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Explicit, Optimal Stability Functionals and Their Application to Cyclic Discretization Methods*

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Abstract — Zusammenfassung

Explicit, Optimal Stability Functionals and Their Application to Cyclic Discretization Methods. The present paper contains a stability concept for discretization methods of a certain, very general class $\mathfrak{M}$, which is optimal (in the sense of yielding the best general, two-sided error bounds) without being more restrictive than any of the classical stability definitions. The optimal stability functional Ψ_h related to it depends on the linear part of the discretization operator, and has the important property that $\Psi_h[\delta]$ may be of order $q+1$, i.e. $\Psi_h[\delta] = \mathcal{O}(h^{q+1})$, even if the local error δ only has order q, $\delta = \mathcal{O}(h^q)$. This result may be used for the construction of methods with maximum order. Its application to linear cyclic methods, for example, furnishes a new approach to the theory of linear M-cyclic k-step methods of maximum order.

Explizite, optimale Stabilitätsfunktionale und ihre Anwendung auf zyklische Diskretisierungsverfahren. Die vorliegende Arbeit enthält eine Stabilitätsdefinition für sehr allgemeine Diskretisierungsverfahren, die insofern optimal ist, als sie die besten, zweiseitigen Fehlerschranken ergibt, ohne dabei restriktiver zu sein, als die klassischen Stabilitätsdefinitionen. Das zugehörige optimale Stabilitätsfunktional Ψ_h hängt in einfacher Weise vom linearen Teil des Diskretisierungsoperators ab und hat die bemerkenswerte Eigenschaft, daß $\Psi_h[\delta]$ die Ordnung $(q+1)$ haben kann, d. h. $\Psi_h[\delta] = \mathcal{O}(h^{q+1})$, auch wenn δ nur die Ordnung q hat. Notwendige und hinreichende Bedingungen hierfür werden abgeleitet. Dieses Ergebnis ist von praktischer Bedeutung bei der Konstruktion von Verfahren maximaler Konvergenzordnung. Insbesondere führt seine Anwendung auf lineare zyklische Verfahren zu einer neuen Darstellung der Theorie M-zyklischer k-Schrittverfahren und zu ihrem tieferen Verständnis.

1. Introduction

1.1. In [8], Spijker gives a general theory of the structure of error estimates for finite-difference methods, and introduces the concept of "minimal stability functionals" for operators that define such methods. In this paper we consider the question, how to find a minimal stability functional which is *optimal*, in the sense of rendering optimal error bounds. Apparently this amounts to asking for a "best" stability concept.

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For semilinear operators, Spijker proposes to factorize the linear part A of the operator, $A=PQ$, and to determine a minimal stability functional Ψ_0 of P; under certain conditions, Ψ_0 is also a minimal stability functional of A. For special P, it can be obtained explicitly and is given by "Spijker's norm". However, for $Q \neq I$ (I: identity), Ψ_0 does not represent the *optimal* stability functional of A, and the stability concept associated with it (e.g. "stability w.r.t. Spijker's norm") is unnecessarily restrictive. In a recent paper [9], Spijker presents optimal error bounds with stability functionals that are defined implicitly for a class $\mathfrak{K}$ of methods which covers the same methods as the class $\mathfrak{M}$ considered in this contribution.

We are interested in *explicit*, optimal stability functionals in order to find those methods of our class that yield *maximum order bounds* for the discretization error (i.e. methods with the highest order of convergence).

1.2. Thus, in this paper, we are less concerned with optimal error bounds as an objective of its own, but focus on a transparent representation of them, in order to develop criteria for new or more effective methods. Our approach yields an explicit representation of the optimal stability functional for discretization methods of a specific class $\mathfrak{M}$. This class is introduced in *paragraph* 2. It contains most of the classical discretization methods for initial value problems of ordinary differential equations (O.D.E.s) as well as methods for other problems; thus, the limitation to $\mathfrak{M}$ does not represent a serious restriction. Here, we focus on methods for O.D.E.s, including, in particular, cyclic methods.

Explicit, optimal stability functionals for methods of the class $\mathfrak{M}$ are given in *paragraph* 3. They are defined by a norm (definition 3.4) that depends on the operator A and generalizes Spijker's norm; but the stability concept related to it is less restrictive and more easily handled (particularly in the case of composite methods, where stability proofs w.r.t. Spijker's norm may be awkward).

The advantage of having an *explicit* expression for the optimal stability functional allows us to *optimize it over specific methods in* $\mathfrak{M}$. This is done in *paragraph* 4; we show that methods with order of consistency q may converge with order $(q+1)$ if very simple conditions are satisfied. This is important for the construction of methods with *maximum order*. Besides, it also gives a better understanding of Spijker's norm, explaining, in particular, why it furnishes high order bounds for the discretization error of primitive[1] cyclic methods (see the following example (1.2 b)), but not for general cyclic methods of maximal order (such as example (1.2 c)).

The application of our results to cyclic methods in *paragraph* 5 yields a new approach to the theory of linear cyclic methods of maximum order, generalizing considerably the results of Donelson and Hansen [3].

1.3. Before entering the subject, we shall illustrate it by *examples*:

Consider the initial value problem

$$y'(x)=f(x, y(x)), \quad y(a)=\eta_0, \quad x \in [a, b]. \tag{1.1}$$

[1] Definition in Stetter [10], p. 316. The notations in this paper are mostly taken from [10].

To avoid cumbersome notations, our presentation is restricted to the scalar case: $\eta_0 \in \mathbb{R}$, $f: [a, b] \times \mathbb{R} \to \mathbb{R}$, without loss of generality. Assume that f satisfies a Lipschitz-condition w.r.t. y uniformly for $x \in [a, b]$.

Let (1.1) be solved numerically with one of the following three methods, where y_j^* denotes the approximation of y at $x = x_j := a + j\,h$, $j = 0\,(1)\,m$ with $h \in (0, b-a]$, m: greatest integer with $m\,h \leq (b-a)$, $f_j^* := f(x_j, y_j^*)$

$$\text{(a)}\quad y_{j+2}^* = y_j^* + 2\,h\,f_{j+1}^*;\; y_0^* = \eta_0;\; y_1^* = \eta_1(h);\; j = 0\,(1)\,m-2 \quad \text{with}^2\; |y(x_1) - \eta_1(h)| = \mathcal{O}(h^2) \tag{1.2 a}$$

$$\text{(b)}\quad \begin{aligned} y_{2j+1}^* &= y_{2j}^* + h\,f_{2j}^*;\; y_0^* = \eta_0 \\ y_{2j+2}^* &= y_{2j+1}^* + h\,f_{2j+2}^* \end{aligned} \qquad j = 0\,(1)\,[\tfrac{m-2}{2}] \tag{1.2 b}$$

$$\text{(c)}\quad \begin{aligned} y_{2j+2}^* &= y_{2j}^* + \tfrac{h}{3}(f_{2j+2}^* + 4\,f_{2j+1}^* + f_{2j}^*) \\ y_{2j+3}^* &= y_{2j+2}^* + \tfrac{h}{12}(5\,f_{2j+3}^* + 8\,f_{2j+2}^* - f_{2j+1}^*) \end{aligned} \qquad j = 0\,(1)\,[\tfrac{m-3}{2}] \tag{1.2 c}$$

$$y_0^* = \eta_0;\; y_1^* = \eta_1(h) \;\text{ with }\; |y(x_1) - \eta_1(h)| = \mathcal{O}(h^4)$$

Method (1.2 a) is the 2-step midpoint rule, (1.2 b) is a primitive linear 2-cyclic 1-step method, and (1.2 c) is a linear 2-cyclic 2-step method due to Donelson/ Hansen [3].

