

ANNALES ACADEMIAE SCIENTIARUM FENNICAE

Series A

I. MATHEMATICA

503

ON A GENERALIZED INTERPOLATION APPROACH
TO THE NUMERICAL INTEGRATION OF
ORDINARY DIFFERENTIAL
EQUATIONS

BY

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HELSINKI 1971
SUOMALAINEN TIEDEAKATEMIA

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Communicated 13 September 1971 by PENTTI LAASONEN

KESKUSKIRJAPAINO
HELSINKI 1971

Preface

The basic idea of this work is the use of interpolation polynomials in connection with the numerical solution of ordinary differential equations. This idea came into my mind during a seminar on discrete variable methods in differential equations conducted by Professor Pentti Laasonen in the autumn of 1969. The main results were obtained during the spring and summer of 1971.

My gratitude is due to Professor Pentti Laasonen for a thorough introduction into numerical analysis, and for kind encouragement and helpful discussions.

I wish to thank the whole staff of the Institute of Mathematics, Helsinki University of Technology, for their help, interest and patient listening to my problems.

The financial assistance of the E. Aaltonen Foundation and the A. Kordelin Foundation and the Helsinki University of Technology made it possible for me to devote my time to this study. This support is gratefully acknowledged.

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1. INTRODUCTION

Consider the vector valued initial value problem on a closed interval $I = [a, b]$:

$$(1.1) \quad \mathbf{x}' = \mathbf{f}(t, \mathbf{x}); \quad \mathbf{x}(a) = \mathbf{x}_0 \quad (' = d/dt).$$

Commonly, an approximate numerical solution of (1.1) is constructed by taking a set of nodes,

$$(1.2) \quad T_M = \{t_i | i = 0, 1, \dots, M; t_0 = a, t_i < t_{i+1}\} \subset I,$$

and associating a vector \mathbf{X}_i with every t_i ($i = 0, 1, \dots, M$). For $n = 0, 1, \dots, M - k$, the vectors \mathbf{X}_i are constructed by means of the difference equations

$$(1.3) \quad \mathbf{F}_n(\mathbf{X}_n, \mathbf{X}_{n+1}, \dots, \mathbf{X}_{n+k}) = \mathbf{0},$$

from which \mathbf{X}_i , with maximum index i , is derived as a function of the known, lower indexed \mathbf{X}_i 's. The operators \mathbf{F}_n are so chosen that \mathbf{X}_i is in some sense an approximation to the solution $\mathbf{x}(t)$ of (1.1) at $t = t_i$.

In the two most widely used classes of discrete variable methods, one-step methods (mainly of the Runge-Kutta type) and linear multistep methods (cf. [23], [31]), the operators \mathbf{F}_n are independent of n . In the latter, the nodes are equally spaced.

Various ideas have been applied for construction of the operators \mathbf{F}_n . The following possibilities may be mentioned as a natural background for the present work.

In derivations that lead to linear multistep methods, the components of $\mathbf{f}(t, \mathbf{x})$ have been replaced by a Lagrange interpolation polynomial, and then integrated, or the components of $\mathbf{x}(t)$ have been approximated by a Lagrange interpolation polynomial, and then differentiated [23]. Dahlquist [13], [23] has generalized the difference equations obtained by these ideas to the classical linear multistep methods, without any close connection with interpolation.

The idea of interpolation has been extended for instance by Salzer [46] and Quade [43], who applied Hermite interpolation in order to derive some linear multistep methods. Unfortunately, these methods are unstable. The idea of interpolation has also been presented by Osborne [38].

Another approach involves the use of truncated Taylor series for the determination of unknown parameters in the operator \mathbf{F}_n . This idea is exemplified by the Runge-Kutta methods.

Inspired by the use of interpolation polynomials for the construction of the operators \mathbf{F}_n , some authors have proposed other different approximating functions for the components of $\mathbf{f}(t, \mathbf{x})$ and $\mathbf{x}(t)$. Instead of polynomials, Brock and Murray [4] have used linear combinations of exponential functions, Gautschi [17] has used trigonometric polynomials, and Lambert and Shaw [28, 29, 30] have applied rational approximations and polynomials, added with a non-polynomial term which can be singular. Loscalzo has studied the application of spline functions to initial value problems (cf. [33] and also [11]).

Lambert [27] has generalized the classical linear multistep methods with constant coefficients to similar methods with mildly varying coefficients. Also Brunner [5, 6, 7] has used coefficients which are linear functions of the step size.

As a rule the nodes t_i have been equidistant, although in some cases it would be very desirable to change the spacing of the nodes. No more than a few multistep methods with varying step size have been presented. We shall mention the method of Nordsieck [36, 39], which is equivalent to the Adams method [23] when the step size is constant. Krogh [26] has made another generalization of the Adams method; in addition to the step size, this also permits the integer k in \mathbf{F}_n to be dependent on n . Krogh's method is suitable for differential equations of higher order as well. A third generalization of the Adams method is that made by Piotrowski [41].

Another way of generalizing the linear multistep methods with constant step size is by means of introducing some additional nodes between the equally spaced nodes. This leads to the so-called hybrid methods introduced by Gragg and Stetter [21], Butcher [8], [10] and Gear [18], and reviewed in [31]. The hybrid methods fall somewhere between linear multistep methods and Runge-Kutta methods. Butcher [9] has presented unifying formalism which covers not only Runge-Kutta and multistep methods but also hybrid methods and some others. Other unifying techniques have been proposed by Gear [20], and Papian and Ball [40].

Our aim here is the construction of some reasonable operators \mathbf{F}_n . As a result we generalize the classical multistep methods, but our starting point is not a linear multistep method with constant coefficients. Our method is based on the idea of Hermite-Birkhoff interpolation [48] by means of generalized polynomials [12]. This idea is present in Dyer [15], too. Let k be a given constant. Then for every index n we associate a generalized polynomial y_{nj} with the j :th component of \mathbf{X}_{n+k} . These polynomials are linear combinations of prescribed continuous functions

with unknown coefficients. To fix these coefficients we require the following

$$(1.4) \quad \begin{cases} y_{nj}(t_{n+i}) = \mu_i X_{n+i}^j & \text{for some values of } i = 0, 1, \dots, k-1, \\ y'_{nj}(t_{n+i}) = \mu'_i f^j(t_{n+i}, \mathbf{X}_{n+i}) & \text{for some values of } i = 0, 1, \dots, k, \end{cases}$$

where the superscript j indicates the j :th component of \mathbf{X}_{n+i} , or \mathbf{f} respectively. The constants μ_i and μ'_i are fixed previously, and usually have values near to one. The value of X_{n+k}^j is then obtained as a function of the known values \mathbf{X}_{n+i} , by stating

$$(1.5) \quad X_{n+k}^j = y_{nj}(t_{n+k}).$$

Thus the operators \mathbf{F}_n have been implicitly constructed. The nodes of T_M may be arbitrarily spaced.

Our basic goal is to discuss a unifying method for constructing the operators \mathbf{F}_n , and to study the consequences of our approach.

In chapter 2 we give the problem and make some preparatory assumptions and definitions.

In chapter 3 we present the basic construction principles (paragraph 3.1) of our generalized polynomial interpolation approach to the initial value problem. These principles implicitly define the operators \mathbf{F}_n .

Given the construction principles, it is natural to ask the circumstances under which the construction is possible. This question is studied in the following paragraph, 3.2, in which we give two existence theorems for our construction. We use some results from the general theory of finite interpolation and Hermite-Birkhoff interpolation. This background material is presented, and applied to our case in Appendix 1.

Paragraph 3.3 is devoted to explicit formulation of our construction. There the connection between our method and the classical linear multi-step methods is brought out. Paragraph 3.4 contains some detailed discussion of the most important case, the use of the usual polynomials as interpolants.

Chapter 4 is very similar to some parts of the book of Henrici [22]. The results of chapter 4 concerning stability, consistency, convergence and errors of our method are obtained by slight modifications of those of Henrici. Therefore we use the notations and definitions of Henrici as far as possible.

Chapter 5 provides illustrative examples of our method and shows how some earlier published methods, and new methods, can be derived by our approach.

Our construction leads to the following results. As a natural assumption of existence and uniqueness related to our method, let us assume that we have as many equations (1.4) as we have coefficients in the expression of y_{nj} , and that (1.4) will determine these constants uniquely. Then (1.5)

leads to an expression similar to linear multistep methods, except that the coefficients and the step size in general are functions of n . If a constant step size h is used, the coefficients of the resulting difference equation are usually functions of h , but independent of n . When the generalized polynomials are «usual» polynomials, and the step size is constant, our method reduces to classical linear multistep methods with constant coefficients.

Our construction will cover most of the linear multistep methods with constant coefficients, the variable step size versions of these methods, and a number of methods based on nonpolynomial approximations. In addition, we are able to discover many new methods.

2. PROBLEM, ASSUMPTIONS, DEFINITIONS

We want to construct numerical solutions to the initial value problem (1.1). The definitions of this chapter are based on Henrici [22]. We assume that $I = [a, b]$ is a closed finite interval of real numbers. The vectors associated with problem (1.1) belong to the real normed Q -dimensional space Y_Q . The components of $\mathbf{x} \in Y_Q$ are denoted by x^1, x^2, \dots, x^Q . Usually the norm of x is defined by

$$(2.1) \quad \|\mathbf{x}\| = \sum_{i=1}^Q |x^i|,$$

but other norms are also applicable.

We assume that $\mathbf{f}(t, \mathbf{x}) \in Y_Q$ and \mathbf{f} is an L -function, i.e. a continuous function from $I \times Y_Q$ to Y_Q , satisfying the uniform Lipschitz-condition

$$(2.2) \quad \|\mathbf{f}(t, \mathbf{x}) - \mathbf{f}(t, \mathbf{z})\| \leq L \|\mathbf{x} - \mathbf{z}\|$$

for all $t \in I$, $\mathbf{x} \in Y_Q$, $\mathbf{z} \in Y_Q$. With these assumptions, the problem (1.1) has a unique solution on I for all $\mathbf{x}_0 \in Y_Q$. For a fixed \mathbf{x}_0 , we denote the solution of (1.1) by $\mathbf{x}(t)$.

Let us denote the set of consecutive integers by $J_n = \{0, 1, \dots, n\}$. Given the set T_M defined in (1.2), we relate a certain vector $\mathbf{X}_i(M) \in Y_Q$ to the solution vector $\mathbf{x}(t_i)$ at every $t_i \in T_M$. The approximation $\mathbf{X}_i(M)$, which is considered as an approximation of $\mathbf{x}(t_i)$, is obtained as a solution of a certain difference equation

$$(2.3) \quad \mathbf{F}_{i-k}(\mathbf{X}_{i-k}(M), \mathbf{X}_{i-k+1}(M), \dots, \mathbf{X}_i(M)) = \mathbf{0},$$

where k is a fixed integer. Here, \mathbf{F} is a given function from J_{M-k} and from the $(k+1)$ -fold Cartesian product of a subset of Y_Q with itself to Y_Q .

Equation (2.3) will define $\mathbf{X}_i(M)$ as a function of the k preceding

approximations $\mathbf{X}_{i-k}(M)$, $\mathbf{X}_{i-k+1}(M)$, \dots , $\mathbf{X}_{i-1}(M)$. Therefore we assume that there exists a proper *starting procedure*, which produces the first k approximations $\mathbf{X}_0(M)$, $\mathbf{X}_1(M)$, \dots , $\mathbf{X}_{k-1}(M)$. It is assumed that these starting vectors have been used, unless otherwise indicated. Naturally, the functions \mathbf{F}_{i-k} are so chosen that $\mathbf{X}_i(M)$ uniquely exists for every $t_i \in T_M$. The explicit expression of \mathbf{F}_i is derived in chapter 3.

On occasion, \mathbf{X}_i is written instead of $\mathbf{X}_i(M)$.

