tilde{a}_i f_{n-i} = h \sum_{i=0}^{\tilde{k}} \tilde{b}_i F(x_{n-i}, f_{n-i}, z_{n-i}),$$

$$z_n = h \sum_{j=0}^n w_{n,j} K_*(x_n, x_j, f_j),$$

$n \geq k^*$,

where $k^* = \max\{\tilde{k}, k\}$. The required starting values are $f_0 = f(x_0)$, f_1, \dots, f_{k^*-1} and $z_0 = 0$, z_1, \dots, z_{k^*-1} . We will denote such methods by $\{\tilde{\rho}, \tilde{\sigma}; S_k; \rho, \sigma\}$ where S_k represents the starting quadrature rules. We have the following convergence theorem.

THEOREM 6.3. *In addition to the conditions for existence and uniqueness of a smooth solution $f(x)$ of (6.3), assume that*

- (i) $\{\tilde{\rho}, \tilde{\sigma}\}$ is a convergent linear k -step method of order \tilde{p} ,
- (ii) the weights $(w_{n,j})$ in (6.13) are the weights of (ρ, σ) -reducible quadrature formulae of order p ,
- (iii) the starting errors e_j ($j = 0(1)k^*-1$) are of order s .

Let $r = \min(\tilde{p}, p, s)$, then

$$e_n = O(h^r), \quad \text{as } h \rightarrow 0, n \rightarrow \infty, nh = x_n - x_0.$$

PROOF. Apply the theorems of LINZ [15]. \square

The stability analysis for fixed $h \neq 0$ is usually analyzed by applying the scheme (6.13) to the test equation (see e.g. BRUNNER & LAMBERT [4]).

$$(6.14) \quad f'(x) = \xi f(x) + \eta \int_0^x f(y) dy, \quad \xi, \eta \in \mathbb{R},$$

This yields

$$(6.15) \quad \left\{ \begin{array}{l} \sum_{i=0}^{\tilde{k}} \tilde{a}_i f_{n-i} = h \sum_{i=0}^{\tilde{k}} \tilde{b}_i (\xi f_{n-i} + \eta z_{n-i}), \\ z_n = h \sum_{j=0}^n w_{n,j} f_j. \end{array} \right.$$

Differencing the last equation by means of the coefficients a_i yields

$$(6.16) \quad \left\{ \begin{array}{l} \sum_{i=0}^{\tilde{k}} \tilde{a}_i f_{n-i} = h \sum_{i=0}^{\tilde{k}} \tilde{b}_i (\xi f_{n-i} + \eta z_{n-i}), \\ \sum_{i=0}^k a_i z_{n-i} = h \sum_{i=0}^k b_i f_{n-i}. \end{array} \right.$$

Therefore the method (6.13) is *stable iff the stability polynomial defined by*

$$\rho(\zeta)[\tilde{\rho}(\zeta) - h\xi\tilde{\sigma}(\zeta)] - h^2\eta\tilde{\sigma}(\zeta)\sigma(\zeta)$$

is a simple von Neumann polynomial. Stability regions can be defined (see [4]) in the $(h\xi, h^2\eta)$ -plane.

Strictly speaking, equation (6.14) is a system of ODEs

$$(6.17) \quad \left\{ \begin{array}{l} f' = \xi f + \eta z, \\ z' = f, \end{array} \right.$$

and the method (6.16) can be regarded as a combination of a LMS method $\{\tilde{\rho}, \tilde{\sigma}\}$ and a LMS method $\{\rho, \sigma\}$ for solving the first and second equation in (6.17), respectively. The stability analysis of such "combined" schemes has been treated previously. In [16] conditions for A-stability were derived, and in [4] stability regions are given for some first and second order methods. In this paper we give the stability regions of two classes of methods with orders ranging from 2 to 6. The methods originate from special choices of the LMS methods $\{\tilde{\rho}, \tilde{\sigma}\}$ and $\{\rho, \sigma\}$. For both classes we have chosen for

$\{\tilde{\rho}, \tilde{\sigma}\}$: the k -step backward differentiation formulae for $k = 2(1)6$.

Methods of Class I are now obtained by taking for

$\{\rho, \sigma\}$: the $(k-1)$ -step Adams-Moulton formulae for $k = 2(1)6$. With suitable starting quadrature rules, these formulae generate the well-known Gregory quadrature rules. The methods of Class I are denoted $\{BD;AM\}$.

Methods of Class II are obtained if we choose

$\{\rho, \sigma\}$: equal to $\{\tilde{\rho}, \tilde{\sigma}\}$. This choice generates the unconventional quadrature rules discussed in section 5. The methods of Class II are denoted $\{BD;BD\}$.

Since k -step BD methods and $(k-1)$ -step AM methods are of order k , both classes are of order k in view of theorem 6.3. In appendix IV the stability regions are presented and, as can be seen, the regions corresponding to the methods of Class II are substantially larger than those of the Class I methods.

7. NUMERICAL STABILITY AND THE ASYMPTOTIC REPETITION FACTOR

In this section we investigate the connection between asymptotic repetition factor and numerical stability of methods for solving second kind Volterra integral equations. We start by recalling the definition of (in)stability employed by NOBLE [19].

DEFINITION 7.1. A step-by-step method for solving a Volterra integral equation is said to be unstable if the error in the computed solution has dominant spurious components introduced by the numerical scheme.