If a k-step method is stable w.r.t. the norm

$$\|\delta\|_h := \max_{0 \leq j \leq m} |\delta_j| \tag{1.3 a}$$

or

$$\|\delta\|_h := \max_{0 \leq l \leq k-1} |\delta_l| + h \sum_{j=k}^{m} |\delta_j| \tag{1.3 b}$$

or

$$\|\delta\|_h := \sum_{l=0}^{k-1} |\delta_l| + h \max_{k \leq j \leq m} \left| \sum_{l=k}^{j} \delta_l \right| \tag{1.3 c}$$

then there are fixed positive numbers C and $h_0 \leq (b-a)$ such that for all $j \leq m$ and all $h \in (0, h_0]$ we have the following upper bounds for the global discretization error

$$|y_j - y_j^*| \leq C\,\|\delta\|_h \qquad j = 0\,(1)\,m \tag{1.4}$$

where δ_j are the local discretization errors. In general, $|\delta_j| = \mathcal{O}(h^{q^{(j)}})$, and $q = \min\limits_{0 \leq j \leq m} q^{(j)}$ is the *order of consistency* of the method. In case of method (1.2 a), e.g., we have, for $y \in \mathbb{C}^3[a, b]$, $q = 2$ and

$$\delta_j := \begin{cases} 0 & \text{for } j = 0 \\ y(x_1) - \eta_1(h) = \mathcal{O}(h^2) & \text{for } j = 1 \\ h^{-1}[y(x_j) - y(x_{j-2}) - 2\,hf(x_{j-1}, y_{j-1})] = \mathcal{O}(h^2) & \text{for } 2 \leq j \leq m \end{cases}$$

(1.3 c) is the *Spijker norm*; it provides the most refined of the three error bounds and yields the most restrictive stability definition. However, in certain cases, the stability requirement imposed by this norm is *too restrictive.* Method (1.2 a), for example, is *unstable* w.r.t. the Spijker norm (see Stetter [10], p. 83).

[2] In what follows, $|\cdot|$ always denotes a norm in $\mathbb{R}^s$ (with $s \in \mathbb{N}$ defined in the context).

It may happen that the global discretization error obtained with Spijker's norm has higher order than that obtained with (1.3 a) or (1.3 b); but this occurs only for special cases (see section 4.8.) as for the primitive cyclic method (1.2 b).

The bound (1.4) for the global discretization error of method (1.2 c), on the other hand, has only order 3 in h for all three norms (1.3 a—c) if $y \in \mathbb{C}^5[a,b]$; it is well-known, however, that for $y \in \mathbb{C}^5[a,b]$ this method converges with order 4, i.e. $|y_j - y_j^*| = \mathcal{O}(h^4)$. This raises the question whether another norm exists, which furnishes a bound of order 4 — if possible a two-sided one — without rendering the method unstable. In paragraph 3 we propose such a norm as a generalization of Spijker's norm.

2. Â-Methods

2.1. In what follows, we consider the class $\mathfrak{M}$ of discretization methods of the form

$$z_0^* = \zeta_0(h); \quad z_j^* = \hat{A}\, z_{j-1}^* + h\,\hat{\Phi}(x_{j-1}, z_{j-1}^*, z_j^*; h), \quad j = 1\,(1)\,p, \tag{2.1}$$

where $\hat{A}$ is a real (k,k)-matrix; $\zeta_0(h)$, $z_j^* \in \mathbb{R}^k$; $h \in (0, h_0] \subseteq (0, b-a)$, and $\hat{\Phi}: [a,b] \times \mathbb{R}^k \times \mathbb{R}^k \times [0, h_0] \to \mathbb{R}^k$. We always assume that (2.1) has a unique solution z_j^* for all $h \in (0, h_0]$. Methods of this class were first considered in Albrecht [1].

2.2. **Definition:** Methods that can be reduced to the above form (2.1) will be called *Â-methods*, if the following conditions are satisfied:

(a) there is a constant $D \geq 1$ such that $\|\hat{A}^j\| \leq D$ for all $j \in \mathbb{N}$ (2.2 a)

(b) $\hat{\Phi}$ is continuous and satisfies the Lipschitz-condition:

$$|\hat{\Phi}(x, u_1, v_1; h) - \hat{\Phi}(x, u_2, v_2; h)| \leq K_1\,|u_1 - u_2| + K_2\,|v_1 - v_2| \tag{2.2 b}$$

with constants $K_1 \geq 0$ and $K_2 \geq 0$ independent of x, h, u_1, u_2, v_1, v_2.

Condition (2.2 a) is satisfied if the eigenvalues of $\hat{A}$ do not exceed 1 in absolute value and if eigenvalues of modulus 1 have only linear elementary divisors. The matrix $\hat{A}$ as well as the method (2.1) is then said to satisfy the *root condition.* This generalizes Dahlquist's classical stability definition for linear k-step methods.

2.3. Obviously all Runge-Kutta methods belong to $\mathfrak{M}$. To give an idea of the variety of other methods that fall into this class consider the following examples.

Example 1: Linear k-step methods of the form

$$\begin{aligned} y_{j+k}^* &= -\sum_{l=0}^{k-1} \alpha_l\, y_{j+l}^* + h \sum_{l=0}^{k} \beta_l\, f(x_{j+l}, y_{j+l}^*) \\ y_l^* &= \eta_l(h), \quad l = 0\,(1)\,k-1; \quad j = 0\,(1)\,m-k, \end{aligned} \tag{2.3}$$

with $y_j^* \in \mathbb{R}$; $f: [a,b] \times \mathbb{R} \to \mathbb{R}$ Lipschitz-continuous, are reduced to (2.1) by setting

$$z_j^* := \begin{pmatrix} y_j^* \\ y_{j+1}^* \\ \vdots \\ y_{j+k-2}^* \\ y_{j+k-1}^* \end{pmatrix} \in \mathbb{R}^k; \quad \hat{A} := \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 \\ -\alpha_0 & -\alpha_1 & -\alpha_2 & \dots & -\alpha_{k-1} \end{pmatrix} \tag{2.4}$$

$$\hat{\Phi}(x_j, z_j^*, z_{j+1}^*; h) := \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \sum_{l=0}^{k} \beta_l f(x_{j+l}, y_{j+l}^*) \end{pmatrix} \in \mathbb{R}^k; \quad \zeta_0(h) := \begin{pmatrix} \eta_0(h) \\ \eta_1(h) \\ \vdots \\ \eta_{k-2}(h) \\ \eta_{k-1}(h) \end{pmatrix}$$

In case of a *system* of n O.D.E.s we have n equations of the form (2.1) with the same $\hat{A}$ and $\hat{\Phi}$. Of course, they could be written as one equation with a $(n\,k, n\,k)$-matrix; however, we intentionally do *not* make use of this possibility.

f is Lipschitz-continuous, therefore $\hat{\Phi}$ satisfies the Lipschitz-condition (2.2 b). Hence, linear k-step methods are $\hat{A}$-methods if their generating matrix $\hat{A}$ satisfies the root condition.