The behaviour of the approximations $\mathbf{X}_i(M)$ will be studied when the density of nodes t_i is increased. Let us denote $h_i = t_i - t_{i-1}$ for $i = 1, 2, \dots, M$ and

$$(2.4) \quad h_M^* = \max_{i=1,2,\dots,M} h_i.$$

We assume that when $M \rightarrow \infty$, $h_M^* \rightarrow 0$ so that Mh_M^* remains bounded above, i.e. there exists a constant C such that

$$(2.5) \quad Mh_M^* \leq C, \quad M = 1, 2, \dots.$$

Further, we must assume that constants C_1 and C_2 exist such that for every M and for every $i = 1, 2, \dots, M-1$

$$(2.6) \quad 0 < C_1 \leq \frac{h_{i+1}}{h_i} \leq C_2.$$

For a fixed M , we define a k -vector \mathbf{h}_n by

$$(2.7) \quad \mathbf{h}_n = (h_{n+1}, h_{n+2}, \dots, h_{n+k})^T \quad \forall n \in J_{M-k}.$$

A starting procedure is called *bounded*, if a constant S exists such that

$$(2.8) \quad \|\mathbf{X}_i(M)\| \leq S, \quad i = 0, 1, \dots, k-1,$$

for all sufficiently large M . A starting procedure is called *compatible* with the given initial value problem (1.1), if

$$\lim_{M \rightarrow \infty} \mathbf{X}_i(M) = \mathbf{x}_0 \quad \text{for } i = 0, 1, \dots, k-1.$$

The procedure for generation of the vectors \mathbf{X}_i , $i \in J_M \setminus J_{k-1}$ is called an approximating method for the numeral solution of the problem (1.1). Since the most essential characteristic of a method is the equation (2.3) we call the method associated with (2.3) an **F**-method.

An approximating **F**-method is called *stable*, if for every L -function \mathbf{f} , and for all starting procedures bounded with some constant S , and with $M > M_0$, a constant S' exists such that

$$\max_{i \in J_M} \|\mathbf{X}_i(M)\| \leq S' \quad \text{for all } M > M_0.$$

Here M_0 is a sufficiently large constant; a more precise statement is given in (3.15). The stability of a method implies that the approximate solution remains uniformly bounded as $M \rightarrow \infty$. However, the bound S' may depend on the bound S of the starting procedures.

An **F**-method is called *consistent*, if for all L -functions \mathbf{f} the following is true: if \mathbf{x} denotes any solution of the differential equation $\mathbf{x}' = \mathbf{f}(t, \mathbf{x})$, then

$$(2.9) \quad \max_{i \in J_{M-k}} \|\mathbf{F}_i(\mathbf{x}(t_i), \mathbf{x}(t_{i+1}), \dots, \mathbf{x}(t_{i+k}))\| = o(h_M^*),$$

when $M \rightarrow \infty$.

An **F**-method is called *convergent*, if for all L -functions \mathbf{f} , and for all initial value vectors $\mathbf{x}_0 \in Y_Q$,

$$(2.10) \quad \lim_{M \rightarrow \infty} \max_{i \in J_M} \|\mathbf{X}_i(M) - \mathbf{x}(t_i)\| = 0,$$

when \mathbf{x} is the solution of the initial value problem (1.1) and the approximation $\mathbf{X}_i(M)$ is obtained by the aid of any bounded and compatible starting procedure.

The *order* of an **F**-method is defined as the largest integer q such that

$$(2.11) \quad \max_{i \in J_{M-k}} \|\mathbf{F}_i(\mathbf{x}(t_i), \mathbf{x}(t_{i+1}), \dots, \mathbf{x}(t_{i+k}))\| = O(h_M^{*q+1})$$

for all solutions \mathbf{x} of all initial value problems (1.1) where \mathbf{f} is continuously differentiable of sufficiently high order.

The error **E** defined by

$$(2.12) \quad \mathbf{E}_i = \mathbf{X}_i - \mathbf{x}(t_i), \quad \forall i \in J_M$$

is called the *discretization error* of the **F**-method. The error is totally defined by the problem (1.1), and the given approximating **F**-method with the starting procedure applied. It is assumed that all the calculations are exact. In practice another error will be caused by approximation of the real numbers by the very special rational numbers used in the computation machinery, whatever it may be. Thus, the actual computation produces a vector $\tilde{\mathbf{X}}_i$, instead of the exact vector \mathbf{X}_i . The difference

$$(2.13) \quad \mathbf{r}_i = \tilde{\mathbf{X}}_i - \mathbf{X}_i, \quad \forall i \in J_M,$$

is called the *round-off error*.

3. CONSTRUCTION OF THE OPERATORS F_n

3.1. Construction principles

Given an L -function \mathbf{f} , a set T_M , a fixed integer k , and vectors $\mathbf{X}_0, \mathbf{X}_1, \dots, \mathbf{X}_{k-1}$ produced by a bounded starting procedure compatible with a given initial value vector \mathbf{x}_0 , our generalized polynomial interpolation method for the initial value problem (1.1) is defined by the following rules of construction:

- i) Assume: given sets $F \subset J_{k-1}$ with $K \geq 1$ elements and $D \subset J_k$ with $L \geq 0$ elements so that $0 \in F \cup D$. Denote $N = K + L$. Assume that the elements $i_j \in F$ and $i'_j \in D$ have been ordered: $i_1 < i_2 < \dots < i_K$, $i'_1 < i'_2 < \dots < i'_L$.
- ii) Assume: given K real numbers μ_i and L real numbers μ'_i associated with the sets F and D , so that for every $i \in F$ we have a fixed μ_i , and for every $i \in D$ we have a fixed μ'_i . The numbers μ_i and μ'_i are called weights. Denote by R the $N \times N$ diagonal matrix with the diagonal elements

$$\mu_{i_1}, \mu_{i_2}, \dots, \mu_{i_K}, \mu'_{i'_1}, \mu'_{i'_2}, \dots, \mu'_{i'_L}.$$

- iii) Assume: given N real functions $g_i \in C[(1-k)h_M^*, h_M^*]$, which generate an N -dimensional Haar subspace Y_N of $C[(1-k)h_M^*, h_M^*]$. Y_N is called a Haar space, if it satisfies the Haar condition (cf. [12]): Any nonzero vector in Y_N vanishes at most at $N - 1$ distinct points in $[(1-k)h_M^*, h_M^*]$. The system $\{g_1, g_2, \dots, g_N\}$ is usually called a Tchebycheff system [1, 25]. Denote an arbitrary element of Y_N by

$$(3.1) \quad y(t) = \sum_{i=1}^N c_i g_i(t).$$

- iv) For $n = 0, 1, \dots, M - k$ and $j = 1, 2, \dots, Q$ pick up functions y_{nj} from Y_N such that

$$(3.2) \quad \begin{cases} y_{nj}(t_{n+v}) = \sum_{i=1}^N c_{ij}(n) g_i(t_{n+v} - t_{n+k-1}) = \mu_\nu X_{n+v}^j & \forall \nu \in F \\ y'_{nj}(t_{n+v}) = \sum_{i=1}^N c'_{ij}(n) g'_i(t_{n+v} - t_{n+k-1}) = \mu'_\nu f_{n+v}^j & \forall \nu \in D. \end{cases}$$

Here, and through the remainder of this paper we denote

$$\mathbf{f}_{n+v} = \mathbf{f}(t_{n+v}, \mathbf{X}_{n+v}).$$

- v) Finally, take

$$(3.3) \quad X_{n+k}^j = y_{nj}(t_{n+k}) \quad j = 1, 2, \dots, Q.$$

The rules above implicitly define the operators \mathbf{F}_n for every $n \in J_{M-k}$. An explicit generalized polynomial interpolation algorithm may be developed by an algorithmization of the picking act in iv) above. Obviously, the construction is of use only if the polynomials y_{nj} satisfying (3.2) will exist independently of T_M , and for arbitrary values of $\mu_\nu X_{n+\nu}^j$ and $\mu'_\nu f_{n+\nu}^j$.

3.2. Existence of the method

The existence of the interpolation polynomials that satisfy (3.2) is guaranteed by

Theorem 1. Given the construction rules i)–iii) of paragraph 3.1 with arbitrary set T_M , any L -function \mathbf{f} and any compatible starting procedure, assume:

- i) Y_N is an N -dimensional Haar subspace of $C^1[(1-k)h_M^*, h_M^*]$ such that the space spanned by the derivatives of the basis functions of Y_N is an $(N-1)$ -dimensional Haar subspace of $C[(1-k)h_M^*, h_M^*]$,
- ii) for any $\nu \in D \setminus F$ either $\nu < \nu_q$ or $\nu > \nu_s$ when we define

$$(3.4) \quad \nu_q = \min_{\nu \in F} \nu \quad \text{and} \quad \nu_s = \max_{\nu \in F} \nu.$$

The conditions i) and ii) above are sufficient for the existence of the polynomials defined by (3.2). The polynomials are unique if they exist. The condition ii) is also necessary if $Y_N = \pi_{N-1}$ (the usual polynomials of degree $N-1$).

Proof. In Appendix 1 we have presented, and modified for our purposes, some results derived from the general theory of finite interpolation and Hermite-Birkhoff interpolation. Theorem 1 is an obvious corollary of Theorems A1–A4 in Appendix 1.

Remark. Condition i) is automatically satisfied by π_{N-1} , but is not necessary in every case. An example of a space for which i) is not valid is the system spanned by $1, \sin \omega t, \cos \omega t, \sin 2\omega t, \cos 2\omega t, \dots$. For spaces not covered by Theorem 1, the existence must be proved case by case.

For the trigonometric polynomials, we are able to prove

Theorem 2. Given the construction rules i)–iii) of paragraph 3.1 with equally spaced set T_M , any L -function \mathbf{f} and any compatible starting procedure, assume:

- i) Y_N is spanned by the N first functions of the sequence

$$(3.5) \quad 1, \sin \omega t, \cos \omega t, \sin 2\omega t, \cos 2\omega t, \dots,$$

where ω is an arbitrary, given frequency parameter that satisfies $2\pi/|\omega| > kh_M^*$;

ii) for any $\nu \in D \setminus F$ either $\nu < \nu_q$ or $\nu > \nu_s$ as in (3.4).

Then the polynomials defined by (3.2) exist, if M is sufficiently large.

Proof. The proof is presented in Appendix 2.

3.3. Details of the algorithm

From now on we assume that the method defined in paragraph 3.1 exists. In such cases, the coefficients $c_{ij}(n)$ in (3.2) can be solved as functions of $X_{n+\nu}^j$ and $f_{n+\nu}^j$.