Since Noble's analysis is asymptotic (as $h \rightarrow 0$) in nature, it is applicable to general second kind Volterra integral equations, that is, without any restrictions on the kernel K and the forcing function g . As a consequence his analysis establishes results with regard to *the suitability of a method for general use*.

Further we can adopt from BAKER & KEECH [3] the definitions of absolute and relative stability, which are related to the test equation

$$f(x) = 1 + \lambda \int_0^x f(y) dy.$$

With respect to this test equation, intervals (or regions) of absolute and relative stability can be determined. Because of its asymptotic character, however, Noble's analysis cannot be used to determine the size of the stability interval. Yet, it yields useful information on the *nature* of the stability interval, such as the existence of an interval of relative stability in the neighbourhood of the origin.

The definition 7.1 is a little vague, since it depends upon the interpretation of the term "dominant". From Noble's paper, however, we have good evidence that there is an equivalence between relative stability and stability in the sense of definition 7.1. This we formalize in the following definition.

DEFINITION 7.2. A quadrature method for solving second kind Volterra integral equations is stable in the sense of Noble if the method has an interval of relative stability of the form $(-\alpha, \beta)$ where $\alpha, \beta > 0$.

Adopting this definition, we then derive from theorem 3.3 and STETTER [21, p.271-275] for our class of methods the following theorem.

THEOREM 7.1. A (ρ, σ) -reducible quadrature method for solving second kind Volterra integral equations is stable in the sense of Noble iff the quadrature weights have an asymptotic repetition factor one.

The validity of this theorem for general quadrature methods is beyond the scope of this paper, and is left as a conjecture.

Stability in the sense of Noble (or relative stability) can be a severe requirement, in particular when the behaviour of the kernel or the solution is known beforehand. For instance when λ or $\partial K / \partial f$ is always negative, relative instability may be *harmless*. In such cases the spurious error components decay to zero; still, they are dominant in the sense that they decay at a smaller rate than the principal error component. The concept of absolute stability is then more appropriate, depending of course on the specific requirements imposed by the problem at hand.

Having indicated the connection between asymptotic repetition factor and relative instability, we give a few examples to demonstrate that there is *no connection between asymptotic repetition factor and absolute stability*.

The first example is an artificially constructed method from KEECH [10] (which is not (ρ, σ) -reducible). The quadrature weights are

$$(w_{n,j}) = \begin{bmatrix} 1/2 & 1/2 & & & & & & & & & \\ 1 & 0 & 1 & & & & & & & & \\ 0 & 2 & 1/2 & 1/2 & & & & & & & \\ 1 & 0 & 2 & 0 & 1 & & & & & & \\ & \cdot & \cdot & \cdot & & & & & & & \\ 0 & 2 & 0 & 2 & \dots & 0 & 2 & 1/2 & 1/2 & & \\ 1 & 0 & 2 & 0 & \dots & 2 & 0 & 2 & 0 & 1 & \\ & \cdot & \cdot & \cdot & & & & & & & \end{bmatrix}$$

The corresponding quadrature method for second kind equations has repetition factor 2 and an interval of absolute stability $(-2, 0)$; it is relatively unstable in the left-hand neighbourhood of the origin, and therefore unstable in the sense of Noble.

The second example is a method which is (ρ, σ) -reducible. We take the explicit LMS method (see LAMBERT [12, p.70])

$$y_n - y_{n-2} = h/2(f_{n-1} + 3f_{n-2}).$$

which has an interval of absolute stability $(-4/3, 0)$. Starting with the weights $w_{0,j} = 0$, $w_{1,0} = 1$, $w_{1,1} = 0$, our construction (2.5) yields the weights (with repetition factor 2)

$$(w_{n,j}) = \frac{1}{2} \begin{bmatrix} 0 \\ 2 & 0 \\ 3 & 1 & 0 \\ 2 & 3 & 1 & 0 \\ 3 & 1 & 3 & 1 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 2 & 3 & 1 & 3 & 1 & \dots & 3 & 1 & 0 \\ 3 & 1 & 3 & 1 & 3 & \dots & 1 & 3 & 1 & 0 \end{bmatrix}$$

Again the method is relatively unstable for small negative $h\lambda$.

In MCKEE & BRUNNER [17] other examples can be found.

8. CONCLUDING REMARKS

In this paper, we have employed linear multistep methods for solving ordinary differential equations to construct quadrature methods for solving functional equations of Volterra type. Of course, other methods for solving ODEs can be used: it is well-known that the use of Runge-Kutta methods yields quadrature methods of extended Runge-Kutta type (see e.g. BAKER [2]). The question whether generalizations of our results are possible if we employ cyclic linear multistep methods, multistep Runge-Kutta methods or other methods for solving ODEs is still open, and the answer to it will be the subject of further research. If such generalizations are possible, it is evident that we have a powerful tool for constructing and analyzing, in a unified way, high-order highly stable methods for solving Volterra type equations.

Further, we have introduced the concept of asymptotic repetition factor, and indicated its connection with the location of the zeros of the polynomial ρ . We have also shown the interrelationship of asymptotic repetition factor, stability in the sense of Noble and relative stability. Moreover, we have demonstrated by means of examples that there is no connection between absolute stability and repetition factor.

Numerical experiments with methods reducible to the backward differentiation methods have been performed for Volterra integro-differential equations and are reported in [8]. Experiments with the same methods for the solution of first and second kind equations will be reported in the near future.