2.4. *Example* 2: With the above notation, $P(EC)^s$ *E-methods* take the form

$$z_j^{*(0)} = A^{(0)} z_{j-1}^* + h\,\Phi^{(0)}(x_{j-1}, z_{j-1}^*; h); \quad z_0^* = \zeta_0(h); \quad j = 1\,(1)\,p = m-k+1$$
$$z_j^{*(i)} = \hat{A}\, z_{j-1}^* + h\,\Phi^{(1)}(x_{j-1}, z_{j-1}^*, z_j^{*(i-1)}; h); \quad i = 1\,(1)\,s$$

$z_j^* = z_j^{*(s)}$; s: number of corrector evaluations.

Substitution yields

$$z_j^* = \hat{A}\, z_{j-1}^* + h\,\hat{\Phi}(x_{j-1}, z_{j-1}^*; h); \quad z_0^* = \zeta_0(h), \quad j = 1\,(1)\,p$$

where $\hat{\Phi}$ is composed of $\Phi^{(0)}$ and $\Phi^{(1)}$ and satisfies the Lipschitz-condition (2.2 b).

Hence, $P(EC)^s$ E-methods are $\hat{A}$-methods if their corrector matrix $\hat{A}$ satisfies the root condition.

2.5. *Example* 3: *Cyclic methods* can also be reduced to the form (2.1), which simplifies considerably their theoretical treatment as will be seen later. Consider, as an example, method (1.2 c); with

$$z_j^* := \begin{pmatrix} y_j^* \\ y_{j+1}^* \end{pmatrix}; \quad A^{(0)} := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad A^{(1)} := \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}; \quad \zeta_0(h) := \begin{pmatrix} \eta_0 \\ \eta_1(h) \end{pmatrix}$$

$$\Phi^{(0)}(x_{2j}, z_{2j}^*, z_{2j+1}^*; h) := \tfrac{1}{3} \begin{pmatrix} 0 \\ f_{2j+2}^* + 4 f_{2j+1}^* + f_{2j}^* \end{pmatrix}$$

$$\Phi^{(1)}(x_{2j+1}, z_{2j+1}^*, z_{2j+2}^*; h) := \tfrac{1}{12} \begin{pmatrix} 0 \\ 5 f_{2j+3}^* + 8 f_{2j+2}^* - f_{2j+1}^* \end{pmatrix}$$

it takes the form

$$z_0^* = \zeta_0(h); \quad z_{2j-1}^* = A^{(0)} z_{2j-2}^* + h\,\Phi^{(0)}(x_{2j-2}, z_{2j-2}^*, z_{2j-1}^*; h)$$
$$z_{2j}^* = A^{(1)} z_{2j-1}^* + h\,\Phi^{(1)}(x_{2j-1}, z_{2j-1}^*, z_{2j}^*; h).$$

Substitution yields with $w_j^* := z_{2j}^*$, $\hat{A} := A^{(1)} A^{(0)} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}$, $\hat{\Phi} := \Phi^{(1)} + A^{(1)} \Phi^{(0)}$:

$$w_0^* = \zeta_0(h); \quad w_j^* = \hat{A}\, w_{j-1}^* + h\,\hat{\Phi}(x_{j-1}, w_{j-1}^*, w_j^*; h); \quad j = 1\,(1)\,p$$

$\hat{\Phi}$ satisfies the Lipschitz-condition (2.2 b); hence method (1.2 c) is an $\hat{A}$-method if $\hat{A} := A^{(1)} A^{(0)}$ satisfies the root condition.

2.6. *Example* 4: Also Gragg and Stetter's [5] *methods with offstep points* can be reduced to $\hat{A}$-methods. Consider, for example, the following 2-stage method (which is *not* cyclic):

$$\hat{z}_j^* = A^{(0)} z_{j-1}^* + h\,\Phi^{(0)}(x_{j-1}, z_{j-1}^*; h); \quad z_0^* = \zeta_0(h) \tag{2.5 a}$$

$$z_j^* = A^{(1)} \hat{z}_j^* + h\,\Phi^{(1)}(x_{j-1}, z_j^*, \hat{z}_j^*; h), \quad j = 1\,(1)\,p \tag{2.5 b}$$

with

$$A^{(0)} := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\hat{a}_0 & -\hat{a}_1 & -\hat{a}_2 \end{pmatrix}; \; A^{(1)} := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -a_0 & -a_1 & -a_2 \end{pmatrix}; \; z_j^* := \begin{pmatrix} y_j^* \\ y_{j+1}^* \\ y_{j+2}^* \end{pmatrix}; \; \hat{z}_j^* := \begin{pmatrix} y_j^* \\ y_{j+1}^* \\ \hat{y}_{j+2}^* \end{pmatrix}$$

$$\Phi^{(0)}(x_j, z_j^*; h) := \begin{pmatrix} 0 \\ 0 \\ \hat{b}_0 f_j^* + \hat{b}_1 f_{j+1}^* + \hat{b}_2 f_{j+2}^* \end{pmatrix}$$

$$\Phi^{(1)}(x_j, z_{j+1}^*, \hat{z}_{j+1}^*; h) := \begin{pmatrix} 0 \\ 0 \\ b_1 f_{j+1}^* + b_2 f_{j+2}^* + \beta_3 f_{j+3}^* + \beta \hat{f}_{j+3}^* \end{pmatrix}$$

$$\hat{f}_j^* := f(\hat{x}_j, \hat{y}_j^*); \; \hat{x}_j\text{: off-step point.}$$

Setting

$$\alpha_0 := -\hat{a}_0\, a_2; \quad \alpha_1 := -\hat{a}_1\, a_2 + a_0; \quad \alpha_2 := -\hat{a}_2\, a_2 + a_1$$

$$\beta_0 := -\hat{b}_0\, a_2; \quad \beta_1 := -\hat{b}_1\, a_2 + b_1; \quad \beta_2 := -\hat{b}_2\, a_2 + b_2$$

it can be seen that (2.5 a/b) is identical with the off-step method:

$$\hat{y}_j^* = -\hat{a}_2\, y_{j-1}^* - \hat{a}_1\, y_{j-2}^* - \hat{a}_0\, y_{j-3}^* + h(\hat{b}_2 f_{j-1}^* + \hat{b}_1 f_{j-2}^* + \hat{b}_0 f_{j-3}^*)$$

$$y_j^* = -\alpha_2\, y_{j-1}^* - \alpha_1\, y_{j-2}^* - \alpha_0\, y_{j-3}^* + h(\beta_3 f_j^* + \beta_2 f_{j-1}^* + \beta_1 f_{j-2}^* + \beta_0 f_{j-3}^* + \beta \hat{f}_j^*)$$

From (2.5 a/b) we obtain by substitution the form (2.1):

$$z_j^* = \hat{A}\, z_{j-1}^* + h\,\hat{\Phi}(x_{j-1}, z_{j-1}^*, z_j^*; h); \quad z_0^* = \zeta_0(h) \tag{2.6}$$

with $\hat{A} := A^{(1)} A^{(0)}$ and $\hat{\Phi} := \Phi^{(1)} + A^{(1)} \Phi^{(0)}$. (2.6) is an $\hat{A}$-method, if $\hat{A}$ satisfies the root condition, which may be the case no matter whether $A^{(0)}$ and $A^{(1)}$ also satisfy it or not (this indicates that the mechanism of increasing the order and avoiding the "Dahlquist barrier" is the same for cyclic methods and for methods with off-step points).