We denote by $\boldsymbol{\theta}_{nj}$ the N -vector, which has components $X_{n+\nu}^j$, $\nu \in F$ and $h_{n+k} f_{n+\nu}^j$, $\nu \in D$. Finally we use the matrix and vector notations

$$(3.6) \quad P_n = \begin{pmatrix} g_1(t_{n+\nu} - t_{n+k-1}) \cdots g_N(t_{n+\nu} - t_{n+k-1}) & \vdots \\ \vdots & \vdots \\ h_{n+k} g_1'(t_{n+\nu} - t_{n+k-1}) \cdots h_{n+k} g_N'(t_{n+\nu} - t_{n+k-1}) & \vdots \\ \vdots & \vdots \end{pmatrix} \begin{cases} K \text{ rows} \\ \nu \in F \\ L \text{ rows} \\ \nu \in D \end{cases}$$

and

$$(3.7) \quad \mathbf{c}_j(n) = (c_{1j}(n), c_{2j}(n), \dots, c_{Nj}(n))^T.$$

Equations (3.2) can be expressed by

$$(3.8) \quad P_n \mathbf{c}_j(n) = R \boldsymbol{\theta}_{nj} \quad j = 1, 2, \dots, Q.$$

Naturally, we have (3.8) for every $n \in J_{M-k}$. The assumption of the existence of the method guarantees that P_n^{-1} exists. Hence we have

$$(3.9) \quad \mathbf{c}_j(n) = P_n^{-1} R \boldsymbol{\theta}_{nj}.$$

Let us denote $\mathbf{g}_n = (g_1(h_{n+k}), \dots, g_N(h_{n+k}))^T$. Then, in view of (3.9), the relation (3.3) is expressed by

$$(3.10) \quad X_{n+k}^j = \mathbf{g}_n^T \mathbf{c}_j(n) = \mathbf{g}_n^T P_n^{-1} R \boldsymbol{\theta}_{nj}.$$

The row vector $\mathbf{g}_n^T P_n^{-1} R$ is independent of j . For fixed n and j , X_{n+k}^j is a linear combination of the components of $\boldsymbol{\theta}_{nj}$. It is therefore possible to write (3.10) in the form

$$(3.11) \quad X_{n+k}^j + \sum_{\nu \in F} \alpha_{\nu n} X_{n+\nu}^j = h_{n+k} \sum_{\nu \in D} \beta_{\nu n} f_{n+\nu}^j.$$

Here, the coefficients $\alpha_{\nu n} = \alpha_\nu(\mathbf{h}_n)$ and $\beta_{\nu n} = \beta_\nu(\mathbf{h}_n)$ in fact depend on \mathbf{h}_n defined in (2.7), and are independent of j so that we also have

$$(3.12) \quad \mathbf{X}_{n+k} + \sum_{\nu \in F} \alpha_\nu(\mathbf{h}_n) \mathbf{X}_{n+\nu} = h_{n+k} \sum_{\nu \in D} \beta_\nu(\mathbf{h}_n) \mathbf{f}_{n+\nu}.$$

Now \mathbf{F}_n has been explicitly defined by (3.12).

We denote the column vectors of P_n^{-1} by \mathbf{p}_{nv} . We have a \mathbf{p}_{nv} corresponding to each equation in (3.2), with $v \in F$ and $v \in D$. By the aid of (3.10) we get

$$(3.13) \quad \begin{cases} \alpha_{vn} = \alpha_v(\mathbf{h}_n) = -\mathbf{g}_n^T \mathbf{p}_{nv} \mu_v & \forall v \in F \\ \beta_{vn} = \beta_v(\mathbf{h}_n) = \mathbf{g}_n^T \mathbf{p}_{nv} \mu'_v & \forall v \in D. \end{cases}$$

By combination of the formulas (3.13) and (3.12) with the construction rules of paragraph 3.1, we have defined our generalized polynomial interpolation algorithm (GPIA) for the initial value problem (1.1).

The algorithm may be computationally poor, since P_n may have nearly equal rows, when M is large, and the nodes in T_M are close to each other. This difficulty can be overcome by means of suitable computational modifications, which will avoid the direct matrix inversion. Despite this inconvenience, the algorithm is theoretically interesting.

The expression (3.12) defines \mathbf{X}_{n+k} explicitly if $k \notin D$. In such cases, GPIA will produce a unique sequence of vectors $\mathbf{X}_k, \mathbf{X}_{k+1}, \dots$, starting from the given vectors $\mathbf{X}_0, \mathbf{X}_1, \dots, \mathbf{X}_{k-1}$. If $k \in D$, \mathbf{X}_{n+k} is defined only implicitly by (3.12), which may be rewritten as

$$(3.14) \quad \mathbf{X}_{n+k} = h_{n+k} \beta_{nk} \mathbf{f}(t_{n+k}, \mathbf{X}_{n+k}) + \mathbf{z} = \mathbf{G}(\mathbf{X}_{n+k}),$$

where \mathbf{z} is a constant vector. If \mathbf{G} is a contracting mapping, (3.14) has a unique solution attained with arbitrary accuracy by the iteration of (3.14) (cf. [37], p. 120).

\mathbf{G} is contractive for every n when $M \rightarrow \infty$, if

$$|h_{n+k} \beta_{nk} \bar{L}| < 1.$$

\bar{L} is the Lipschitz-constant defined in (2.2). The condition of contractiveness is fulfilled, if we are able to assume that $|\beta_{nk}| \leq \beta_k^*$ for every fixed t_n when $M \rightarrow \infty$. For a moment, let us make this assumption. Then, with fixed M we have

$$|h_{n+k} \beta_{nk} \bar{L}| \leq h_{M/\beta_k^*}^* \bar{L}$$

and a constant M_0 exists such that

$$(3.15) \quad h_{M/\beta_k^*}^* \bar{L} < 1 \text{ for every } M > M_0.$$

In what follows, we assume that a constant β_k^* exists such that

$$(3.16) \quad |\beta_{nk}| \leq \beta_k^* \quad \forall n \in J_{M-k}, \quad \forall M > M_0.$$

From (3.12) we see that our method may reduce to a linear multistep method with constant coefficients, if we have an equidistant T_M , and the coefficients $\alpha_v(\mathbf{h}_n)$ and $\beta_v(\mathbf{h}_n)$ are independent of \mathbf{h}_n .

If T_M is equidistant with spacing h , the elements of P_n and \mathbf{g}_n are functions of h , only, and we write $P_n = P(h)$, $\mathbf{g}_n = \mathbf{g}(h)$ and consequently

$$(3.17) \quad \mathbf{X}_{n+k} + \sum_{v \in F} \alpha_v(h) \mathbf{X}_{n+v} = h \sum_{v \in D} \beta_v(h) \mathbf{f}_{n+v} .$$

Formula (3.17) defines a linear multistep method with constant coefficients, but we have different coefficients with different step size h .

3.4. Polynomial approximations

Interpolation with π_{N-1} leads to the simplest case.

3.4.1. Arbitrary nodes

If $Y_N = \pi_{N-1}$, the elements of the j :th column of P_n in (3.6) are homogeneous functions of \mathbf{h}_n , and of degree $j - 1$. Thus, the elements of the j :th row of P_n^{-1} are homogeneous functions of degree $-j + 1$. When P_n^{-1} is multiplied by $\mathbf{g}_n^T = (1, h_{n+k}, \dots, h_{n+k}^{N-1})$, as was done in (3.10), the elements of the resulting vector are homogeneous functions of degree zero. Consequently the coefficients $\alpha_v(\mathbf{h}_n)$ and $\beta_v(\mathbf{h}_n)$ in (3.12) are homogeneous functions of \mathbf{h}_n and of degree zero.

Let us denote by $d(\mathbf{h}_n)$ the determinant of P_n . Then, each coefficient $\alpha_v(\mathbf{h}_n)$ and $\beta_v(\mathbf{h}_n)$ is a quotient of a continuous homogeneous function of \mathbf{h}_n divided by $d(\mathbf{h}_n)$. $d(\mathbf{h}_n)$ is a continuous function of \mathbf{h}_n when $\mathbf{h}_n > \mathbf{0}$, and moreover $d(\mathbf{h}_n) \neq 0$ by assumption, when $\mathbf{h}_n > \mathbf{0}$.

Thus, the coefficients $\alpha_v(\mathbf{h}_n)$ and $\beta_v(\mathbf{h}_n)$ are unique for every $n \in J_{M-k}$ and every M . However, the limits of these coefficients will depend on the way by which the nodes are distributed in $[a, b]$, when $M \rightarrow \infty$. For example, assume that we have $h_{i+1}/h_i = \gamma$ for every $i = 1, 2, \dots, M - 1$ and every M . Then for every M ,

$$\begin{cases} \alpha_v(\mathbf{h}_n) = \alpha_v(\gamma) \\ \beta_v(\mathbf{h}_n) = \beta_v(\gamma) , \end{cases}$$

i.e. the coefficients are constants, but may depend on γ . The limiting values of the coefficients may thus depend on the way in which the limit has been achieved. An illustrative example is given in (5.7).

If the weights are nonzero, formula (3.11) can be written as

$$(3.18) \quad X_{n+k}^j + \sum_{v \in F} \frac{\alpha_{vm}}{\mu_v} \mu_v X_{n+v}^j = h_{n+k} \sum_{v \in D} \frac{\beta_{vm}}{\mu_v} \mu_v' f_{n+v}^j .$$

In view of Theorem A1 (Appendix 1) the result of Hermite-Birkhoff interpolation is unique if it exists. Therefore, if we have $x \in \pi_{N-1}$, and

$$(3.19) \quad \begin{cases} x(t_{n+v} - t_{n+k-1}) = \mu_\nu X_{n+v}^j & \forall \nu \in F \\ x'(t_{n+v} - t_{n+k-1}) = \mu'_\nu f_{n+v}^j & \forall \nu \in D \end{cases}$$

then

$$(3.20) \quad x(t_{n+k} - t_{n+k-1}) = X_{n+k}^j.$$

Now, by means of (3.19), (3.20) and the selection of $x(t) = 1, t, t^2, \dots, t^{N-1}$, after the proper divisions by h_{n+k} (3.18) yields

$$(3.21) \quad 1 + \sum_{\nu \in F} \frac{\alpha_{\nu n}}{\mu_\nu} = 0,$$

$$(3.22) \quad 1 + \sum_{\nu \in F} \frac{\alpha_{\nu n}}{\mu_\nu} \frac{t_{n+v} - t_{n+k-1}}{h_{n+k}} = \sum_{\nu \in D} \frac{\beta_{\nu n}}{\mu'_\nu}$$

and generally

$$(3.23) \quad 1 + \sum_{\nu \in F} \frac{\alpha_{\nu n}}{\mu_\nu} \frac{(t_{n+v} - t_{n+k-1})^i}{h_{n+k}^i} = \sum_{\nu \in D} \frac{\beta_{\nu n}}{\mu'_\nu} i \frac{(t_{n+v} - t_{n+k-1})^{i-1}}{h_{n+k}^{i-1}},$$

when $i = 0, 1, \dots, N - 1$.

3.4.2. Equidistant nodes

When T_M is equidistant with spacing h , we have $P(h) = PH$, and $\mathbf{g}(h) = (1, h, h^2, \dots, h^{N-1})^T$. Here, P is an $N \times N$ -matrix independent of h , and has a form

$$(3.24) \quad P = \left(\begin{array}{cccccc} 1 & \nu - k + 1 & (\nu - k + 1)^2 & \dots & (\nu - k + 1)^{N-1} & \\ \vdots & \vdots & \vdots & & \vdots & \\ \vdots & \vdots & \vdots & & \vdots & \\ 0 & 1 & 2(\nu - k + 1) & \dots & (N - 1)(\nu - k + 1)^{N-2} & \\ \vdots & \vdots & \vdots & & \vdots & \\ \vdots & \vdots & \vdots & & \vdots & \end{array} \right) \left. \begin{array}{l} \text{rows} \\ \nu \in F \\ \text{rows} \\ \nu \in D \end{array} \right\}$$

H is an $N \times N$ -diagonal matrix with diagonal elements $1, h, h^2, \dots, h^{N-1}$ (the common multipliers for the columns of $P(h)$). Therefore, we get

$$\mathbf{g}^T(h)P^{-1}(h) = \mathbf{g}^T(h)H^{-1}P^{-1} = \boldsymbol{\delta}^T P^{-1},$$

in which we have defined $\boldsymbol{\delta} = (\delta_i)$ as an N -vector with unit elements.

We denote $P^{-1} = (\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_N)$ where a column vector \mathbf{p}_ν corresponds to each of the values $\nu \in F$ and $\nu \in D$. Hence, in correspondence with (3.13), independently of h , we derive

$$(3.25) \quad \begin{cases} \alpha_\nu = -\mu_\nu \boldsymbol{\delta}^T \mathbf{p}_\nu & \forall \nu \in F \\ \beta_\nu = \mu'_\nu \boldsymbol{\delta}^T \mathbf{p}_\nu & \forall \nu \in D. \end{cases}$$

Thus, we have proved

Theorem 3. Every generalized polynomial interpolation method reduces to a unique linear multistep method of form (3.17) with the constant coefficients (3.25), if $Y_N = \pi_{N-1}$ and T_M is equally spaced.