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APPENDIX I: The starting quadrature rules

Here, we summarize for $k = 2(1)6$ interpolatory quadrature rules for obtaining the starting values I_0, \dots, I_{k-1} for (2.1). These rules are based on equidistant abscissae $x_j = x_0 + jh$. We have determined the weights $(w_{i,j}^{(k)})_{i,j=0}^{k-1}$ such that each quadrature rule is of maximal precision. We have put $w_{i,j}^{(k)} = w_{i,j}^*/D_k$, where $w_{i,j}^*$ and D_k are listed below (we have omitted the weights $w_{0,j}$ since these are all zero). Further, we list the order p and the error constant $C_i^{(k)}$ defined by

$$Q_i^{(k)}[\phi] = h \sum_{j=0}^{k-1} w_{i,j}^{(k)} \phi(x_j) - \int_{x_0}^{x_i} \phi(t) dt = C_i^{(k)} h^p \phi^{(p-1)}(\xi),$$

where $\xi \in [x_0, x_{k-1}]$ (this implies that a starting rule of order p is of precision $p-2$). The quadrature rules listed here can also be deduced from the block methods given by ROSSER [20, p.446-447].

k	D_k	j	$w_{j,0}^*$	$w_{j,1}^*$	$w_{j,2}^*$	$w_{j,3}^*$	$w_{j,4}^*$	$w_{j,5}^*$	p	$C_j^{(k)}$
2	2	1	1	1					3	1/12
3	12	1	5	8	-1				4	-1/24
		2	4	16	4				5	1/90
4	24	1	9	19	-5	1			5	19/720
		2	8	32	8	0			5	1/90
		3	9	27	27	9			5	3/80
5	720	1	251	646	-264	106	-19		6	-3/160
		2	232	992	192	32	-8		6	-1/90
		3	243	918	648	378	-27		6	-3/160
		4	224	1024	384	1024	224		7	8/945
6	1440	1	475	1427	-798	482	-173	27	7	863/60480
		2	448	2064	224	224	-96	16	7	37/3780
		3	459	1971	1026	1026	-189	27	7	29/2240
		4	448	2048	768	2048	448	0	7	8/945
		5	475	1875	1250	1250	1875	475	7	275/12096

APPENDIX II: The proof of theorem 6.1

PROOF. We will prove convergence at an arbitrary point $x \in [x_0, X]$. Let $Mh = x - x_0$ and $x_n = x_0 + nh$. Recall from (6.4) that f_n satisfies the scheme

$$(1) \quad h \sum_{j=0}^n w_{n,j} K(x_n, x_j) f_j = g(x_n), \quad n = k(1)M.$$

The exact solution of the integral equation satisfies

$$(2) \quad h \sum_{j=0}^n w_{n,j} K(x_n, x_j) f(x_j) = g(x_n) + T_n, \quad n = k(1)M,$$

where the truncation error T_n is given by

$$(3) \quad T_n = h \sum_{j=0}^n w_{n,j} K(x_n, x_j) f(x_j) - \int_{x_0}^{x_n} K(x_n, y) f(y) dy.$$

Subtracting (2) from (1) yields the equation for the global error

$$e_j = f_j - f(x_j)$$

$$(4) \quad h \sum_{j=0}^n w_{n,j} K(x_n, x_j) e_j + T_n = 0, \quad n = k(1)M,$$

where the errors in the starting values e_0, \dots, e_{k-1} are, by assumption, of order h^S . We will prove that $|e_M| = O(h^P) + O(h^S)$, as $h \rightarrow 0$ and $M \rightarrow \infty$ while $Mh = x - x_0$, and proceed as follows:

For $n \geq 2k$ and $i = O(1)k$ multiply the $(n-i)$ -th equation in (4) by a_i and take the summation over i to obtain

$$(5) \quad \sum_{i=0}^k a_i \sum_{j=0}^{n-i} w_{n-i,j} K(x_{n-i}, x_j) e_j + (1/h) \sum_{i=0}^k a_i T_{n-i} = 0, \quad n = 2k(1)M.$$

We will use the following abbreviations:

$$K^{(p,q)}(x,y) := \frac{\partial^{p+q}}{\partial x^p \partial y^q} K(x,y);$$

$$K_{n,j}^{(p,q)} := K^{(p,q)}(x_n, x_j); \quad K_{n,j} := K(x_n, x_j).$$

Expanding $K_{n-i,j}$ in a Taylor series about $x = x_n$ yields

$$(6) \quad K_{n-i,j} = K_{n,j} - ihK_{n,j}^{(1,0)} + i^2 h^2 \theta_{n-i,j}^2,$$

where, due to the smoothness of K , $|\theta_{n-i,j}| \leq \theta = \frac{1}{2} \max |K_{xx}|$. Substituting (6) into (5) and using the relations (2.4) for the weights, we arrive at

$$(7) \quad \begin{aligned} \sum_{i=0}^k b_i K_{n,n-i} e_{n-i} &= h \sum_{i=0}^k i a_i \sum_{j=0}^{n-i} w_{n-i,j} K_{n,j}^{(1,0)} e_j + \\ &- h^2 \sum_{i=0}^k i^2 a_i \sum_{j=0}^{n-i} w_{n-i,j} \theta_{n-i,j} e_j + \\ &- (1/h) \sum_{i=0}^k a_i T_{n-i}, \quad n = 2k(1)M. \end{aligned}$$

Expanding $K_{n,n-i}$ in a Taylor series about $y = x_n$ yields

$$(8) \quad K_{n,n-i} = K_{n,n} - ih\chi_{n,n-i},$$

where $|\chi_{n,n-i}| \leq \chi = \max |K_y|$.