2.7. *Example* 5: Linear multiderivative methods are *not* $\hat{A}$-methods. Consider, however, the *summed form* (see Henrici [6], p. 329) of linear methods for the special equation $y'' = f(x, y)$ given by

$$y_{j+k}^* = -\sum_{l=0}^{k-2} \alpha_l\, y_{j+l+1}^* + h \sum_{l=0}^{k} \beta_l\, F_{j+l} \tag{2.7}$$

$$F_{j+k}=F_{j+k-1}+hf^*_{j+k};\quad f_j^*:=f(x_j, y_j^*);$$
$$F_{-1}:=H;\, H\text{: constant (see [6]).}$$

This multiderivative method is reduced to (2.1) by setting

$$z_j^*:=\begin{pmatrix} y^*_{j+1} \\ \vdots \\ y^*_{j+k-1} \\ F_{j+k-1}\end{pmatrix}\in\mathbb{R}^k;\qquad \hat{A}:=\begin{pmatrix} 0 & 1 & 0 \dots & 0 & 0 \\ 0 & 0 & 1 \dots & 0 & 0 \\ \dots & & & & \\ 0 & 0 & 0 \dots & 1 & 0 \\ -\alpha_0 & -\alpha_1 & -\alpha_2 \dots & -\alpha_{k-2} & 0 \\ 0 & 0 & 0 \dots & 0 & 1 \end{pmatrix}$$

$$\hat{\Phi}(x_j, z_j^*, z_{j+1}^*; h):=\begin{pmatrix} 0 \\ \vdots \\ 0 \\ \sum_{l=0}^{k}\beta_l F_{j+l} \\ f^*_{j+k}\end{pmatrix}\in\mathbb{R}^k.$$

Hence, all methods of the form (2.7) are $\hat{A}$-methods if $\hat{A}$ satisfies the root condition (as in the previous examples, $\hat{\Phi}$ satisfies the Lipschitz-condition (2.2 b) if f is Lipschitz-continuous).

2.8. The above examples show that the concept of $\hat{A}$-methods allows us to treat a great variety of different methods in the same theoretical way. In fact, it is not easy to indicate widely used methods that are not $\hat{A}$-methods. A prominent class of non-$\hat{A}$-methods are the multiderivative methods (see, however, example 5) and methods with varying coefficients or varying stepsize.

Note, that the difference in the treatment of one-step and multistep methods vanishes, as all $\hat{A}$-methods are reduced to the one-step form (2.1). As will be seen, this notation is very helpful in the formulation of our results, in particular of the stability concept proposed in section 3 and the theoretical approach to composite (especially cyclic) methods.

3. An Optimal Stability Functional for Â-Methods

In this paragraph, we present a stability functional for $\hat{A}$-methods which permits two-sided error bounds and which is optimal in a sense to be defined.

3.1. For each $h\in(0, h_0]$ let $\mathbb{G}_h$ denote the space of the grid functions $z: I_h\to\mathbb{R}^k$, $I_h:=\{x_0, x_1, \dots, x_p\}$, with the norm $\|\cdot\|_h$. Let Ψ_h denote a real functional on $\mathbb{G}_h$. We associate the mapping $U_h\colon \mathbb{G}_h\to\mathbb{G}_h$ with an $\hat{A}$-method by

$$U_h[z](x_j):=\begin{cases} z_0-\zeta_0(h) & \text{for } j=0 \\ h^{-1}\{z_j-\hat{A}\,z_{j-1}-h\,\hat{\Phi}(x_{j-1}, z_{j-1}, z_j; h)\} & \text{for } j=1\,(1)\,p\end{cases}\tag{3.1}$$

3.2. **Definition:** ([8], [10]): Method (2.1) is called *stable with respect to the functional* Ψ_h if there are fixed positive numbers C and $h_1\in(0, h_0]$ such that

$$\|z-z^*\|_h\le C\,\Psi_h[\delta]\tag{3.2}$$

holds for all $h \in (0, h_1]$ and all $z, z^*, \delta \in \mathbb{G}_h$ satisfying

$$U_h[z](x_j) = \delta_j \tag{3.3 a}$$

$$U_h[z^*](x_j) = o. \tag{3.3 b}$$

Ψ_h then is called a *stability functional* for the method.
Frequently Ψ_h is a norm; therefore, one often uses the expression *stable w.r.t. the norm* Ψ_h.

Commonly used stability functionals are (cf. (1.3 a—c))

$$\Psi_h^*[z] := \max_{0 \le j \le p} |z_j| \qquad (\text{"maximum norm"}) \tag{3.4 a}$$

$$\Psi_h^{**}[z] := |z_0| + h \sum_{j=1}^{p} |z_j| \tag{3.4 b}$$

$$\Psi_h^I[z] := \max_{0 \le j \le p} \left\{ \left| z_0 + h \sum_{l=1}^{j} z_l \right| \right\} \qquad (\text{"Spijker's norm"})^3 \tag{3.4 c}$$

3.3. If z denotes the exact solution of a problem under consideration, e.g. (1.1), then inequality (3.2) furnishes a bound for the global error due to the *local discretization errors* δ_j. If, furthermore, $|\delta_j| = \mathcal{O}(h^{q^{(j)}})$, $q^{(j)} \in \mathbb{N}$, then $q := \min_{0 \le j \le p} q^{(j)}$ is called *order of consistency* of method (2.1).

Likewise, the δ_j may be interpreted as *local perturbations* (such as rounding) occurring during the calculation of the approximations z_j^*; (3.2) then gives a bound for their global effect. Besides, we are interested in *two-sided estimates* of the form

$$C_1 \Psi_h[\delta] \le \| z - z^* \|_h \le C_2 \Psi_h[\delta]. \tag{3.5}$$

3.4. **Definition:** Let $\mathbb{G}_h$ have the maximum norm $\| \cdot \|_h^*$ defined by (3.4 a)[4]; then a method is called $\tilde{A}$-*stable* if it is stable w.r.t. the functional

$$\Psi_h^{\tilde{A}}[\delta] := \| w \|_h^* \quad \text{with} \quad w_j := \tilde{A}^j \delta_0 + h \sum_{l=1}^{j} \tilde{A}^{j-l} \delta_l; \quad \delta_j \in \mathbb{R}^k. \tag{3.6}$$

This functional, depending on a (k, k)-matrix $\tilde{A}$, will be called $\tilde{A}$-*norm* and denoted by $\| \delta \|_h^{\tilde{A}}$.

For $\tilde{A} = I$, $\Psi_h^{\tilde{A}}$ reduces to Spijker's norm (3.4 c).

3.5. The practical value of this stability concept depends on the answers to the following questions:

(1) Which methods are $\tilde{A}$-stable?

(2) Does an $\tilde{A}$-norm furnish better error bounds than other norms, e.g. Spijker's norm?

(3) Does it permit two-sided error bounds?

These questions will be answered in the following sections.

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[3] This form of Spijker's norm is slightly more refined than (1.3 c).

[4] The transition to other norms in $\mathbb{G}_h$ is simple, and indicated in section 3.12.