It may be asked whether there always exists an equally spaced polynomial interpolation method, which corresponds to a given linear multistep method. By correspondence we mean that the two methods produce the same sequence $\mathbf{X}_k, \mathbf{X}_{k+1}, \dots$ of solution vectors, if the starting values are the same for both methods. We shall examine this problem.

Given a linear multistep method with constant coefficients,

$$(3.26) \quad \mathbf{X}_{n+k} + \sum_{v=0}^{k-1} \alpha_v \mathbf{X}_{n+v} = h \sum_{v=0}^k \beta_v \mathbf{f}_{n+v},$$

let us define

$$(3.27) \quad F = \{v | \alpha_v \neq 0\}, \quad D = \{v | \beta_v \neq 0\} \quad \text{and}$$

$$(3.28) \quad \tilde{F} = \{v | v \in F \text{ or } v \in D \text{ and } v_q < v < v_s\},$$

when v_q and v_s are defined in (3.4).

It should be recalled that matrix P of an equally spaced polynomial interpolation method, as written in (3.24), is totally defined by F and D . Similarly, \tilde{F} with K elements and D with L elements given by (3.27) and (3.28) will define an $N \times N$ -matrix \tilde{P} , when $N = K + L$. \tilde{P}^{-1} exists by Theorem 1. We denote the column vectors of \tilde{P}^{-1} by $\tilde{\mathbf{p}}_v$. If we are able to state

$$(3.29) \quad \begin{cases} \mu_v = 0 & \forall v \in \tilde{F} \setminus F \\ \mu_v = -\frac{\alpha_v}{\delta^T \tilde{\mathbf{p}}_v} & \forall v \in F \\ \mu'_v = \frac{\beta_v}{\delta^T \tilde{\mathbf{p}}_v} & \forall v \in D \end{cases}$$

we have generated a unique, equally spaced polynomial interpolation method, defined by the weights (3.29), the sets \tilde{F} and D in (3.28) and (3.27), and which corresponds to (3.26).

Let us call

$$(3.30) \quad \delta^T \tilde{\mathbf{p}}_v \neq 0 \quad \text{for } \forall v \in \tilde{F} \text{ and } \forall v \in D$$

the *inversion condition*. Hence we proved

Theorem 4. A linear multistep method (3.26) corresponds to a unique

equally spaced polynomial interpolation method defined by (3.27), (3.28) and (3.29) if and only if the inversion condition (3.30) is satisfied.

The meaning of the inversion condition will be studied elsewhere.

The role of the weight matrix R is clarified to some extent by our next theorem. From (3.23) we are able to conclude that in the equidistant case, where $h_{n+k} = h$ and $t_{n+v} - t_{n+k-1} = (v - k + 1)h$, the following is true:

Theorem 5. Every equally spaced polynomial interpolation method with unit matrix R reduces to a consistent linear multistep method of the order $N - 1$.

Theorem 5 becomes evident if the definition of consistency is recalled and it is observed that (3.21) and (3.22) are necessary and sufficient conditions for consistency in linear multistep methods (cf. [22], Theorem 3.4).

Theorem 5 has an immediate consequence, first discovered by Dahlquist ([13], Theorem 2):

Corollary. There exists a linear k -step method of the order $2k$.

For the proof, it should be observed that the equally spaced polynomial interpolation method with $F = J_{k-1}$, $D = J_k$ exists by Theorem 1 and has $N = 2k + 1$.

If a weight differs from unity, the order of the method will automatically be lower than the maximum otherwise possible. However, the nonunity weights may be useful, if we are seeking a method with properties other than the maximum order. See [31]. For an example, see also paragraph 5.1.1.

4. STABILITY, CONSISTENCY, CONVERGENCE, ERRORS

4.1. Preliminaries

In this chapter we shall examine the conditions of stability, consistence and convergence of our method and derive some bounds for the errors (2.12) and (2.13). Our starting point is the equation (3.12), here repeated as

$$(4.1) \quad \mathbf{X}_{n+k} + \sum_{v \in F} \alpha_v(\mathbf{h}_n) \mathbf{X}_{n+v} = h_{n+k} \sum_{v \in D} \beta_v(\mathbf{h}_n) \mathbf{f}_{n+v}.$$

In our case the coefficient functions $\alpha_v(\mathbf{h}_n)$ and $\beta_v(\mathbf{h}_n)$ are the special functions defined by (3.13), although the equation (4.1) is more general, permitting the coefficients to be arbitrary functions of \mathbf{h}_n . Thus (4.1) includes the methods of Lambert [27] and Brunner [5, 6, 7].

The following results can be proved only on the assumption that the coefficient functions $\alpha_\nu(\mathbf{h}_n)$, (as in [27]) will have the form

$$(4.2) \quad \alpha_\nu(\mathbf{h}_n) = \alpha_\nu + h_{n+k} a_\nu(\mathbf{h}_n), \quad \forall \nu \in F,$$

where α_ν is constant, and functions $a_\nu(\mathbf{h}_n)$ are bounded by constants a_ν^* such that

$$(4.3) \quad |a_\nu(\mathbf{h}_n)| \leq a_\nu^*, \quad \forall \nu \in F, \quad \forall n \in J_{M-k}.$$

Further, we must assume that constants β_ν^* exist such that

$$(4.4) \quad |\beta_\nu(\mathbf{h}_n)| \leq \beta_\nu^*, \quad \forall \nu \in D, \quad \forall n \in J_{M-k}.$$

In (3.16) we have already made this assumption for $\nu = k$.

Our results are heavily based on a lemma due to Henrici ([22], Lemma 3.2). The lemma has been slightly modified so that the arbitrary spacing of T_M can be taken into account. We present the following

Lemma. Let

$$\varrho(z) = \sum_{i=0}^k \alpha_{k-i} z^{k-i}$$

be a polynomial with real coefficients, $\alpha_k \neq 0$. (Subsequently they are the coefficients α_ν of (4.2).) Let $\mathbf{B}^{(i)}$ ($i = 0, 1, \dots, k$) be $k+1$ given sequences of functions from Y_Q to Y_Q defined on J_{M-k} such that, for suitable constants $B^{(i)} \geq 0$,

$$\|\mathbf{B}_j^{(i)}(\mathbf{Z})\| \leq B^{(i)} \|\mathbf{Z}\|, \quad i = 0, 1, \dots, k \quad \forall j \in J_{M-k},$$

for all vectors $\mathbf{Z} \in Y_Q$. Also, let \mathbf{A} be a sequence of vectors in Y_Q defined on J_{M-k} , and $\{h_i\}$ ($i = 1, 2, \dots, M$) be a sequence of positive real numbers, and take h_M^* as in (2.4). Write the difference equation

$$(4.5) \quad \sum_{i=0}^k \alpha_{k-i} \mathbf{Z}_{m+k-i} = h_{m+k} \sum_{i=0}^k \mathbf{B}_m^{(k-i)}(\mathbf{Z}_{m+k-i}) + A_m.$$

Denote by ω the maximum of the moduli of the roots of the polynomial $\varrho(z)$. If all the roots of modulus ω have multiplicity 1, and if

$$h_M^* < |\alpha_k| B^{(k)-1},$$

then for every solution \mathbf{Z} of difference equation (4.5) satisfying

$$\|\mathbf{Z}_n\| \leq \omega^n \bar{H}, \quad n = 0, 1, \dots, k-1,$$

for some constant \bar{H} , the inequality

$$(4.6) \quad \|\mathbf{Z}_n\| \leq \omega^n \Gamma^*(A \bar{H} + A_n) e^{nh_M^* \Gamma^* B}$$

holds for $n = 0, 1, \dots, M$, where

$$A = \sum_{i=1}^k i\omega^{k-i}|\alpha_{k-i}|;$$

$$B = \sum_{i=0}^k \omega^i B^{(i)};$$

$$A_n = \begin{cases} 0, & n = 0, 1, \dots, k-1 \\ \sum_{i=0}^{n-k} \omega^{-i} \|A_i\|, & n = k, k+1, \dots, M; \end{cases}$$

and

$$I^* = I(1 - h_M^* |\alpha_k|^{-1} B^{(k)})^{-1},$$

if we define

$$I = \sup_{n=0,1,2,\dots} |\gamma_n| \text{ (which exists) and } \left(\sum_{i=0}^k \omega^{k-i} |\alpha_{k-i} z^i| \right)^{-1} = \sum_{i=0}^{\infty} \gamma_i z^i.$$

If any root of modulus ω has multiplicity > 1 , then for every $\hat{\omega} > \omega$ and for

$$|h_M^*| < |\alpha_k| \hat{\omega}^{-k} B^{(k)-1},$$

the inequality

$$(4.8) \quad \|\mathbf{Z}_n\| \leq \hat{\omega}^n \hat{I}^* (\hat{A} \hat{H} + \hat{A}_n) e^{nh_M^* \hat{I}^* \hat{B}}$$

holds for $n = 0, 1, \dots, M$, where

$$\hat{A} = \sum_{i=0}^k (2k+1-2i) \hat{\omega}^{i+1} |\alpha_i|,$$

$$\hat{B} = 2\hat{\omega} \sum_{i=0}^k \hat{\omega}^i B^{(i)},$$

$$\hat{H} = \max(\bar{H}, \hat{\omega}^{-k} \|\mathbf{Z}_k\|),$$

$$\hat{A}_n = 2\hat{\omega} \sum_{i=0}^{n-k} \hat{\omega}^{-i} \|A_i\| \text{ and}$$

$$\hat{I}^* = \hat{I}(1 - h_M^* |\alpha_k|^{-1} B^{(k)})^{-1}, \text{ if we define}$$

$$\hat{I} = \sup_{i=0,1,2,\dots} |\hat{\gamma}_i|, \quad \hat{\varrho}(z) = (z - \hat{\omega})\varrho(z) \text{ and } z^{-k} \hat{\varrho}^{-1}(\hat{\omega}/z) = \sum_{i=0}^{\infty} \hat{\gamma}_i z^i.$$

Proof. The proof runs completely in parallel to that of [22] (Lemma 3.2), if the constant h of [22] is estimated by h_M^* in the obvious way.

4.2. Stability

Assumptions (4.2) and (4.3) allow us to prove that the stability of method (4.1) is a consequence of a purely algebraic property of the polynomial $\varrho(z)$. According to [22], we say that any polynomial

$$\varrho(z) = \sum_{i=0}^k \alpha_{k-i} z^{k-i} \quad \text{with } \alpha_k \neq 0$$

satisfies the *root condition* if its k roots z_i satisfy $|z_i| \leq 1$, $i = 1, 2, \dots, k$, and if the roots of modulus 1 have multiplicity 1.

With the aid of (4.2), we write the difference equation (4.1) in the form

$$(4.8) \quad \mathbf{X}_{n+k} + \sum_{v \in F} \alpha_v \mathbf{X}_{n+v} = h_{n+k} \left[\sum_{v \in D} \beta_v(\mathbf{h}_n) \mathbf{f}_{n+v} - \sum_{v \in F} a_v(\mathbf{h}_n) \mathbf{X}_{n+v} \right],$$

and associate with it the polynomial $\varrho(z)$ with coefficients α_v . We take $\alpha_v = 0$ of $v \notin F$, otherwise α_v is taken from (4.8). Clearly $\alpha_k = 1$.

We can now prove as in [22]

Theorem 6. Method (4.8) is stable if the polynomial ϱ associated with it satisfies the root condition.