Substitution of (8) into (7), and division by $K_{n,n}$ gives us

$$(9) \quad \begin{aligned} \sum_{i=0}^k b_i e_{n-i} &= h \sum_{i=1}^k d_{n,n-i}^{(1)} e_{n-i} + h \sum_{j=0}^{n-k-1} d_{n,j}^{(2)} e_j \\ &- h^2 \sum_{j=0}^{n-1} d_{n,j}^{(3)} e_j - T_n^*, \quad n = 2k(1)M, \end{aligned}$$

where we have introduced the abbreviations:

$$(10.a) \quad d_{n,n-i}^{(1)} := i b_i \chi_{n,n-i} / K_{n,n} + d_{n,n-i}^{(2)},$$

$$(10.b) \quad d_{n,j}^{(2)} := \sum_{i=1}^k i a_i w_{n-i,j} K_{n,j}^{(1,0)} / K_{n,n},$$

$$(10.c) \quad d_{n,j}^{(3)} := \sum_{i=1}^k i^2 a_i w_{n-i,j} \theta_{n-i,j} / K_{n,n},$$

$$(10.d) \quad T_n^* := \sum_{i=0}^k a_i T_{n-i} / (hK_{n,n}).$$

Since $w_{n,j}$, $\chi_{n,j}$, $\theta_{n,j}$ and $K_{n,j}^{(1,0)}$ are uniformly bounded and $|K_{n,n}| \geq \kappa = \min_{x \in [x_0, X]} |K(x, x)| \neq 0$, we readily see that the expressions defined in (10.a-c) are uniformly bounded.

Without loss of generality we assume that $b_0 \neq 0$. (If $b_0 = 0$ and b_j is the first non-zero coefficient, then equation (9) actually defines the error equation for e_{n-j} . In such a case the proof of this theorem requires no essential modifications.) As in HENRICI [7, p.242] we define the coefficients γ_n ($n \geq 0$) as the solution of the difference equation

$$(11) \quad \sum_{i=0}^k b_i \gamma_{n-i} = 0, \quad n \geq 1, \quad \gamma_{-k+1} = \dots = \gamma_{-1} = 0, \quad \gamma_0 = 1/b_0.$$

Since, by assumption, $\sum_{i=0}^k b_i \zeta^{k-i}$ is a simple von Neumann polynomial, the coefficients $|\gamma_n|$ are uniformly bounded.

Next we take a fixed N ($2k \leq N \leq M$), multiply (9) by γ_{N-n} for each $n = 2k(1)N$ and sum over n . For the left-hand side of (7) we then obtain

$$(12) \quad \sum_{n=2k}^k \gamma_{N-n} \sum_{i=0}^k b_i e_{n-i} = e_N + \sum_{n=2k}^{N-1} \left(\sum_{i=0}^k b_i \gamma_{N-n-i} \right) e_n + \sum_{n=k}^{2k-1} \left(\sum_{i=0}^k b_i \gamma_{N-n-i}^* \right) e_n = e_N + \sum_{j=k}^{2k-1} \left(\sum_{i=0}^k b_i \gamma_{N-j-i}^* \right) e_j,$$

by virtue of (11), and where γ_n^* is defined

$$\gamma_n^* := \begin{cases} \gamma_n & \text{if } n \leq N-2k, \\ 0 & \text{if } n > N-2k. \end{cases}$$

For the right-hand side of (9) the following 4 terms appear

$$(13) \quad h \sum_{n=2k}^N \gamma_{N-n} \sum_{i=1}^k d_{n,n-i}^{(1)} e_{n-i} = h \sum_{j=k}^{2k-1} \left(\sum_{i=1}^k d_{j+i,j}^{(1)} \gamma_{N-j-i}^* \right) e_j + h \sum_{j=2k}^{N-1} \left(\sum_{i=1}^k d_{j+i,j}^{(1)} \gamma_{N-j-i} \right) e_j;$$

$$(14) \quad h \sum_{n=2k}^N \gamma_{N-n} \sum_{j=0}^{n-k-1} d_{n,j}^{(2)} e_j = h \sum_{j=0}^{k-1} \left(\sum_{n=2k}^N d_{n,j}^{(2)} \gamma_{N-n} \right) e_j + \\ + h \sum_{j=k}^{N-k-1} \left(\sum_{n=j+k+1}^N d_{n,j}^{(2)} \gamma_{N-n} \right) e_j;$$

$$(15) \quad h^2 \sum_{n=2k}^N \gamma_{N-n} \sum_{j=0}^{n-1} d_{n,j}^{(3)} e_j = h^2 \sum_{j=0}^{2k-1} \left(\sum_{n=2k}^N d_{n,j}^{(3)} \gamma_{N-n} \right) e_j + \\ + h^2 \sum_{j=2k}^{N-1} \left(\sum_{n=j+1}^N d_{n,j}^{(3)} \gamma_{N-n} \right) e_j;$$

and finally

$$(16) \quad \sum_{n=2k}^N \gamma_{N-n} T_n^*.$$

The second term in the last expression of (12) is bounded by $A_1 \sum_{j=k}^{2k-1} |e_j|$, since b_i and γ_n^* are uniformly bounded.

The term (13) is bounded by $hA_2 \sum_{j=k}^{N-1} |e_j|$, since $d_{n,j}^{(1)}$ and γ_n are uniformly bounded.

The term (15) is bounded by $hA_3 \sum_{j=0}^{N-1} |e_j|$, since $d_{n,j}^{(3)}$ and γ_n are uniformly bounded and $Nh \leq X - x_0$. (Note that the constants A_i are independent of N .)