3.6. **Theorem:** *All $\hat{A}$-methods are $\hat{A}$-stable.*

3.7. *Proof*: From (3.3 a/b) we have

$$z_j = \hat{A} z_{j-1} + h \hat{\Phi}(x_{j-1}, z_{j-1}, z_j; h) + h \delta_j; \quad z_0 = \zeta_0 + \delta_0$$

$$z_j^* = \hat{A} z_{j-1}^* + h \hat{\Phi}(x_{j-1}, z_{j-1}^*, z_j^*; h); \qquad z_0^* = \zeta_0, \quad j = 1\,(1)\,p$$

Hence

$$q_j = \hat{A} q_{j-1} + h \delta_j + h e_j \tag{3.7}$$

where

$$q_j := z_j - z_j^*; \quad e_j := \hat{\Phi}(x_{j-1}, z_{j-1}, z_j; h) - \hat{\Phi}(x_{j-1}, z_{j-1}^*, z_j^*; h). \tag{3.8}$$

By induction:

$$q_j = \left(\hat{A}^j \delta_0 + h \sum_{l=1}^{j} \hat{A}^{j-l} \delta_l\right) + h \sum_{l=1}^{j} \hat{A}^{j-l} e_l, \quad j = 0\,(1)\,p \tag{3.9}$$

With (2.2 a/b) we obtain

$$|q_j| \le \|\delta\|_h^{\hat{A}} + h D \sum_{l=1}^{j} (K_1 |q_{l-1}| + K_2 |q_l|) \tag{3.10}$$

and for $h D K_2 < 1$ induction yields:

$$\begin{aligned} |q_j| &\le \frac{(1 + h u)^{j-1}}{(1 - h D K_2)} (\|\delta\|_h^{\hat{A}} + h D K_1 |q_0|); \quad u := \frac{D(K_1 + K_2)}{(1 - h D K_2)} \\ &\le \frac{e^{(b-a)u}}{(1 - h D K_2)} (1 + h D K_1) \|\delta\|_h^{\hat{A}} \end{aligned} \tag{3.11}$$

since $(1 + h u)^j \le e^{hju} \le e^{(b-a)u}$ and $|q_0| = |\delta_0| \le \|\delta\|_h^{\hat{A}}$. Hence, (3.2) is satisfied for all $h \in (0, h_1]$ with $h_1 < (D K_2)^{-1}$.

3.8. Theorem 3.6. implies that $\Psi_h^{\hat{A}}$ is a *stability functional* for $\hat{A}$-methods. Thus, to have $\hat{A}$-stability we only require (2.2 a/b), which is not more than any reasonable other (in particular Dahlquist's) stability concept demands. In view of this fact, one may be inclined to doubt whether the stability definition 3.4. can furnish better error bounds than the classical concepts for methods of practical importance. This, however, is the case, as is illustrated by the following simple examples:

(a) One can show (section 5.2.) that the bound (3.11) obtained with the $\hat{A}$-norm (with $\hat{A} = A^{(1)} A^{(0)}$) for the global discretization error of method (1.2 c) has *order* 4 (whereas the norms (3.4 a—c) only yield the order 3).

(b) The 2-step midpoint-rule (1.2 a) is stable w.r.t. the $\hat{A}$-norm, $\hat{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and unstable w.r.t. Spijker's norm. More general: All weakly stable linear k-step methods are unstable w.r.t. Spijker's norm; they are stable, however, w.r.t. the $\hat{A}$-norm, hence allowing (two-sided) error bounds of the form (3.5).

However, for Adams-methods where[5] (cf. (2.4))

[5] The author is indebted to one of the referees for calling his attention to this case.

$$\hat{A} := \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \quad \delta_j = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ d_j \end{pmatrix} \in \mathbb{R}^k \tag{3.12}$$

we have $\| \delta \|_h^{\hat{A}} = \| \delta \|_h^I$, as is best seen by writing down explicitly the relation (3.6). This explains why the Spijker-norm performs so well for Adams-methods, as observed by Stetter ([10], p. 84).

For the *general case*, however, the $\hat{A}$-norm represents the most natural choice for the functional Ψ_h, as is clearly indicated by (3.9). In fact, as will be seen in section 3.10., it is *optimal* in the following sense:

3.9. **Definition:** Let Ψ_h be a stability functional of an $\hat{A}$-method with Ψ_h independent of $\hat{\Phi}$. Then we call Ψ_h *optimal* if the following conditions hold for all $\delta \in \mathbb{G}_h$ and all $h \in (0, h_1]$:

(a)
$$\| z - z^* \|_h = \Psi_h[\delta] \tag{3.13 a}$$

for all $\hat{\Phi}(x, u, v; h)$ that are independent of u and v.

(b) For any $\varepsilon > 0$ exists a $\gamma > 0$ such that

$$(1-\varepsilon)\, \Psi_h[\delta] < \| z - z^* \|_h < (1+\varepsilon)\, \Psi_h[\delta] \tag{3.13 b}$$

for all $\hat{\Phi}$ with $K_1 + K_2 < \gamma$.

3.10. **Theorem:** *Let $\mathbb{G}_h$ carry the maximum norm; then $\Psi_h[\delta] = \| \delta \|_h^{\hat{A}}$ is optimal and permits the following two-sided error bounds for all $\hat{A}$-methods:*

$$C_1 \| \delta \|_h^{\hat{A}} \le \max_{0 \le j \le p} | z_j - z_j^* | \le C_2 \| \delta \|_h^{\hat{A}} \tag{3.14}$$

where $h \in (0, h_1]$, $h_1 < (D K_2)^{-1}$ (see section 3.7.)

$$C_1 = [1 + (b-a)\, D\, (K_1 + K_2)]^{-1}$$

$$C_2 = e^{(b-a)u} (1 - h D K_2)^{-1} (1 + h D K_1); \quad u := \frac{D (K_1 + K_2)}{(1 - h D K_2)}$$

3.11. *Proof*: (3.13 a) is a consequence of equation (3.9), and (3.13 b) is satisfied if (3.14) holds. The right hand side of (3.14) is already proved by (3.11). To prove the left hand side we consider (3.9):

$$\left(\hat{A}^j \delta_0 + h \sum_{l=1}^{j} \hat{A}^{j-l} \delta_l \right) = q_j - h \sum_{l=1}^{j} \hat{A}^{j-l} e_l$$

$$\begin{aligned} \| \delta \|_h^{\hat{A}} &\le \max_{0 \le j \le p} | q_j | + \max_{0 \le j \le p} \left\{ h D \sum_{l=1}^{j} (K_1 | q_{l-1} | + K_2 | q_l |) \right\} \\ &\le \max_{0 \le j \le p} | q_j | \{ 1 + h p D (K_1 + K_2) \} \\ &\le \max_{0 \le j \le p} | q_j | \{ 1 + (b-a) D (K_1 + K_2) \} \end{aligned}$$

Hence

$$C_1 \| \delta \|_h^{\hat{A}} \le \max_{0 \le j \le p} | q_j |.$$

3.12. We saw in the previous sections that an optimal stability functional for $\hat{A}$-methods is given by the $\hat{A}$-norm if $\mathbb{G}_h$ carries the maximum norm. A generalization to *other norms in* $\mathbb{G}_h$ is obviously obtained by considering the functional

$$\Psi_h^{\hat{A}} := \| w \|_h \quad \text{with} \quad w_j := \hat{A}^j \delta_0 + h \sum_{l=1}^{j} \hat{A}^{j-l} \delta_l. \tag{3.15}$$

Substitution of (3.6) by (3.15) generalizes the stability definition 3.4.