Proof. The proof runs in parallel to the sufficiency proof of Theorem 3.3 in [22]. We denote by \mathbf{X} the family of solutions of (4.8) with fixed $M > M_0$ and with any bounded starting vectors that satisfy

$$\|\mathbf{X}_i(M)\| \leq S, \quad i = 0, 1, \dots, k-1.$$

The difference equation (4.8) is then written in the form

$$\mathbf{X}_{n+k} + \sum_{v \in F} \alpha_v \mathbf{X}_{n+v} = h_{n+k} \left\{ \sum_{v \in D} \beta_v(\mathbf{h}_n) [\mathbf{f}_{n+v} - \mathbf{f}(t_{n+v}, \mathbf{0})] - \sum_{v \in F} a_v(\mathbf{h}_n) \mathbf{X}_{n+v} \right\} + \mathbf{A}_n,$$

where

$$\mathbf{A}_n = h_{n+k} \sum_{v \in D} \beta_v(\mathbf{h}_n) \mathbf{f}(t_{n+v}, \mathbf{0}).$$

We see that our Lemma is applicable. Functions $\mathbf{B}_n^{(i)}$ are defined by

$$(4.9) \quad \mathbf{B}_n^{(i)}(\mathbf{X}_{n+i}) = \beta_i(\mathbf{h}_n) [\mathbf{f}_{n+i} - \mathbf{f}(t_{n+i}, \mathbf{0})] - a_i(\mathbf{h}_n) \mathbf{X}_{n+i}$$

for every $i \in F \cup D$, when the coefficients not present in (4.8) are taken as zeros. Thus

$$(4.10) \quad B^{(i)} = \beta_i^* \bar{L} + a_i^*.$$

By the continuity of \mathbf{f} , we have

$$\|\mathbf{A}_n\| \leq h_M^* \beta^* f, \quad \text{where } f = \max_{t \in [a, b]} \|\mathbf{f}(t, \mathbf{0})\| \quad \text{and}$$

$$(4.11) \quad \beta^* = \sum_{v \in D} \beta_v^*.$$

Hence, if $\varrho(z)$ has a root of modulus 1, Lemma yields

$$(4.12) \quad \|\mathbf{X}_n\| \leq \Gamma^* (AS + nh_M^* \beta^* f) e^{nh_M^* \Gamma^* B},$$

where A is as in Lemma,

$$(4.13) \quad B = \bar{L}\beta^* + a^*,$$

$$(4.14) \quad a^* = \sum a_v^*$$

and I^* is defined by the aid of (4.10) as in Lemma. Here A_n has been approximated upwards. Clearly, $\|\mathbf{X}_n\|$ in (4.12) is uniformly bounded for every $n \in J_M$ and every $M > M_0$, since we have assumed in (2.5) that $Mh_M^* \leq C$.

If $\varrho(z)$ has no root of modulus 1, we can apply the second part of Lemma taking $\hat{\omega} = 1$. The resulting estimate is similar to (4.12), with somewhat different values of the constants A , S , I^* and B . Consequently the sufficiency of the root condition for stability has been proved.

4.3. Consistency

The consistency of method (4.1), with the restrictions (4.2), (4.3) and (4.4), is a consequence of some simple conditions in relation to the coefficients of (4.1). In the same way as in [22] (Theorem 3.4), we have

Theorem 7. Method (4.8) is consistent if and only if the following conditions are satisfied:

$$(4.15) \quad 1 + \sum_{v \in F} \alpha_v = 0,$$

$$(4.16) \quad \sum_{v \in F} \alpha_v(\mathbf{h}_n) \rightarrow 0, \quad \forall n \in J_{M-k}, \quad M \rightarrow \infty,$$

$$(4.17) \quad 1 + \sum_{v \in F} \alpha_v(\mathbf{h}_n) \frac{t_{n+v} - t_{n+k-1}}{h_{n+k}} - \sum_{v \in D} \beta_v(\mathbf{h}_n) \rightarrow 0, \quad \forall n \in J_{M-k}, \quad M \rightarrow \infty.$$

Proof. Again, as in [22], we are able to conclude as follows. We denote the modulus of continuity of $\mathbf{x}' = \mathbf{f}(t, \mathbf{x})$ by γ . Then for the solution \mathbf{x} of the differential equation $\mathbf{x}' = \mathbf{f}(t, \mathbf{x})$, we have

$$(4.18) \quad \mathbf{x}(t+s) = \mathbf{x}(t) + s\mathbf{x}'(t) + s\gamma(s)\boldsymbol{\theta},$$

where $\boldsymbol{\theta}$ is a vector of which the components are less than or equal to 1 in the modulus.

We must establish that (2.9) holds for (4.8). Here

$$\begin{aligned} \mathbf{F}_i(\mathbf{x}) &= \mathbf{F}_i(\mathbf{x}(t_i), \mathbf{x}(t_{i+1}), \dots, \mathbf{x}(t_{i+k})) = \\ &= \mathbf{x}(t_{i+k}) + \sum_{v \in F} (\alpha_v + h_{i+k} a_v(\mathbf{h}_i)) \mathbf{x}(t_{i+v}) - h_{i+k} \sum_{v \in D} \beta_v(\mathbf{h}_i) \mathbf{x}'(t_{i+v}), \end{aligned}$$

and by the aid of (4.18), we can write:

$$\begin{aligned}
(4.19) \quad \mathbf{F}_i(\mathbf{x}) &= [1 + \sum_{\nu \in F} (\alpha_\nu + h_{i+k} a_\nu(\mathbf{h}_i))] \mathbf{x}(t_{i+k-1}) \\
&+ [h_{i+k} + \sum_{\nu \in F} (\alpha_\nu + h_{i+k} a_\nu(\mathbf{h}_i))(t_{i+\nu} - t_{i+k-1}) - h_{i+k} \sum_{\nu \in D} \beta_\nu(\mathbf{h}_i)] \mathbf{x}'(t_{i+k-1}) \\
&+ [h_{i+k} + \sum_{\nu \in F} |\alpha_\nu + h_{i+k} a_\nu(\mathbf{h}_i)| |t_{i+\nu} - t_{i+k-1}|] \chi(t_{i+k} - t_i) \boldsymbol{\theta} \\
&+ h_{i+k} \sum_{\nu \in D} |\beta_\nu(\mathbf{h}_i)| \chi(t_{i+k} - t_i) \boldsymbol{\theta}.
\end{aligned}$$

Here, $\boldsymbol{\theta}$ is not the same as in (4.8). Obviously $\|\mathbf{F}_i(\mathbf{x})\|$ is $o(h_M^*)$ if (4.15), (4.16) and (4.17) are satisfied. The necessity of (4.15) and (4.16) follows from the fact that if $\mathbf{x}' = \mathbf{0}$, then $\mathbf{x}(t) \equiv \mathbf{a}$ (a constant vector), and we must have

$$[1 + \sum_{\nu \in F} (\alpha_\nu + h_{i+k} a_\nu(\mathbf{h}_i))] / h_M^* \rightarrow 0, \quad \forall n \in J_{M-k}, \quad M \rightarrow \infty.$$

Following this the necessity of (4.17) is observable on taking $\mathbf{x}' = \mathbf{c}$ (a nonzero constant vector). This leads to the requirement that the coefficient of $\mathbf{x}'(t_{i+k-1})$ in (4.19) divided by h_M^* must tend to zero as $M \rightarrow \infty$. So, the theorem has been proved.

Remark. Sufficient conditions for consistency are also obtained if (4.16) is replaced by

$$(4.20) \quad \sum_{\nu \in F} a_\nu(\mathbf{h}_n) = 0, \quad \forall n \in J_{M-k}, \quad \forall M > M_0,$$

or if (4.17) is replaced by either

$$(4.21) \quad 1 + \sum_{\nu \in F} \alpha_\nu \frac{t_{n+\nu} - t_{n+k-1}}{h_{n+k}} = \sum_{\nu \in D} \beta_\nu(\mathbf{h}_n), \quad \forall n \in J_{M-k}, \quad \forall M > M_0,$$

or

$$(4.22) \quad 1 + \sum_{\nu \in F} \alpha_\nu(\mathbf{h}_n) \frac{t_{n+\nu} - t_{n+k-1}}{h_{n+k}} = \sum_{\nu \in D} \beta_\nu(\mathbf{h}_n), \quad \forall n \in J_{M-k}, \quad \forall M > M_0.$$

4.4. Convergence

The main result of this chapter will now be proved as

Theorem 8. Method (4.8) is convergent if (4.15), (4.20), (4.22) and the root condition are satisfied.

Proof. The basic idea has been presented in [22] and [27]. From (4.19) we get

$$(4.23) \quad \|\mathbf{F}_i(\mathbf{x}(t_i), \mathbf{x}(t_{i+1}), \dots, \mathbf{x}(t_{i+k}))\| \leq C_M h_M^* \chi(k h_M^*),$$

where

$$C_M = 1 + \sum_{\nu \in F} (k - 1 - \nu) (|\alpha_\nu| + h_M^* \alpha_\nu^*) + \sum_{\nu \in D} \beta_\nu^* .$$

We denote by $\mathbf{X}(M)$ the solutions of the difference equation (4.8) with any bounded and compatible starting values that have

$$\|\mathbf{X}_i(M)\| \leq S, \quad i = 0, 1, \dots, k - 1 .$$

Thus, we have

$$\mathbf{F}_i(\mathbf{X}_i, \mathbf{X}_{i+1}, \dots, \mathbf{X}_{i+k}) = 0 .$$

By stating as in (2.12) that

$$\mathbf{E}_i = \mathbf{X}_i(M) - \mathbf{x}(t_i), \quad \forall i \in J_M,$$

we obtain

$$\begin{aligned} (4.24) \quad & \mathbf{F}_i(\mathbf{X}_i, \mathbf{X}_{i+1}, \dots, \mathbf{X}_{i+k}) - \mathbf{F}_i(\mathbf{x}(t_i), \mathbf{x}(t_{i+1}), \dots, \mathbf{x}(t_{i+k})) \\ &= \mathbf{E}_{i+k} + \sum_{\nu \in F} (\alpha_\nu + h_{i+k} \alpha_\nu(\mathbf{h}_i)) \mathbf{E}_{i+\nu} - h_{i+k} \sum_{\nu \in D} \beta_\nu(\mathbf{h}_i) [\mathbf{f}_{i+\nu} - \mathbf{f}(t_{i+\nu}, \mathbf{x}(t_{i+\nu}))] = \mathbf{A}_i, \end{aligned}$$

where

$$\|\mathbf{A}_i\| \leq C_M h_M^* \chi(k h_M^*)$$

by (4.23).

We write (4.24) in the form

$$\begin{aligned} \mathbf{E}_{i+k} + \sum_{\nu \in F} \alpha_\nu \mathbf{E}_{i+\nu} &= h_{i+k} \sum_{\nu=0}^k \{ \beta_\nu(\mathbf{h}_i) [\mathbf{f}(t_{i+\nu}, \mathbf{x}(t_{i+\nu})) + \mathbf{E}_{i+\nu}] - \mathbf{f}(t_{i+\nu}, \mathbf{x}(t_{i+\nu})) \} \\ &\quad - a_\nu(\mathbf{h}_i) \mathbf{E}_{i+\nu} \} + \mathbf{A}_i = h_{i+k} \sum_{\nu=0}^k \mathbf{B}_i^{(\nu)}(\mathbf{E}_{i+\nu}) + \mathbf{A}_i \end{aligned}$$

and apply Lemma with $\mathbf{Z} = \mathbf{E}$, $\omega = 1$,

$$B^{(\nu)} = \beta_\nu^* \bar{L} + \alpha_\nu^*$$

as in (4.10), and

$$\bar{H} = \max_{0 \leq j \leq k-1} \|\mathbf{X}_j(M) - \mathbf{x}_0\| + \max_{0 \leq j \leq k-1} \|\mathbf{x}(t_j) - \mathbf{x}_0\| = \bar{H}(M) .$$

Moreover, with the observation that A is as in Lemma, B is as in (4.13), I^* is defined by the aid of (4.10) as in Lemma,

$$(i - k + 1)h_M^* \leq Mh_M^* \leq C$$

by (2.5), and

$$\mathbf{A}_i \leq i h_M^* C_M \chi(k h_M^*),$$

we get

$$(4.25) \quad \|\mathbf{E}_i\| \leq \Gamma^*(A\bar{H}(M) + CC_{M\chi}(kh_M^*))e^{C\Gamma^*B}.$$

Since $\bar{H}(M) \rightarrow 0$, $\chi(kh_M^*) \rightarrow 0$, and C_M remains bounded as $M \rightarrow \infty$, we get

$$\lim_{M \rightarrow \infty} \max_{i \in J_M} \|\mathbf{E}_i\| = 0,$$

and consequently method (4.8) is convergent, and the theorem is proved.