The task of finding uniform bounds for the terms (14) and (16) appears to be more involved and requires careful attention to details. We have isolated certain subproblems which appear as lemmas in Appendix III.

Consider the first term of the right-hand side of (14); for each $j = 0(1)k-1$ we have to show that

$$\left| \sum_{n=2k}^N d_{n,j}^{(2)} \gamma_{N-n} \right|$$

is bounded uniformly in N . Recall from (10.b) that $d_{n,j}^{(2)}$ is defined as a finite sum of terms. Therefore, it is sufficient to prove that for each $i = 1(1)k$

$$\left| \sum_{n=2k}^N \gamma_{N-n} w_{n-i,j} K_{n,j}^{(1,0)} / K_{n,n} \right|$$

is bounded uniformly in N . Since, by assumption, $K^{(1,0)}(x, x_j)/K(x, x)$ is continuously differentiable, it follows from application of Lemma 3.b, that it is sufficient to prove that for each $j = 0(1)k-1$ and each $i = 1(1)k$

$$(17) \quad \left| \sum_{n=m}^N \gamma_{N-n} w_{n-i, j} \right|$$

is uniformly bounded for all m and N ($2k \leq m \leq N$). If we define $\delta_n := w_{n-i, j}$ for fixed i and j , then δ_n satisfies $\sum_{i=0}^k a_i \delta_{n-i} = 0$. Moreover γ_n satisfies (11), and, hence, application of Lemma 2.b establishes the uniform boundedness of (17).

Next we consider the second term of the right-hand side of (14). Similar reasoning as above (using Lemma 3.b), yields that we have to prove that for each $j = k(1)N-k-1$

$$\left| \sum_{n=m}^N \gamma_{N-n} w_{n-i, j} \right|$$

is uniformly bounded in m and N , ($j+k+1 \leq m \leq N$). Moreover, we have to show that this uniform bound is *independent of j* , since j runs through a set the upperbound of which depends upon N . This we prove as follows.

For $j = k$, one proves, as we did for (17), that there exists a constant D_k independent of m and N such that

$$(18) \quad \left| \sum_{n=m}^N \gamma_{N-n} w_{n-i, k} \right| \leq D_k, \quad (2k+1 \leq m \leq N).$$

For $j > k$, one has to find a uniform upperbound for

$$\left| \sum_{n=m}^N \gamma_{N-n} w_{n-i, j} \right|,$$

independent of m^* and N ($j+k+1 \leq m^* \leq N$), and independent of j . Recall from (2.8) that $w_{n-i, j} = w_{n-i-j+k, k}$. Therefore,

$$(19) \quad \left| \sum_{n=m}^N \gamma_{N-n} w_{n-i, j} \right| = \left| \sum_{n=m}^{N^*} \gamma_{N^*-n} w_{n-i, k} \right|,$$

where $N^* = N-j+k$ and $2k+1 \leq m \leq N^*$. The last expression in (19), however, is bounded by D_k by virtue of the result (18).

Hence, we have shown that (14) is bounded by $hA_4 \sum_{j=0}^{N-k-1} |e_j|$.

Finally, we investigate the term (16). If we define $\psi(x,y) := K(x,y)f(y)$, then the truncation error T_{n-i} defined in (3) is given by the quadrature error in the approximation of the integral of the function $\psi(x_{n-i}, \cdot)$ on the interval $[x_0, x_{n-i}]$ (see (4.1)); that is

$$T_{n-i} = Q_{n-i}[\psi(x_{n-i}, \cdot)].$$

Expanding the function $\psi(x_{n-i}, y)$ in a Taylor series about $x = x_n$ the truncation error can be split into

$$\begin{aligned} T_{n-i} &= Q_{n-i}[\psi(x_n, \cdot)] - ihQ_{n-i}[\psi^{(1,0)}(x_n, \cdot)] \\ &\quad + \frac{1}{2}i^2 h^2 Q_{n-i}[\psi^{(2,0)}(\xi_{n-i}, \cdot)], \quad \xi_{n-i} \in [x_{n-i}, x_n]. \end{aligned}$$

Next we form $\sum_{i=0}^k a_i T_{n-i}$ and obtain the following terms:

$$\sum_{i=0}^k a_i Q_{n-i}[\psi(x_n, \cdot)] = -C_{p+1} h^{p+1} \psi^{(0,p)}(x_n, x_n) + O(h^{p+2}),$$

by virtue of (4.2);

$$\begin{aligned} h \sum_{i=0}^k i a_i Q_{n-i}[\psi^{(1,0)}(x_n, \cdot)] &= \\ - \sum_{i=0}^k i a_i C_{p+1} / \sigma(1) h^{p+1} \{ \psi^{(1,p-1)}(x_n, x_{n-i}) - \psi^{(1,p-1)}(x_n, x_0) \} + O(h^{p+2}) &= \\ - C_{p+1} h^{p+1} \{ \psi^{(1,p-1)}(x_n, x_n) - \psi^{(1,p-1)}(x_n, x_0) \} + O(h^{p+2}), & \end{aligned}$$

by virtue of (4.5), and

$$\frac{1}{2} h^2 \sum_{i=0}^k i^2 a_i Q_{n-i}[\psi^{(2,0)}(\xi_{n-i}, \cdot)] = O(h^{p+2}).$$