4. Maximum Order Bounds for the Discretization Error

Having achieved an explicit expression for the optimal stability functional $\Psi_h[\delta] = \Psi_h^{\hat{A}}[\delta]$, we now may *optimize it over* $\hat{A}$ to find $\hat{A}$-methods with maximum order of convergence. As a result, we obtain theorem 4.3. and its corollary 4.7. which are of major practical interest for the construction of high order composite methods for O.D.E.s, in particular, of cyclic methods, as will be seen in paragraph 5. It should be noted, however, that they hold for *all* types of discretization methods which are $\hat{A}$-methods; hence, there may be interesting other applications.

4.1. **Lemma:** *Let* $\mu_1 = 1$, $\mu_i \neq 1$ $(i = 2(1)k)$ *be the eigenvalues of the* (k, k)*-matrix* $\hat{A}$, $\{u(\mu_i), i = 1(1)k\}$ *a normal eigenbasis in* $\mathbb{R}^k$, $p^T \neq o$ *a left-eigenvector of* $\hat{A}$ *to the eigenvalue* μ_1, *i.e.* $p^T \hat{A} = p^T$ *and*

$$t := \sum_{i=1}^{k} d_i\, u(\mu_i).$$

Then $d_1 = 0$, *if and only if* $p^T t = 0$.

The *proof* is a consequence of $p^T u(\mu_i) = 0$ for $i \neq 1$.

4.2. It is a remarkable property of the $\hat{A}$-norm that $\| \delta \|_h^{\hat{A}}$ may have order $(q+1)$ in h, $\| \delta \|_h^{\hat{A}} = \mathcal{O}(h^{q+1})$, even if δ_j $(j = 1(1)p)$ only have order q. This is due to the following theorem:

4.3. **Theorem:** (*a*) *For all* $h \in (0, h_0]$ *let* $\delta_j \in \mathbb{R}^k$ *have the form*

$$\delta_0 = \mathcal{O}(h^{q+1}), \tag{4.1}$$

$$\delta_j = h^q g(x_j)\, t + \mathcal{O}(h^{q+1}), \quad j = 1(1)p, \tag{4.2}$$

with $q \in \mathbb{N}$, *a constant vector* $t \in \mathbb{R}^k$, *and a grid function* $g: I_h \to \mathbb{R}$.

(*b*) *Let the eigenvalues of* $\hat{A}$ *satisfy*

$$\mu_1 = 1, \quad |\mu_i| < 1, \quad i = 2(1)k. \tag{4.3}$$

Then

$$\| \delta \|_h^{\hat{A}} = \mathcal{O}(h^{q+1}) \tag{4.4}$$

if and only if one of the following two conditions holds:

$$p^T t = 0 \quad \text{where} \quad p^T \hat{A} = p^T, \quad p \in \mathbb{R}^k \backslash o. \tag{4.5 a}$$

$$\left|\sum_{l=1}^{j} g(x_l)\right| \le c \quad \textit{with a constant } c>0 \textit{ independent of } h \textit{ and } j \le p^{6} \tag{4.5 b}$$

4.4. *Proof*: With (4.1/2) and $t=\sum_{i=1}^{k} d_i u(\mu_i)$ we obtain

$$\|\delta\|_h^{\hat{A}} = \max_{0\le j\le p} \left|\hat{A}^j \delta_0 + h^{q+1} \sum_{l=1}^{j} \hat{A}^{j-l} g(x_l) \sum_{i=1}^{k} d_i u(\mu_i) + \mathcal{O}(h^{q+1})\right|$$

$$= \max_{0\le j\le p} |S_j h^{q+1} + \mathcal{O}(h^{q+1})|$$

with

$$S_j := d_1 \left\{\sum_{l=1}^{j} g(x_l)\right\} u(1) + \sum_{i=2}^{k} d_i \sum_{l=1}^{j} g(x_l) \left\{\sum_{r=0}^{r_i-1} P_{ir}(l)\,\hat{A}^r\right\} \mu_i^{j-l} u(\mu_i) \tag{4.6}$$

where $P_{ir}(l)$ are polynomials of degree (r_i-1). Due to assumption (b) and lemma 4.1., S_j is bounded for all $h\in(0,h_0]$ and all[6] $j\le p$ if and only if (4.5 a) or (4.5 b) holds.

4.5. **Definition:** Conditions (4.5 a) and (4.5 b) will be called *order conditions*.

4.6. *Remarks*: (1) The left-eigenvector p^T need not be calculated! (4.5 a) is satisfied if the $(k, k+1)$-matrix $(\hat{A}-I, t)$ has rank $r=k-1$.

(2) M. N. Spijker suggested[7] to replace (4.2) by the slightly more general assumption

$$\delta_j = h^q\, t(x_j) + \mathcal{O}(h^{q+1}). \tag{4.2)*}$$

The order conditions (4.5 a/b) then reduce to *one* condition:

$$\left|\sum_{l=1}^{j} p^T t(x_l)\right| \le c. \tag{4.5)*}$$

The proof 4.4. basically remains the same if one considers $p^T t(x_l) = d_1(x_l)\, p^T u(1)$.

(3) In certain cases, assumption (4.3) may be replaced by the weaker requirement (2.2 a). In the case of Spijker's norm, for example, we have $\hat{A}=I$ and assumption (4.3) is not satisfied; yet,

$$S_j = \left(\sum_{l=1}^{j} g(x_l)\right) \sum_{i=1}^{k} d_i u(\mu_i)$$

is bounded, if and only if (4.5 b) holds.

(4) The order condition (4.5 a) is of greater practical significance than (4.5 b), as is seen in paragraph 5.

Compare theorem 4.3. with Stetter's theorem 5.4.3. in [10], p. 314, which permits *several* essential roots; the results in his paragraph 5.4.2. already point into the direction of our results.

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[6] Note that p depends on h.

[7] Private communication.

4.7. The following corollary is a consequence of theorem 3.10.; it states which $\hat{A}$-methods with order of consistency q (in the sense of section 3.3.) converge *with order* $(q+1)$:

Corollary: *Let an $\hat{A}$-method and its local discretization errors δ_j satisfy assumptions (a) and (b) of theorem 4.3. Then it converges with order $(q+1)$, and the upper and lower bounds (3.14) for the global discretization error also have order $(q+1)$, if and only if an order condition is satisfied.*

4.8. Note that order condition (4.5 b) is *independent of* $\hat{A}$; hence, it indicates the only cases where bounds obtained *with Spijker's norm* have order $(q+1)$, and corresponds to Spijker's idea ([7], [8]) of constructing (primitive cyclic) methods with order of convergence $(q+1)$ and stages of order q (see example (1.2b)).
We shall see in the next section that condition (4.5 a) generalizes considerably Donelson and Hansen's approach [3] to cyclic methods of maximum order.

5. Examples and Applications to Cyclic Methods

This paragraph contains examples and outlines how to use our results for a new approach to cyclic methods with maximum order.