4.5. Asymptotic behaviour of errors

The asymptotic behaviour of the discretization error \mathbf{E}_i at a fixed $t = t_i$, $M \rightarrow \infty$, can be estimated if the method used is consistent, the root condition is satisfied, and the method is of order q . We make these assumptions in this chapter.

The assumption of order is written

$$(4.26) \quad \max_{n \in J_M} \|\mathbf{F}_n(\mathbf{x}(t_n), \mathbf{x}(t_{n+1}), \dots, \mathbf{x}(t_{n+k}))\| \leq C_{q+1}^* h_M^{*q+1},$$

where the constant C_{q+1}^* depends on the constants α_i , a_i^* and β_i^* of the method, and on

$$\max_{t \in [a, b]} \|\mathbf{x}^{(q+1)}(t)\|,$$

where $\mathbf{x}^{(q+1)}$ is the continuous $(q+1)$:th derivative of the solution \mathbf{x} . The result is then stated (again as in [22], Theorem 4.1) as

Theorem 9. Let the method (4.8), satisfying the root condition, be of order q , and let the solution \mathbf{x} of the problem (1.1) have a continuous derivative of order $q+1$. Let \mathbf{X} be the solutions of (4.8) with the bounded and compatible starting values $\mathbf{X}_i(M)$, $i = 0, 1, \dots, k-1$, and put

$$\mu(M) = \max_{0 \leq i \leq k-1} \|\mathbf{X}_i(M) - \mathbf{x}(t_i)\|.$$

The discretization error then satisfies

$$(4.27) \quad \|\mathbf{E}_n\| \leq \Gamma^*(A\mu(M) + CC_{q+1}^* h_M^{*q})e^{C\Gamma^*B},$$

where Γ^* , A , B and C are defined as in the proof of Theorem 8, and C_{q+1}^* is defined by (4.26).

Proof. The proof is similar to that of Theorem 8. The only exception is that $\bar{H}(M)$ is now replaced by $\mu(M)$, and $C_{M\chi}(kh_M^*)$ is replaced by $C_{q+1}^* h_M^{*q}$. Details are omitted.

We notice that if the starting values are sufficiently accurate, i.e. $\mu(M) = O(h_M^{*g})$, the discretization error is $O(h_M^{*g})$.

In numerical computations, rounding operations occur, so that the vectors \mathbf{X}_i are in fact replaced by vectors $\tilde{\mathbf{X}}_i = \mathbf{X}_i + \mathbf{r}_i$. The vectors \mathbf{r}_i are called accumulated round-off errors. The perturbed vectors $\tilde{\mathbf{X}}_i$ will satisfy the difference equation

$$(4.28) \quad \tilde{\mathbf{X}}_{i+k} + \sum_{\nu \in F} (\alpha_\nu + h_{i+k} a_\nu(\mathbf{h}_i)) \tilde{\mathbf{X}}_{i+\nu} - h_{i+k} \sum_{\nu \in D} \beta_\nu(\mathbf{h}_i) \mathbf{f}(t_{i+\nu}, \tilde{\mathbf{X}}_{i+\nu}) = \boldsymbol{\varepsilon}_i,$$

where the vector $\boldsymbol{\varepsilon}_i$ is called the local round-off error. To obtain (4.28) we must of course apply method (4.8).

We assume that the local errors are bounded, i.e.

$$\|\boldsymbol{\varepsilon}_i\| \leq \varepsilon > 0, \quad \forall i \in J_M.$$

Subtracting from (4.28) the corresponding relation (4.8), we get

$$\mathbf{r}_{i+k} + \sum_{\nu \in F} (\alpha_\nu + h_{i+k} a_\nu(\mathbf{h}_i)) \mathbf{r}_{i+\nu} - h_{i+k} \sum_{\nu \in D} \beta_\nu(\mathbf{h}_i) [\mathbf{f}(t_{i+\nu}, \tilde{\mathbf{X}}_{i+\nu}) - \mathbf{f}_{i+\nu}] = \boldsymbol{\varepsilon}_i.$$

Recalling the assumption that method (4.8) satisfies the root condition, and observing that $\mathbf{r}_i = \mathbf{0}$, $i = 0, 1, \dots, k-1$, we can apply Lemma with $\omega = 1$, as in the proof of Theorem 6. Hence we have (in correspondence with Henricis Theorem 5.1)

Theorem 10. The accumulated round-off error of method (4.8), satisfying the root condition, and applied to the initial value problem (1.1), is estimated by

$$(4.29) \quad \|\mathbf{r}_i\| \leq \frac{\Gamma^* \varepsilon C}{h_M^*} e^{CI^*B}, \quad \forall i \in J_M,$$

where Γ^* , B and C are the same as in the proof of Theorem 6.

5. APPLICATIONS

In this chapter we shall consider what kind of methods can be constructed by our generalized polynomial interpolation approach. The treatment is illustrative rather than exhaustive.

5.1. Polynomial approximations

5.1.1. Equidistant nodes

From Theorem 3 we see that our methods will reduce to classical linear multistep methods with constant coefficients, when T_M is equidistant with spacing h , and we use 'usual' polynomial interpolants. In such cases

our method is totally defined by the given sets F and D , the integer k , and the weight matrix R . Sets F and D must satisfy the condition ii) of Theorem 1 for an existing method. For the theory of stability, consistency and convergence of the methods we refer to Henrici [22, 23] for more complete results than those presented here in chapter 4.

As far as we know, the problem of stability of a given polynomial interpolation method can be solved only by conversion of the method into the equivalent multistep method, followed by examination of the root condition.

When a search is being made for polynomial interpolation methods, the most natural course is that of taking unit weights associated with the given sets F and D . In such cases, the order of the resulting method will be as high as possible, and the method is always consistent, as is stated by Theorem 5. Clearly, we thus rediscover the classical methods based on numerical integration (see [23]), by taking a unit matrix R , and using the sets of Table 5.1.

Table 5.1.

Method	F	D	k
Adams-Bashforth	$\{k-1\}$	$\{0, 1, \dots, k-1\}$	$1, 2, \dots$
Adams-Moulton	$\begin{cases} \{0\} \\ \{k-1\} \end{cases}$	$\begin{cases} \{1\} \\ \{0, 1, \dots, k\} \end{cases}$	$\begin{cases} 1 \\ 1, 2, \dots \end{cases}$
Nyström	$\begin{cases} \{0\} \\ \{k-2\} \end{cases}$	$\begin{cases} \{1\} \\ \{0, 1, \dots, k-1\} \end{cases}$	$\begin{cases} 2 \\ 2, 3, \dots \end{cases}$
Milne-Simpson (generalized)	$\begin{cases} \{0\} \\ \{0\} \\ \{k-2\} \end{cases}$	$\begin{cases} \{2\} \\ \{1, 2\} \\ \{0, 1, \dots, k\} \end{cases}$	$\begin{cases} 2 \\ 2 \\ 2, 3, \dots \end{cases}$

Similarly we rediscover the classical methods based on numerical differentiation (the methods 5–48 of [23]) by means of Table 5.2.

Table 5.2.

Method	F	D	k
D0	$\{0, 1, \dots, k-1\}$	$\{k\}$	$1, 2, \dots$
D1	$\{0, 1, \dots, k-1\}$	$\{k-1\}$	$1, 2, \dots$
D2	$\begin{cases} \{1\} \\ \{0, 1, \dots, k-1\} \end{cases}$	$\begin{cases} \{0\} \\ \{k-2\} \end{cases}$	$\begin{cases} 2 \\ 2, 3, \dots \end{cases}$
D3	$\begin{cases} \{2\} \\ \{1, 2\} \\ \{0, 1, \dots, k-1\} \end{cases}$	$\begin{cases} \{0\} \\ \{0\} \\ \{k-3\} \end{cases}$	$\begin{cases} 3 \\ 3 \\ 3, 4, \dots \end{cases}$

The coefficients α_ν and β_ν of these methods are obtained by use of matrix P of type (3.24). In P , we have a row for each $\nu \in F$ and $\nu \in D$.

Corresponding columns appear in P^{-1} . The coefficients α_v and β_v are the sums of the elements of these columns.

We notice that the existence of the classical methods is guaranteed by the fact that either F or D has only one element. It is also worthy of note that methods $D0$ with $k = 2, 3, 4, 5, 6$ are the stiffly stable (see [31]) methods proposed by Gear [19].

If the weights in R differ from unity, the maximum possible order is not reached, as is seen from (3.21), (3.22) and (3.23). However if the order of a multistep method is relaxed by one, we arrive at a one-parameter family of methods, as proposed e.g. in [45] and [24] (see also [31]). The nonunity weights may serve as this parameter as well as a parameter introduced into coefficients α_v and β_v . The parameter can then be used to modify the method to obtain useful properties other than high order. Naturally, the idea of parameters is easily generalized to more than one parameter.

As an example of nonunity weights we give a method of type $D0$ ($k = 4$) and two of its also stiffly stable modifications proposed by Jain and Srivastava [24]. The basic formula of order 4 is

$$(5.1) \quad 25X_{n+4} = 48X_{n+3} - 36X_{n+2} + 16X_{n+1} - 3X_n + 12hf_{n+4},$$

when written for the scalar problem as in [24]. Jain and Srivastava give, among others, the following two third-order versions of (5.1):

$$(5.2) \quad 150X_{n+4} = 262X_{n+3} - 159X_{n+2} + 54X_{n+1} - 7X_n + 78hf_{n+4},$$

$$(5.3) \quad 10X_{n+4} = 14X_{n+3} - 3X_{n+2} - 2X_{n+1} + X_n + 6hf_{n+4}.$$

Formulas (5.2) and (5.3) can be obtained by means of $F = \{3, 2, 1, 0\}$, $D = \{4\}$, and the weights $\mu_3, \mu_2, \mu_1, \mu_0$ and μ'_4 . The weights are the ratios of coefficients (5.2) and (5.3) to those of (5.1). The three decimal values of these weights are:

Formula	μ_3	μ_2	μ_1	μ_0	μ'_4
(5.2)	.910	.736	.563	.389	1.083
(5.3)	.729	.208	-.313	-.833	1.250

The behaviour of these weights is understood by reference to an illustrative approach made by Gear [19].

The problem of finding the proper nonunity weights is not treated here, but certainly calls for further study.

The meaning of the inversion condition (3.30) is clarified by the following examples. Let us assume that we have a given k -step method with coefficients $\alpha_v \neq 0$ and $\beta_v \neq 0$ and the corresponding sets F and D . We assume that F and D are such that there exists a polynomial inter-

polation method defined by them. F and D define the matrix P of type (3.24).

When the inversion condition is met, the sums of the elements of the columns in P^{-1} are nonzero and the weights corresponding to coefficients α_ν and β_ν are obtainable by (3.29).

However, in some cases, zero sums exist and the corresponding weights are not defined. This phenomenon occurs, for instance, when $F = \{0\}$ and $D = \{0, 1\}$ (Nyström's method with $k = 2$) or $F = \{0\}$ and $D = \{1, 2\}$ (Milne-Simpson method with $k = 2$) or $F = \{1\}$ and $D = \{0, 1, 2, 3\}$ (Milne-Simpson method with $k = 3$). Thus, given these pairs of sets F and D with the corresponding nonzero coefficients α_ν and β_ν , it is impossible to find a corresponding polynomial interpolation method.

However, the polynomial interpolation methods with sets F and D mentioned above, and with unity weights, will produce the classical methods mentioned. But these methods have a zero coefficient, reducing them to methods obtainable by unity weights in connection with the pairs $F = \{0\}$, $D = \{1\}$ (Nyström's method with $k = 2$, the mid-point rule) or $F = \{0\}$, $D = \{0, 1, 2\}$ (Milne-Simpson method with $k = 2$, the familiar Simpson formula). The explanation is that these methods possess a higher accuracy than would normally be expected (cf. [23], chapter 5.1–2).