Hence T_n^* defined by (10.d) has the form

$$\begin{aligned} T_n^* &= -(1/K_{n,n}) h^p C_{p+1} \{ \psi^{(0,p)}(x_n, x_n) - \psi^{(1,p-1)}(x_n, x_n) + \\ (20) \quad &\quad \psi^{(1,p-1)}(x_n, x_0) \} + O(h^{p+1}). \end{aligned}$$

Note that we have to prove that (16) is uniformly bounded. It is easily seen that the terms of $O(h^{p+1})$ in (20) yield, due to the boundedness of γ_n , a term of $O(h^p)$ in (16). Omitting, therefore, the $O(h^{p+1})$ -terms in (20) and observing that the functions $\psi^{(0,p)}(x,x)/K(x,x)$, $\psi^{(1,p-1)}(x,x)/K(x,x)$ and $\psi^{(1,p-1)}(x,x_0)/K(x,x)$ are continuously differentiable on $[x_0, X]$, application of Lemma 3.a yields that the expression (16) is uniformly bounded if $|\sum_{n=2k}^N \gamma_{N-n} T_n^*|$ is uniformly bounded for all m and N , ($2k \leq m \leq N$). This, however, follows directly from Lemma 2.a. Hence, we have shown that

$$\left| \sum_{n=2k}^N \gamma_{N-n} T_n^* \right| \leq A_5 h^p.$$

Piecing the bits together, we have shown that

$$|e_N| \leq A_5 h^p + A_6 \sum_{j=0}^{2k-1} |e_j| + h A_7 \sum_{j=2k}^{N-1} |e_j|, \quad N = 2k(1)M,$$

where A_5, A_6 and A_7 are independent of h and N (and thus independent of M). The solution of this recursive inequality is well-known to be (see e.g. HENRICI [7, p.244], BAKER [1, p.925])

$$(21) \quad |e_M| \leq \{A_5 h^p + A_6 \sum_{j=0}^{2k-1} |e_j|\} \exp(A_7(x-x_0)), \quad x-x_0 = Mh,$$

The errors e_0, \dots, e_{k-1} are $O(h^s)$. The error e_k is defined in (4) and is readily seen to be $O(h^s) + O(h^{-1}T_k)$. From (4.5) we derive that

$$\begin{aligned} T_k &= -C_{p+1}/\sigma(1)h^p \{\psi^{(1,p-1)}(x_k, x_k) - \psi^{(1,p-1)}(x_k, x_0)\} + O(h^{p+1}) \\ &= -C_{p+1}/\sigma(1)kh^{p+1} \psi^{(1,p)}(x_k, \xi_k) + O(h^{p+1}) \\ &= O(h^{p+1}), \end{aligned}$$

and, therefore $e_k = O(h^s) + O(h^p)$. Similarly one shows that the errors e_{k+1}, \dots, e_{2k-1} are $O(h^s) + O(h^p)$, and together with (21) this establishes that $|e_M| = O(h^s) + O(h^p)$. This completes the proof. \square

APPENDIX III: Lemmas

In the following lemmas \mathbb{C} denotes the set of complex numbers, and \mathbb{Z}^+ the set of non-negative integers; $\rho(\zeta)$ and $\sigma(\zeta)$ are the polynomials (with real coefficients) $\sum a_i \zeta^{k-i}$ and $\sum b_i \zeta^{k-i}$, respectively.

In the proof of theorem 6.1 the lemmas 2.a, 2.b, 3.a and 3.b are used; the proof of these lemmas uses the lemmas 1.a and 1.b.

LEMMA 1.a: Let $c_n = n^\alpha \zeta^n$, where $\zeta \in \mathbb{C}$ and $\alpha \in \mathbb{Z}^+$. If $|\zeta| \leq 1$, $\zeta \neq 1$ and $\alpha = 0$ whenever $|\zeta| = 1$, then $\left| \sum_{n=m}^N c_{N-n} \right|$ is uniformly bounded for all m and N ($m \leq N$).

PROOF. It is elementary to prove that, under the conditions stated above, $\left| \sum_{n=0}^N n^\alpha \zeta^n \right|$ is uniformly bounded for all N . The statement of the lemma follows from the observation that $\sum_{n=m}^N c_{N-n} = \sum_{n=0}^{N-m} c_n$. \square

LEMMA 2.a: Let γ_n satisfy the difference equation $\sum_{i=0}^k b_i \gamma_{n-i} = 0$. If $\sigma(\zeta)$ is a simple von Neumann polynomial with $\sigma(1) \neq 0$, then $\left| \sum_{n=m}^N \gamma_{N-n} \right|$ is uniformly bounded for all m and N ($m \leq N$).

PROOF. γ_n can be written as a finite sum of terms of the form $n^\alpha \zeta^n$, where ζ is a zero of σ and α is related to the multiplicity of that zero. Applying Lemma 1.a to each term completes the proof. \square

Next we give a "two-dimensional" analogue of the lemmas 1.a and 2.a.

LEMMA 1.b: Let $c_n = n^\alpha \zeta^n$ and $d_n = n^\beta \xi^n$, where $\zeta, \xi \in \mathbb{C}$ and $\alpha, \beta \in \mathbb{Z}^+$. If $|\zeta| \leq 1$, $|\xi| \leq 1$, $\zeta \neq \xi$, $\alpha = 0$ whenever $|\zeta| = 1$ and $\beta = 0$ whenever $|\xi| = 1$, then $\left| \sum_{n=m}^N c_{N-n} d_n \right|$ is uniformly bounded for all m and N ($m \leq N$).