5.1. *Example* 1: In the case of a linear k-step method with order q we have the local discretization errors

$$\delta_0 = z_0 - \zeta_0(h); \quad \delta_j = h^q\, y^{(q+1)}(x_j)\, t + \mathcal{O}(h^{q+1}) \quad j = 1\,(1)\,p$$

with $t = (0, 0, \dots, 0, c_{q+1})^T \in \mathbb{R}^k$; c_{q+1}: error constant, and $\hat{A}$ is the Frobenius matrix given in (2.4). Then, $p^T = (p_1, p_2, \dots, p_{k-1}, 1)$, hence (4.5 a) only holds for $c_{q+1} = 0$ whereas (4.5 b), in general, cannot be satisfied. Hence, as could be expected, no linear k-step method with order of consistency q converges with order $(q+1)$.

5.2. The situation is different, however, for composite methods, as may be seen from the following simple *example* 2:

Consider the general 2-cyclic 2-step method:

$$y^*_{2j+2} + \alpha_1^{(0)} y^*_{2j+1} + \alpha_0^{(0)} y^*_{2j} = h\,(\beta_2^{(0)} f^*_{2j+2} + \beta_1^{(0)} f^*_{2j+1} + \beta_0^{(0)} f^*_{2j}) \tag{5.1 a}$$

$$y^*_{2j+3} + \alpha_1^{(1)} y^*_{2j+2} + \alpha_0^{(1)} y^*_{2j+1} = h\,(\beta_2^{(1)} f^*_{2j+3} + \beta_1^{(1)} f^*_{2j+2} + \beta_0^{(1)} f^*_{2j+1}) \tag{5.1 b}$$

$$y^*_0 = \eta_0; \qquad y^*_1 = \eta_1(h)$$

with stages of order $q^{(0)}$ resp. $q^{(1)}$. As in section 2.5., both stages can be written in the form (2.1). With

$$z_j := \begin{pmatrix} y_j \\ y_{j+1} \end{pmatrix}; \; A^{(0)} := \begin{pmatrix} 0 & 1 \\ -\alpha_0^{(0)} & -\alpha_1^{(0)} \end{pmatrix}; \; A^{(1)} := \begin{pmatrix} 0 & 1 \\ -\alpha_0^{(1)} & -\alpha_1^{(1)} \end{pmatrix} \text{ and } q := \min(q^{(0)}, q^{(1)})$$

we have

$$z_{2j-1} = A^{(0)} z_{2j-2} + h\,\Phi^{(0)}(x_{2j-2}, z_{2j-2}, z_{2j-1}; h) + \\ + \begin{pmatrix} 0 \\ c_{q+1}^{(0)} \end{pmatrix} y^{(q+1)}(x_{2j})\, h^{q+1} + \mathcal{O}(h^{q+2}),$$

$$z_{2j} = A^{(1)} z_{2j-1} + h\,\Phi^{(1)}(x_{2j-1}, z_{2j-1}, z_{2j}; h) + \begin{pmatrix} 0 \\ c_{q+1}^{(1)} \end{pmatrix} y^{(q+1)}(x_{2j})\, h^{q+1} + \mathcal{O}(h^{q+2}),$$

where $c_{q+1}^{(r)}$ denotes the error constant of the r^{th} stage, if $q^{(r)}=q$, and $c_{q+1}^{(r)}=0$, if $q^{(r)}>q$, $r=0,1$.

With $w_j := z_{2j}$ and $\hat{\Phi} := \Phi^{(1)} + A^{(1)}\Phi^{(0)}$ we obtain by substitution:

$$w_j = A^{(1)} A^{(0)} w_{j-1} + h\,\hat{\Phi}(x_{j-1}, w_{j-1}, w_j; h) + h^{q+1} y^{(q+1)}(x_j)\, t + \mathcal{O}(h^{q+2}),$$

$$j = 1(1)\left[\tfrac{m-1}{2}\right],$$

with

$$t = \begin{pmatrix} 0 \\ c_{q+1}^{(1)} \end{pmatrix} + A^{(1)} \begin{pmatrix} 0 \\ c_{q+1}^{(0)} \end{pmatrix} = \begin{pmatrix} c_{q+1}^{(0)} \\ c_{q+1}^{(1)} - \alpha_1^{(1)} c_{q+1}^{(0)} \end{pmatrix}.$$

Thus, the

$$\delta_j = h^q y^{(q+1)}(x_j)\, t + \mathcal{O}(h^{q+1}) \tag{5.2}$$

have the form (4.2); hence, if (4.3) holds and the starting vector has order $(q+1)$, and if (see remark (1) of section 4.6.):

$$\operatorname{rank}(A^{(1)} A^{(0)} - I, t) = k - 1, \tag{5.3}$$

then method (5.1) has order $(q+1)$.

Using $\alpha_0^{(i)} + \alpha_1^{(i)} + 1 = 0$ (due to consistency) it is easily seen that (5.3) holds if

$$\begin{vmatrix} 1+\alpha_0^{(0)} & c_{q+1}^{(0)} \\ \alpha_1^{(1)} & c_{q+1}^{(1)} \end{vmatrix} = 0 \tag{5.4}$$

Method (1.2 c), for example, satisfies this condition.

Example 2 shows how corollary 4.7. may be used for the construction of composite methods with maximum order, especially of cyclic methods. In a similar manner, one may obtain the following general results (see Albrecht [2]):

5.3. **Theorem:** *Let a M-cyclic k-step method have (not necessarily stable) stages with order* $q^{(r)}$, $r=0(1)M-1$, *and starting values of order* $(q+1)$, *with* $q := \min_{0\le r\le M-1} q^{(r)}$. *Let the eigenvalues* μ_i *of* $\hat{A} := A^{(M-1)} A^{(M-2)} \dots A^{(1)} A^{(0)}$ *satisfy* $\mu_1 = 1$, $|\mu_i| < 1$, $i = 2(1)k$. *Then it converges with order* $(q+1)$ *for all* $y \in \mathbb{C}^{q+1}[a,b]$, *if* $p^T t = 0$ *(see 4.5 a) where* $p^T \hat{A} = p^T$, $p \neq o$,

$$t := c^{(M-1)} + A^{(M-1)} c^{(M-2)} + A^{(M-1)} A^{(M-2)} c^{(M-3)} + \dots + A^{(M-1)} \dots A^{(1)} c^{(0)} \tag{5.5}$$

$$c^{(r)} := (0, 0, \dots, 0, c_{q+1}^{(r)})^T \in \mathbb{R}^k$$

$$c_{q+1}^{(r)} := \textit{error constant of the r-th stage if } q^{(r)} = q, \textit{ otherwise } 0. \tag{5.6}$$

Note that the method may be stable although its stages are unstable which represents the main advantage of composite methods. It is due to the fact that $\hat{A}$ may satisfy condition (4.3) although some or all $A^{(i)}$ don't and implies that the "Dahlquist barrier" does not hold for composite methods.