Another difficulty involved in finding the polynomial interpolation method that corresponds to a given multistep method occurs if the given sets F and D are such that existence condition ii) of Theorem 1 is not satisfied. The corresponding interpolation method is constructed by taking, instead of F , the set \tilde{F} defined in (3.28) and then applying the formulas (3.29).

As an example, consider the 3-step methods defined by $F = \{0, 2\}$, $D = \{1\}$. Let us assume that they are stable and consistent. They are then given by

$$(5.4) \quad \mathbf{X}_{n+3} = (1 - a)\mathbf{X}_{n+2} + a\mathbf{X}_n + h(1 + 2a)\mathbf{f}_{n+1},$$

where $-1/2 < a \leq 1$. When $a = 0, 1$ and a double zero are the roots of $\varrho(z)$. All the roots of $\varrho(z)$ are of modulus 1 in the method with $a = 1$. Methods (5.4) are of order 1.

The matrix P defined by F and D is singular, but if we take $\tilde{F} = \{0, 1, 2\}$ and $D = \{1\}$, we derive a linear multistep method, which is, with unity weights, of type $D2$ ($k = 2$) and is written as

$$(5.5) \quad \mathbf{X}_{n+3} = 6\mathbf{X}_{n+2} - 3\mathbf{X}_{n+1} - 2\mathbf{X}_n - 6h\mathbf{f}_{n+1}.$$

Hence method (5.4) is obtained by use of the weights

$$\begin{cases} \mu_2 = (1 - a)/6 \\ \mu_1 = 0 \\ \mu_0 = -a/2 \\ \mu'_1 = -(1 + 2a)/6. \end{cases}$$

It is very illustrative to consider the case of $a = 1/2$. Formula (5.4) is then written

$$(5.6) \quad \mathbf{X}_{n+3} = 1/2(\mathbf{X}_{n+2} + \mathbf{X}_n) + 2h\mathbf{f}_{n+1}.$$

This is equivalent to the polynomial interpolation method, which makes use of a 3-degree polynomial formed with the aid of the values in $1/12\mathbf{X}_{n+2}$, $\mathbf{0}$, $-1/4\mathbf{X}_n$ and $-1/3\mathbf{f}_{n+1}$. At first glance, the weights do not seem very reasonable, although (5.6) is closely related to Euler's method.

5.1.2. Arbitrary nodes

When T_M is arbitrary, the situation becomes rather difficult, and the properties of the methods generated by the polynomial interpolation are not known completely. The existence of a method is fully prescribed by the sets F and D . The coefficients of a method are functions of \mathbf{h}_n , and are derived by inversion of the matrix P_n . This is a tedious process for $N > 4$. However, for the conditions of stability, consistency and convergence, we must know the properties of coefficients $\alpha_v(\mathbf{h}_n)$ and $\beta_v(\mathbf{h}_n)$. In particular, we must hope that these coefficients have a certain form, and that they are bounded as required in (4.2), (4.3) and (4.4), to ensure that we can use the results of chapter 4.

The situation is here illustrated by only a few examples. The methods of Piotrowski [41] are easily obtainable by our approach with sets F and D devoted to Adams methods. Thus, we get the formulas

$$(5.7) \quad \mathbf{X}_{n+k} = \mathbf{X}_{n+k-1} + h_{n+k} \sum_{r=0}^k \beta_{nr} \mathbf{f}_{n+r}$$

with coefficients β_{nr} : Among others we have

$$\text{a) } k = 2, \quad \beta_{n2} = 0,$$

$$\beta_{n1} = 1 + \frac{h_{n+2}}{2h_{n+1}}, \quad \beta_{n0} = -\frac{h_{n+2}}{2h_{n+1}}.$$

$$\text{b) } k = 2,$$

$$\begin{aligned}\beta_{n2} &= \frac{1}{2} - \frac{1}{6} \frac{h_{n+2}}{h_{n+2} + h_{n+1}}, \\ \beta_{n1} &= \frac{1}{2} + \frac{1}{6} \frac{h_{n+2}}{h_{n+1}}, \\ \beta_{n0} &= -\frac{1}{6} \frac{h_{n+2}^2}{h_{n+1}(h_{n+2} + h_{n+1})},\end{aligned}$$

c) $k = 3$, $\beta_{n3} = 0$,

$$\begin{aligned}\beta_{n2} &= 1 + \frac{h_{n+3}(2h_{n+3} + 6h_{n+2} + 3h_{n+1})}{6h_{n+2}(h_{n+2} + h_{n+1})}, \\ \beta_{n1} &= -\frac{h_{n+3}(2h_{n+3} + 3h_{n+2} + 3h_{n+1})}{6h_{n+2}h_{n+1}}, \\ \beta_{n0} &= \frac{h_{n+3}(2h_{n+3} + 3h_{n+2})}{6h_{n+1}(h_{n+2} + h_{n+1})}.\end{aligned}$$

Recall assumption (2.6). The coefficients are clearly bounded, as required in (4.3) and (4.4). Furthermore they have the property $\sum_{\nu=0}^k \beta_{n\nu} = 1$. The methods are thus convergent for every T_M that satisfies (2.5) and (2.6). However, the limit of a coefficient $\beta_{n\nu}$ will depend on the way in which the limit is achieved when $M \rightarrow \infty$. For instance, consider method a), and take T_M such that $\frac{h_{n+2}}{h_{n+1}} = \gamma$ for every n , $M \rightarrow \infty$. The limits of β_{n1} and β_{n0} are functions of γ , which may be an arbitrary positive constant.

The methods of Krogh [26] include the generalized Adams methods mentioned above. Moreover, Krogh has suggested the use of a variable step number k .

The mid-point rule (Nyström's method with $F = \{0\}$, $D = \{1\}$, $k = 2$) has a varying step size analogy

$$(5.8) \quad \mathbf{X}_{n+2} = \mathbf{X}_n + h_{n+2} \left(1 + \frac{h_{n+1}}{h_{n+2}} \right) \mathbf{f}_{n+1}.$$

The root condition is satisfied, but for consistency we must demand that

$$\lim_{M \rightarrow \infty} \frac{h_{n+1}}{h_{n+2}} = 1 \text{ for every } n.$$

This means that the only reasonable spacing of T_M is equidistant.

A similar phenomenon appears in the usual Milne-Simpson method with $F = \{0\}$, $D = \{0, 1, 2\}$, $k = 2$, which has the coefficients

$$\left\{ \begin{array}{l} \alpha_{n0} = 1, \\ \beta_{n2} = \frac{1}{3} + \frac{1}{6} \frac{h_{n+1}}{h_{n+2}} - \frac{1}{6} \left(\frac{h_{n+1}}{h_{n+2}} \right)^2, \\ \beta_{n1} = \frac{3}{2} + \frac{1}{2} \frac{h_{n+1}}{h_{n+2}} + \frac{1}{6} \left(\frac{h_{n+1}}{h_{n+2}} \right)^2 - \frac{5}{6} \frac{h_{n+2}}{h_{n+1}}, \\ \beta_{n0} = \frac{1}{6} + \frac{1}{3} \frac{h_{n+1}}{h_{n+2}} - \frac{1}{6} \frac{h_{n+2}}{h_{n+1}}. \end{array} \right.$$

Here

$$\sum_{\nu=0}^2 \beta_{n\nu} = 2 + \frac{h_{n+1}}{h_{n+2}} - \frac{h_{n+2}}{h_{n+1}}.$$

For a consistent method we must require that

$$\lim_{M \rightarrow \infty} \sum_{\nu=0}^2 \beta_{n\nu} = 2 \text{ for every } n,$$

and thus the limit spacing must be equidistant.

5.2. Generalized polynomial approximations

In order to simplify the notation we discuss the equidistant T_M , only. The existence of the methods depends on the space Y_N used. As was proved in Theorem 2, the trigonometric polynomials are applicable. Gautschi [17] has studied these methods in some detail. He has derived his formulas in the form of power series. By our approach the results are obtained in a closed form.

For comparison we give the coefficients of an Adams-Bashforth and Adams-Moulton method: Adams-Bashforth: $F = \{1\}$, $D = \{0, 1\}$, $k = 2$

$$\left\{ \begin{array}{l} \alpha_1 = 1, \\ \beta_1 = \frac{1}{\omega h} \sin \omega h + \frac{\cos \omega h}{\sin \omega h} (1 - \cos \omega h), \\ \beta_0 = \frac{-1}{\omega h} \frac{1 - \cos \omega h}{\sin \omega h}; \end{array} \right.$$

Adams-Moulton: $F = \{0\}$, $D = \{0, 1\}$, $k = 1$

$$\begin{cases} \alpha_0 = 1, \\ \beta_1 = \beta_0 = \frac{1}{\omega h} \frac{1 - \cos \omega h}{\sin \omega h}. \end{cases}$$

When expanded into their Taylor series these coefficients are equivalent to those of Gautschi. Here ω is the frequency parameter (see [17]).

As would be expected the exponential functions will give rise to similar formulas. Let us take $g_1 = 1$, $g_2 = e^{\omega t}$ and $g_3 = e^{-\omega t}$. The Adams-Moulton type formula with $F = \{0\}$, $D = \{0, 1\}$ and $k = 1$ then has the coefficients $\alpha_0 = 1$,

$$\beta_1 = \beta_0 = \frac{\cosh \omega h - 1}{\omega h \sinh \omega h}.$$

A detailed discussion of different nonpolynomial approximations does not fall within the scope of this paper.

Appendix 1: Results from the theory of interpolation

1. General problem of finite interpolation

The problem of selecting the polynomials y_{nj} that satisfy (3.2) is an example of the general problem of finite interpolation [14]. The problem is stated as follows: given an N -dimensional linear space Y_N , with a basis $\{g_1, g_0, \dots, g_N\}$, and N linear functionals $\psi_i, i = 1, 2, \dots, N$ defined on Y_N . Is it possible to find an element $y \in Y_N$ such that

$$(A.1) \quad \psi_i y = w^i, \quad i = 1, 2, \dots, N$$

for an arbitrary N -array \mathbf{w} of given values w^i ? In the present case, the functionals ψ_i are the evaluation functionals at points $t_{n+v}, v \in F$, and the derivative evaluation functionals at points $t_{n+v}, v \in D$. Values w^i are the values $\mu_v X_{n+v}^i$ and $\mu'_v f_{n+v}^i$. The problem occurs for any $n \in J_{M-k}$.

The known results (cf. [14], chapter 2.2) concerning the general problem of finite interpolation needed here are given without proof as

Theorem A1. There exists $y \in Y_N$ satisfying (A.1) for arbitrary values w^i if and only if the functionals ψ_i are linearly independent, i.e. the generalized Gram determinant $|\psi_i g_j|$ ($i, j = 1, 2, \dots, N$) is non-vanishing. In that case, the solution is unique.

The basic difficulty in the application of Theorem A1 is that the generalized Gram determinant may be complicated. However, if by some means we can show that (A.1) has a solution for arbitrary w^i 's, then by Theorem A1 we know that it is unique.

2. Hermite-Birkhoff interpolation by polynomials

A more powerful result is obtained by the observation that our interpolation problem is an example of a generalized Hermite-Birkhoff interpolation. The name HB (Hermite-Birkhoff)-interpolation was first used by Schoenberg [48] in connection with $Y_N = \pi_{N-1}$ (the polynomials of degree $\leq N - 1$), although the problem was initially treated by Birkhoff [3] and Polya [42]. The modern contribution to the theory of HB-interpolation with π_{N-1} is due to Sharma and Prasad [49], Atkinson and Sharma [2], Ferguson [16], Schechter [47] and Lorentz and Zeller [32], see also Mathson [34]. The use of spline functions as interpolant has been discussed by Ritter [44].