PROOF. We consider only the case that $|\zeta| \leq |\xi|$. (The case $|\zeta| > |\xi|$ is treated along similar lines.) Defining $w = \zeta/\xi$ we may write

$$\sum_{n=m}^N c_{N-n} d_n = \xi^N \sum_{n=m}^N (N-n)^\alpha n^\beta w^{N-n}.$$

Note that $|w| \leq 1$ and $w \neq 1$ since $\zeta \neq \xi$. Next we distinguish between the cases $|\xi| = 1$ and $|\xi| < 1$.

(i) $|\xi| = 1$. In this case $\beta = 0$ and thus

$$\left| \sum_{n=m}^N c_{N-n} d_n \right| = \left| \sum_{n=m}^N (N-n)^\alpha w^{N-n} \right|,$$

which is uniformly bounded in view of Lemma 1.a.

(ii) $|\xi| < 1$. In this case we write

$$\begin{aligned} \left| \sum_{n=m}^N c_{N-n} d_n \right| &= \left| \xi^N N^{\alpha+\beta} \right| \left| \sum_{n=m}^N \left(\frac{N-n}{N}\right)^\alpha \left(\frac{n}{N}\right)^\beta w^{N-n} \right| \\ &\leq \left| \xi^N N^{\alpha+\beta+1} \right|, \end{aligned}$$

which is readily seen to be uniformly bounded. \square

LEMMA 2.b: Let γ_n and δ_n satisfy the difference equation $\sum_{i=0}^k b_i \gamma_{n-i} = 0$ and $\sum_{i=0}^k a_i \delta_{n-i} = 0$, respectively. If the polynomials ρ and σ have no common factor and are simple von Neumann, then $\left| \sum_{n=m}^N \gamma_{N-n} \delta_n \right|$ is uniformly bounded for all m and N ($m \leq N$).

PROOF. γ_n can be written as a linear combination of terms of the form $c_n = n^\alpha \zeta^n$. Likewise, δ_n has components of the form $d_n = n^\beta \xi^n$. Hence, the product $\gamma_{N-n} \delta_n$ has terms of the form $c_{N-n} d_n$. Applying Lemma 2.a to each of the terms $\left| \sum_{n=m}^N c_{N-n} d_n \right|$ completes the proof. \square

We also need the following lemmas.

LEMMA 3.a: Let the function ϕ be continuously differentiable on $[x_0, X]$; let $x_n = x_0 + nh$ and $Nh \leq X - x_0$ and let $\{\gamma_n\}_{n=0}^\infty$ be a sequence of complex numbers. Then $\left| \sum_{n=n_0}^N \gamma_{N-n} \phi(x_n) \right|$ is uniformly bounded for all N if $\left| \sum_{n=m}^N \gamma_{N-n} \right|$ is uniformly bounded for all m and N ($n_0 \leq m \leq N$).

PROOF. Let $\Gamma_{N-n} := \sum_{j=n}^N \gamma_{N-j}$, $\Gamma_0 := \gamma_0$, $\Gamma_{-1} := 0$. Then

$$\begin{aligned} \sum_{n=n_0}^N \gamma_{N-n} \phi(x_n) &= \sum_{n=n_0}^N (\Gamma_{N-n} - \Gamma_{N-n-1}) \phi(x_n) \\ &= \Gamma_{N-n_0} \phi(x_{n_0}) + \sum_{n=n_0+1}^N \Gamma_{N-n} (\phi(x_n) - \phi(x_{n-1})) \end{aligned}$$

$$= \Gamma_{N-n_0} \phi(x_{n_0}) + \sum_{n=n_0+1}^N \Gamma_{N-n} h \phi'(\xi_n), \quad \xi_n \in [x_{n-1}, x_n].$$

Therefore

$$\left| \sum_{n=n_0}^N \gamma_{N-n} \phi(x_n) \right| \leq \Gamma^* (\max |\phi| + (X-x_0) \max |\phi'|),$$

where Γ^* is the uniform bound of $\left| \sum_{n=m}^N \gamma_{N-n} \right|$. \square

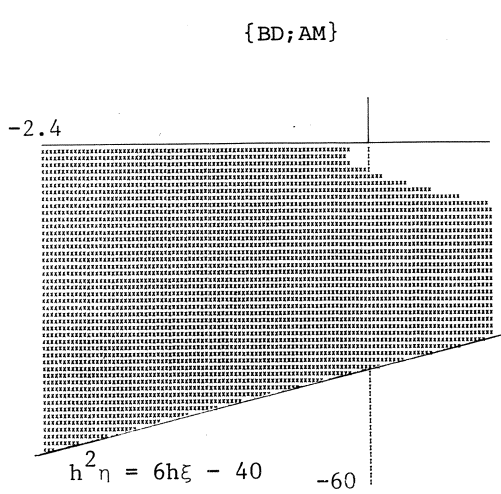
The "two-dimensional" analogue of lemma 3.a reads:

LEMMA 3.b: In addition to Lemma 3.a, let $\{\delta_n\}_{n=0}^{\infty}$ be a sequence of complex numbers. Then $\left| \sum_{n=n_0}^N \gamma_{N-n} \delta_n \phi(x_n) \right|$ is uniformly bounded for all N if $\left| \sum_{n=m}^N \gamma_{N-n} \delta_n \right|$ is uniformly bounded for all m and N ($n_0 \leq m \leq N$).