For $M=k$, we have the following special case of theorem 5.3.:

5.4. **Theorem:** *In the case of linear k-cyclic k-step methods with stages of order q, the order condition* (4.5 a) *reduces to the requirement* (*compare with* (5.4)):

$$\det\begin{pmatrix} 1+\alpha_0^{(0)} & \alpha_1^{(0)} & \dots & \alpha_{k-2}^{(0)} & c_{q+1}^{(0)} \\ \alpha_{k-1}^{(1)} & 1+\alpha_0^{(1)} & \dots & \alpha_{k-3}^{(1)} & c_{q+1}^{(1)} \\ \dots & \dots & \dots & \dots & \dots \\ \alpha_2^{(k-2)} & \alpha_3^{(k-2)} & \dots & 1+\alpha_0^{(k-2)} & c_{q+1}^{(k-2)} \\ \alpha_1^{(k-1)} & \alpha_2^{(k-1)} & \dots & \alpha_{k-1}^{(k-1)} & c_{q+1}^{(k-1)} \end{pmatrix}=0 \tag{5.7}$$

where $\alpha_i^{(j)}$ $(i=0\,(1)\,k)$ *denote the coefficients of the j-th stage with* $\alpha_k^{(j)}=1$, $j=0\,(1)\,k-1$, *and* $c_{q+1}^{(j)}$ *as in* (5.6).

In the special case $q=2k-1$, one may show that $c_{2k}^{(j)}=c\,(1+\alpha_0^{(j)})$, $j=0\,(1)\,k-1$; condition (5.7) then reduces to

$$\det\begin{pmatrix} 1+\alpha_0^{(0)} & \alpha_1^{(0)} & \dots & \alpha_{k-2}^{(0)} & (1+\alpha_0^{(0)}) \\ \alpha_{k-1}^{(1)} & 1+\alpha_0^{(1)} & \dots & \alpha_{k-3}^{(1)} & (1+\alpha_0^{(1)}) \\ \dots & \dots & \dots & \dots & \dots \\ \alpha_2^{(k-2)} & \alpha_3^{(k-2)} & \dots & 1+\alpha_0^{(k-2)} & (1+\alpha_0^{(k-2)}) \\ \alpha_1^{(k-1)} & \alpha_2^{(k-1)} & \dots & \alpha_{k-1}^{(k-1)} & (1+\alpha_0^{(k-1)}) \end{pmatrix}=0 \tag{5.8}$$

(5.8) represents the general form of three (rather complicated) equations obtained for the special cases $k=2$, 3, and 4 by Donelson and Hansen [3].

Finally, it is easy to show [2] that if a linear M-cyclic k-step method satisfies an order condition, then any *cyclic* permutation of its stages also satisfies one.

5.5. k-cyclic k-step methods with maximum order $2k$ have very small stability regions, which makes them useless for practical application. Therefore, it is more advisable to employ (5.7) for the construction of methods with order $<2k$ that have favourable additional properties, e.g. *stiff stability* (in the sense of Gear [4]).

Example 3: The linear 3-cyclic 3-step method given by $(r=0, 1, 2)$

$$\begin{aligned} &\alpha_0^{(r)}=-\alpha_1^{(r)}-\alpha_2^{(r)}-1; && \alpha_3^{(r)}=1 \\ &\beta_0^{(r)}=\tfrac{1}{24}(9\,\alpha_1^{(r)}+8\,\alpha_2^{(r)}+9);; && \beta_1^{(r)}=\tfrac{1}{24}(19\,\alpha_1^{(r)}+32\,\alpha_2^{(r)}+27) \\ &\beta_2^{(r)}=\tfrac{1}{24}(-5\,\alpha_1^{(r)}+8\,\alpha_2^{(r)}+27); && \beta_3^{(r)}=\tfrac{1}{24}(\alpha_1^{(r)}+9) \end{aligned} \tag{5.9}$$

with the values

$$\begin{aligned} &\alpha_1^{(0)}=-0{,}956; && \alpha_1^{(1)}=1{,}363; && \alpha_1^{(2)}=4{,}591 \\ &\alpha_2^{(0)}=-0{,}375; && \alpha_2^{(1)}=-2{,}659; && \alpha_2^{(2)}=-4{,}1600389843\dots \end{aligned}$$

is an $\hat{A}$-method. Its (unstable) stages have order 4 and relation (5.7) is satisfied for $k=3$, $q=4$; hence the method *converges with order* 5. An analysis of its stability region $R(H), H:=\lambda h$, shows that it is simply connected and contains $H_1=\{H : \operatorname{Re} H<-2\}$ and its closure contains $H=0$; i.e. the method is *stiffly stable.* This interesting aspect of cyclic methods is investigated in a forthcoming paper of Mihelčić.

5.6. As shown in this paragraph, theorem 4.3. is particularly useful for cyclic methods; however, it is as well applicable to *other* composite methods, as is indicated by the following *example.*

Consider the composite 2-step *generalized Nordsieck procedure*:

$$\begin{aligned} y_j^* &= \tfrac{1}{2} y_{j-1}^* + \tfrac{1}{2} \bar{y}_{j-2}^* + \tfrac{h}{8}(3 f_j^* + 8 f_{j-1}^* + f_{j-2}^*) \\ \bar{y}_{j-1}^* &= \tfrac{1}{2} y_{j-1}^* + \tfrac{1}{2} \bar{y}_{j-2}^* + \tfrac{h}{24}(-f_j^* + 8 f_{j-1}^* + 5 f_{j-2}^*), \quad j = 2(1)m. \\ y_0^* &= \bar{y}_0^* = \eta_0; \quad y_1^* = \eta_1(h) \text{ with } |\eta_1(h) - y(x_1)| = \mathcal{O}(h^4). \end{aligned} \tag{5.10}$$

With

$$z_j^* := \begin{pmatrix} y_j^* \\ \bar{y}_{j-1}^* \end{pmatrix}, \quad \hat{A} := \tfrac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad \hat{\phi}_j := \tfrac{1}{24}\begin{pmatrix} 9 f_j^* + 24 f_{j-1}^* + 3 f_{j-2}^* \\ -f_j^* + 8 f_{j-1}^* + 5 f_{j-2}^* \end{pmatrix}$$

it reduces to $z_j^* = \hat{A} z_{j-1}^* + h \hat{\phi}_j$. $\hat{A}$ satisfies the root condition and $\hat{\phi}$ the Lipschitz condition (2.2 b); hence, (5.10) is an $\hat{A}$-method.

Each of the stages in (5.10) has order of consistency $q=3$ with the error constants $c_4^{(0)} = \frac{1}{48}$ and $c_4^{(1)} = -\frac{1}{48}$, respectively. As $p^T = (1, 1)$ and $t = (c_4^{(0)}, c_4^{(1)})^T$, our order condition $p^T t = 0$ is satisfied hence the method converges with order $(q+1) = 4$.

The particular method (5.10) can be obtained by modifying an Adams-Moulton method of order 4 (see e.g. Stetter [10], p. 361), thus it is already known to have order 4. For general methods of the above type, however, it would be difficult to prove the exact order of convergence *without* theorem 4.3.

6. Conclusion

We saw that the possibility to obtain explicit optimal stability functionals led to a new stability concept and enabled us to find $\hat{A}$-methods with maximum order bounds and thus of maximum order. Although we only made use of this result for the construction of high order (composite) methods for the solution of O.D.E.s, it may be interesting to look for applications of theorem 4.3. to other discretization methods, particularly for partial differential equations [2].

Revising this paper, the author wants to mention the contribution of R. Skeel [11] which in the meantime came to his attention. Skeel also considers methods of the class $\mathfrak{M}$, and obtains results similar to theorem 3.10. and theorem 4.3. His stability functional $\| [E]^{-1} R \|_\infty$, however, seems not to be optimal in the sense of definition 3.9.

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