For π_{N-1} , the HB-problem is stated as follows: given

i) $k + 1$ nodes (real or complex)

$$(A.2) \quad t_0 < t_1 < \dots < t_k,$$

ii) a so-called incidence matrix $E = (e_{ij})$, $i = 0, 1, \dots, k$, $j = 0, 1, \dots, N - 1$, with elements e_{ij} that are 0 or 1,

iii) a set $e = \{(i, j) | e_{ij} = 1\}$ with N elements,

iv) N real numbers u_{ij} , $(i, j) \in e$.

Then find $y \in \pi_{N-1}$ such that

$$(A.3) \quad y^{(j)}(t_i) = u_{ij}, \quad (i, j) \in e, \quad \left(y^{(j)} = \frac{d^j y}{dt^j} \right).$$

The matrix E is called free [32] or poised [48, 49, 2, 16, etc.], if (A.3) has a solution for each selection of numbers u_{ij} and points (A.2).

Let us denote $m_j = \sum_{i=0}^k e_{ij}$ and $M_j = \sum_{i=0}^j m_i$, $j = 0, 1, 2, \dots, N - 1$.

Schoenberg [48] proved that each free matrix E satisfies the *Pólya condition*

$$(A.4) \quad M_j \geq j + 1, \quad j = 0, 1, \dots, N - 1.$$

According to [32], a sequence of 1's on the i :th row of E

$$(A.5) \quad e_{ij} = \dots = e_{iq} = 1, \quad j \leq q,$$

is called a maximal sequence, if it is not contained in any longer sequence of 1's. A maximal sequence is called supported, if there exists $i_1 < i < i_2$ and $j_1 < j$, $j_2 < j$, for which $e_{i_1 j_1} = e_{i_2 j_2} = 1$.

Sufficient conditions for free matrices E are stated in

Theorem A2. (Lorentz and Zeller [32]). An incidence matrix E is free if it satisfies the Pólya condition, and if each of its supported sequences has an even number of elements.

An equivalent theorem is proved in [2].

When the preceding results are applied to our problem with conditions (3.2), we have $m_0 = K \geq 1$ (F is nonempty), $M_1 = N$ and $e_{ij} = 0$ for $j > 1$. The Pólya condition is thus fulfilled.

Matrix E may contain three types of rows. They can start by

$$(A.6) \quad \begin{array}{ll} \text{i)} & 1 \ 1 \ 0 \ \dots \\ \text{ii)} & 1 \ 0 \ 0 \ \dots \\ \text{iii)} & 0 \ 1 \ 0 \ \dots \end{array}$$

Theorem A2 is useless if E has supported sequences with an odd number of elements. This may occur only if rows of type iii) exist, since the rows of type i) and ii) cannot have supported sequences (no e_{ij} exists with $j < 0$). If we have a j :th row with $e_{j0} = 0$, $e_{j1} = 1$, this implies that we have required

$$(A.7) \quad y'(t_j) = u_{j1}$$

without any requirement for $y(t_j)$. To avoid the odd supported sequences, it is necessary and sufficient to avoid the requirement (A.7) for a bare derivative at a point t_j , if t_j has the following property: t_j lies between t_{i_1} and t_{i_2} such that we have a requirement both for $y(t_{i_1})$ and $y(t_{i_2})$ (i.e. $e_{i_1 0} = e_{i_2 0} = 1$).

Lorentz and Zeller [32] called

$$(A.8) \quad M_j \geq j + 2, \quad j = 0, 1, \dots, N - 2$$

the *strong Pólya condition*. They also proved the following

Theorem A3. (Lorentz and Zeller). Let E be an incidence matrix that satisfies the strong Pólya condition (A.8), and has a row consisting of a single supported one. Then E is not free.

In our case (3.2) only single supported ones may exist. If $m_0 = K = 1$, the strong Pólya condition is not fulfilled. In such cases, E has no supported sequences and is always free. If $m_0 = K > 1$, the strong Pólya condition is filled and theorem A3 is applicable.

3. Hermite-Birkhoff interpolation by generalized polynomials

The HB-interpolation problem can be generalized if, instead of π_{N-1} , any other N -dimensional linear space Y_N is taken. Sufficient conditions, similar to those of Theorem A2 for the existence of the solution of the generalized problem, are not known. With the exception of the basic condition for the generalized Gram determinant in Theorem A1, the only

result known by us is that of Matthews [35]. Fortunately, it is sufficient for our purposes.

We shall present a slightly generalized version of [35] here as

Theorem A4. Let Y_N be an N -dimensional Haar subspace of $C^1[a, b]$ such that the space spanned by the derivatives of the basis functions of Y_N is an $(N - 1)$ -dimensional Haar subspace of $C[a, b]$, denoted by Y'_{N-1} . Take $I = [a, b]$. Then, for any distinct set

$$T_F = \{t_\nu | \nu = 1, 2, \dots, j; t_1 < t_2 < \dots < t_j\} \subset I,$$

and any distinct set

$$T_D = \{t_{\nu_i} | i = 1, 2, \dots, p; t_{\nu_i} \in T_F \text{ or } t_{\nu_i} < t_1 \text{ or } t_{\nu_i} > t_j\} \subset I,$$

such that $j + p \leq N$, and for any set of real numbers,

$$\{u_1, u_2, \dots, u_j, u_{\nu_1}, u_{\nu_2}, \dots, u_{\nu_p}\},$$

an $y \in Y_N$ exists such that

$$(A.9) \quad \begin{cases} y(t_i) = u_i, & i = 1, 2, \dots, j, \\ y'(t_{\nu_i}) = u_{\nu_i}, & i = 1, 2, \dots, p. \end{cases}$$

Proof. The proof is equivalent to that given by Matthews [35] and has accordingly been omitted. The only difference in the theorems is that our set T_D may be a little larger than the corresponding set of Matthews. Matthews has $T_D \subset T_F$. We permit points in T_D outside the interval $[t_1, t_j]$ defined by set T_F . However, this does not disturb the reasoning based on Rolle's theorem in [35].

Remarks. The result of Theorem A4 is equivalent to that of Theorem A2, when Theorem A2 is applied to our special interpolation problem with conditions (3.2). The uniqueness of y in Theorem A4 is warranted, if $j + p = N$, as a consequence of Theorem A1. The Haar condition posed for Y_N and Y'_{N-1} makes Y_N very similar to π_{N-1} . The necessity of the Haar condition is easily understood if we recall that the proofs of Theorems A2 and A3 are heavily based on the number of zeros of polynomials and their derivatives. This also applies to the generalized polynomials in the proof of Theorem A4.

Appendix 2: Proof of Theorem 2

Cf. [17]. We change the basis of Y_N as follows:

$$(A.10) \quad \begin{array}{ccc} \text{New basis} & & \text{Old basis} \\ \left\{ \begin{array}{l} 1 \\ \left(\frac{\sin ut}{uh_M^*}\right)^{2i-1} \cos ut \\ \left(\frac{\sin ut}{uh_M^*}\right)^{2i} \end{array} \right. & & \begin{array}{l} 1 \\ \sin i\omega t \\ \cos i\omega t \end{array} \end{array} \quad \begin{array}{l} \\ i = 1, 2, \dots \\ i = 1, 2, \dots \end{array}$$

Here, we have defined $u = \omega/2$. The fact that the new functions form a basis is an immediate consequence of the known trigonometric identity

$$\sin^{2i}(x/2) = [(1 - \cos x)/2]^i,$$

from which it follows that

$$(A.11) \quad \sin^{2i}(x/2) = \sum_{j=1}^i s_{ij}(1 - \cos jx), \quad i = 1, 2, \dots,$$

where s_{ij} are suitable constants, and in particular $s_{ii} \neq 0$. Differentiation on both sides in (A.11) gives

$$(A.12) \quad \sin^{2i-1}(x/2) \cos(x/2) = \sum_{j=1}^i j/i s_{ij} \sin jx, \quad i = 1, 2, \dots$$

If we take $x = \omega t$, $u = \omega/2$ and multiply the identities (A.11) and (A.12) by suitable constants $(uh_M^*)^{-2i}$ or $(uh_M^*)^{-2i+1}$, it is seen that the new functions form a useful basis obtained by a linear transformation from the old one.

Let our basis functions now be denoted by g_1, g_2, \dots, g_N and the evaluation functionals of (3.2) by ψ_ν for every $\nu \in F$ and every $\nu \in D$. For a fixed n , the generalized Gram determinant $|\psi_\nu g_i|$ that corresponds to (3.2) contains elements of type

$$(A.13) \quad \begin{cases} g_i(t_{n+\nu} - t_{n-k+1}) & \nu \in F, \quad i = 1, 2, \dots, N \\ g_i'(t_{n+\nu} - t_{n-k+1}) & \nu \in D, \quad i = 1, 2, \dots, N \end{cases}$$

With a fixed T_M let us define $\theta_{n\nu}$ so that

$$(A.14) \quad t_{n+\nu} - t_{n-k+1} = \theta_{n\nu} h_M^*.$$

Then, for all n and ν we have $1 - k \leq \theta_{n\nu} \leq 1$.

The elements of $|\psi_\nu g_i|$ in (A.13) are explicitly of the type

$$(A.15) \quad \left\{ \begin{array}{l} \left[\frac{\sin (u \theta_{n\nu} h_M^*)}{u h_M^*} \right]^{2i-1} \cos (u \theta_{n\nu} h_M^*) \\ \left[\frac{\sin (u \theta_{n\nu} h_M^*)}{u h_M^*} \right]^{2i} \end{array} \right\} \nu \in D$$

$$\left\{ \begin{array}{l} \left[\frac{\sin (u \theta_{n\nu} h_M^*)}{u h_M^*} \right]^{2i-2} (2i \cos^2 (u \theta_{n\nu} h_M^*) - 1) \\ 2i \left[\frac{\sin (u \theta_{n\nu} h_M^*)}{u h_M^*} \right]^{2i-1} \cos (u \theta_{n\nu} h_M^*) \end{array} \right\} \nu \in F$$

We can now make the following observations:
 For any integers $j \geq 0, i \geq 1$ as $\tau \rightarrow 0$

$$(A.16) \quad \left\{ \begin{array}{l} \frac{d^j}{d\theta^j} \left[\left(\frac{\sin \tau\theta}{\tau} \right)^{2i-1} \cos \tau\theta \right] \rightarrow \frac{d^j \theta^{2i-1}}{d\theta^j} \quad \text{and} \\ \frac{d^j}{d\theta^j} \left(\frac{\sin \tau\theta}{\tau} \right)^{2i} \rightarrow \frac{d^j \theta^{2i}}{d\theta^j} \end{array} \right.$$

the convergence being uniform with respect to θ in any finite interval. By taking $\tau = u h_M^*$ and letting $M \rightarrow \infty$, we can see that also $\tau \rightarrow 0$. Since $\theta_{n\nu}$ does not depend on Y_N , the elements of our generalized Gram determinant will have the same limits (if they exist) as the elements of the corresponding generalized Gram determinant obtained by means of the elements of π_{N-1} divided by the proper powers of h_M^* . For the existence of these limits we must assume that $\theta_{n\nu}$ is independent of n when M is large. This is true if the spacing of T_M is equidistant when M is large.

Thus we can conclude that if the condition ii) of Theorem 2 is satisfied, and T_M is equidistant, when $M > M_1$ (a sufficiently large constant), the generalized Gram determinant $|\psi_i g_i|$ has a nonzero limit. Hence, by the continuity of functionals ψ_ν , the determinant remains nonzero for $u h_M^*$ sufficiently small, i.e. for M sufficiently large. The application of Theorem A1 finishes our proof.

Remarks. The results of Theorem 2 are very similar to those of Gautschi (cf. [17], Theorem 2). Gautschi also provides estimates for the smallness of ωh_M^* . One rough estimate given in [17] is

$$(A.17) \quad 0 < |\omega h_M^*| < \frac{\pi}{p^2},$$

where p is an integer such that our N corresponds to $2p + 1$. Thus, the requirement for M_1 is very modest.

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