PROOF. Similar to the proof of lemma 3.a. \square

APPENDIX IV: Stability regions

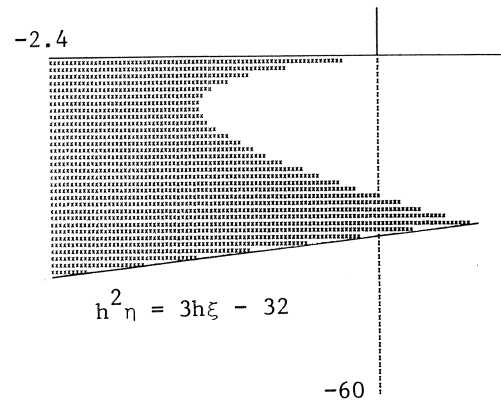
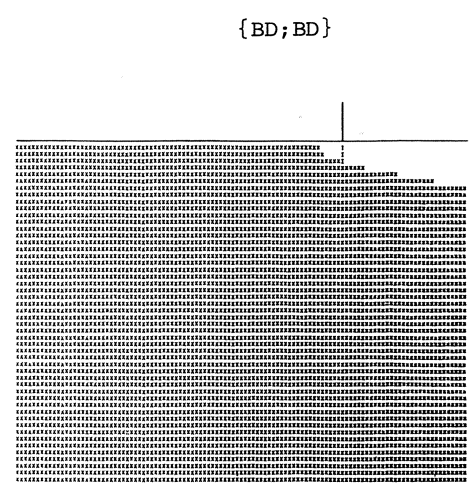
We present here the stability regions in the $(h\xi, h^2\eta)$ -plane of the {BD;AM} and the {BD;BD} methods. The shaded areas indicate stability. Since the integral equation itself is stable only in the third quadrant, we have confined ourselves to this quadrant (and a small strip in the fourth quadrant). The regions are displayed for $k = 3, 4, 5$ and 6 (for $k = 2$ the stability region contains the *whole* third quadrant). These regions can also be found in [8].



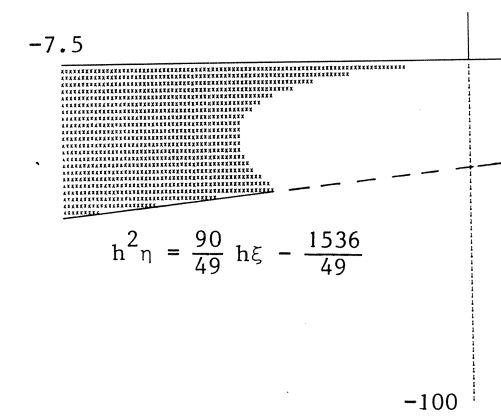
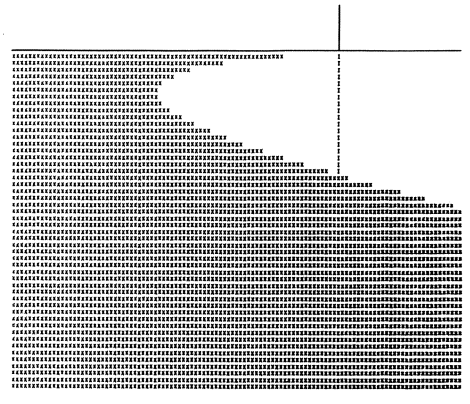
h^2_{η}

$h\xi$

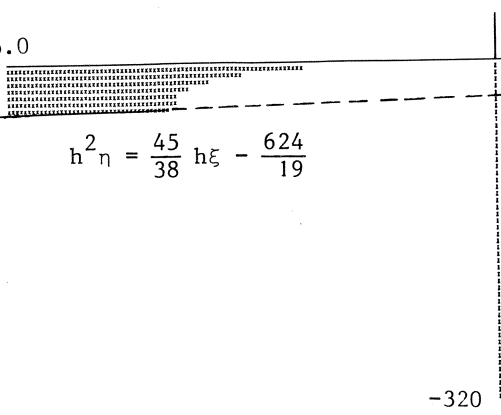
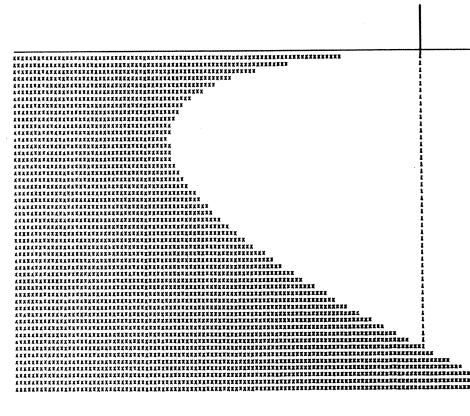
$k = 3$
units:
→ 0.03
↑ 1.2



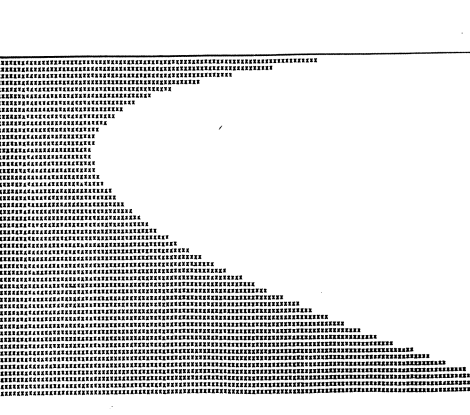
$k = 4$
units:
→ 0.03
↑ 1.2



$k = 5$
units:
→ 0.075
↑ 2.0



$k = 6$
units:
→ 0.125
↑ 6.4



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