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Stepsize restrictions for stability in the numerical solution of ordinary and partial differential equations

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Abstract: This paper deals with the stability analysis of one-step methods for the numerical solution of initial value problems. Both stiff ordinary and partial differential equations are included.

The problem is considered how to restrict the stepsize in the methods in order that they behave stable. We review and extend some recent results on this problem that are based on the use of stability regions in the complex plane.

We focus on differential equations that are essentially more general than the classical test equation $U'(t) = \lambda \cdot U(t)$ (with λ a complex constant). Further, the emphasis is on stability of the methods with respect to the maximum norm.

Keywords: Numerical analysis, initial value problems, stiff ordinary differential equations, partial differential equations, stability, contractivity, maximum norm.

1. Introduction

1.1. The purpose of the paper

This paper is concerned with step-by-step methods for the numerical solution of initial value problems. Both methods for partial differential equations and methods for (stiff) ordinary differential equations are dealt with.

An important question in the step-by-step solution of initial value problems is to predict whether the numerical process will behave stable or not. Classical tools to assess this stability a priori include the famous Von Neumann condition (for partial differential equations) and the so-called stability regions in the complex plane (for ordinary differential equations). Both of these tools are based on the behaviour of the numerical methods when applied to very simple linear test problems. A weakness of these tools is the fact that the above assessment can fail to be relevant to initial value problems that are more realistic and more complicated than the test problems.

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Recently stability regions have been used in rigorously proving stability of numerical methods applied to stiff ordinary differential equations that are essentially more general than the simple, classical test equations (see e.g. [2,6,11,19,30]). Due to the framework in which the proofs are given, these stability results are applicable as well to some methods for partial differential equations where the Von Neumann condition can fail.

The purpose of this paper is to review and extend some of these results and closely related ones. Our discussion is illustrated in the numerical solution of a diffusion-convection problem. We confine our considerations to so-called one-step methods and to linear differential equations that are essentially more general than the test equations mentioned above. Further we focus on stability results with respect to the important maximum norm. For multistep methods, nonlinear differential equations or norms generated by an inner product we refer to [3,4,18,20,25,30].

1.2. Organization of the paper

In Section 2 we formulate the numerical process to be studied in this paper.

In Section 3 we introduce three kinds of stability for this process, viz. weak stability, strong stability and contractivity.

Section 4 is devoted to an obvious, but very unreliable manner in which the stability region may be used for assessing a priori the stability behaviour of the process.

Section 5 provides general conditions for weak stability, which are applied later on in Section 6. Section 5 is a bit technical and can be skipped by the reader who is not so much interested in the proofs.

The Sections 6, 7 are devoted to reliable criteria for weak stability, strong stability and contractivity with respect to the maximum norm. The criteria are formulated in terms of two quantities r and R, which depend on the numerical method but not on the given initial value problem.

Section 8 reviews recent results on the possible size of r and R.

2. Step-by-step methods

In this paper we deal mainly with numerical procedures that can be written in the form

$$u_n = \varphi(hA)u_{n-1} + p_n, \quad n = 1, 2, 3, \ldots . \tag{2.1}$$

Here $h > 0$ denotes a so-called stepsize and A is a real square matrix of order $s \geqslant 1$. Further φ is a given rational function with $\varphi(0) = \varphi'(0) = 1$ and $\varphi(z) = P(z)/Q(z)$ where P, Q are polynomials with real coefficients and no common zero. We say that $\varphi(hA)$ exists and we write $\varphi(hA) = P(hA)Q(hA)^{-1}$ whenever the matrix $Q(hA)$ is regular. In the above, p_n are given vectors in the s-dimensional real vectorspace $\mathbb{R}^s$, whereas $u_n \in \mathbb{R}^s$ are numerical approximations computed in a step-by-step fashion from (2.1) starting from a given $u_0 \in \mathbb{R}^s$.

Many known numerical methods for solving ordinary differential equations, such as Runge–Kutta methods and Rosenbrock methods (cf. [5]), result, when applied to the initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = AU(t) + p(t), \quad t \geqslant 0, \qquad U(0) = u_0,$$

into a procedure of type (2.1). In this situation u_n is an approximation to the true solution $U(t) \in \mathbb{R}^s$ at $t = nh$.

Further, many numerical schemes for solving initial boundary-value problems in partial differential equations can be written in the form (2.1). As an illustration we consider the problem

$$U_t(x, t) = a(x)U_{xx}(x, t) + b(x)U_x(x, t) + c(x)U(x, t) + d(x), \tag{2.2a}$$

$$U(0, t) = f(t), \qquad U_x(1, t) = 0, \tag{2.2b}$$

$$U(x, 0) = e(x) \tag{2.2c}$$

where $0 < x < 1$, $0 < t$ and a, b, c, d, e, f are given functions with

$$a(x) > 0, \qquad b(x) \leqslant 0, \qquad c(x) \leqslant 0.$$

We choose $\Delta t = h > 0$, $\Delta x = s^{-1}$ and consider the approximation of $U(j\,\Delta x, n\,\Delta t)$ by quantities u_j^n. The following finite difference scheme has been constructed by standard principles (cf. [16,22]).

$$\begin{aligned}(\Delta t)^{-1}&\left(u_j^n - u_j^{n-1}\right)\\ &= (\Delta x)^{-2} a(j\,\Delta x)\left\{\theta\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + (1-\theta)\left(u_{j-1}^{n-1} - 2u_j^{n-1} + u_{j+1}^{n-1}\right)\right\}\\ &\quad + (\Delta x)^{-1} b(j\,\Delta x)\left\{\theta\left(u_j^n - u_{j-1}^n\right) + (1-\theta)\left(u_j^{n-1} - u_{j-1}^{n-1}\right)\right\}\\ &\quad + c(j\,\Delta x)\left\{\theta u_j^n + (1-\theta)u_j^{n-1}\right\} + d(j\,\Delta x),\end{aligned} \tag{2.3a}$$

$$u_0^{n-1} = f((n-1)\,\Delta t), \qquad u_{s+1}^{n-1} = u_{s-1}^{n-1}, \tag{2.3b}$$

$$u_j^0 = e(j\,\Delta x) \tag{2.3c}$$

where $j = 1, 2, \dots, s$ and $n = 1, 2, 3, \dots$ whereas θ is a given parameter. If $\theta = 0$, the above scheme reduces to the well-known explicit upwinded finite difference scheme (cf. [16]). The choices $\theta = \frac{1}{2}$, $\theta = 1$ correspond to the Crank–Nicolson scheme and to the, fully implicit, Laasonen scheme, respectively (cf. [16,22]). It is easily verified that the scheme (2.3a), (2.3b) is of type (2.1) with $u_n = (u_1^n, u_2^n, \dots, u_s^n)^{\mathrm{T}}$, $A = (\alpha_{ij})$,

$$\left.\begin{aligned}&\alpha_{i,i-1} = s^2 a(i\,\Delta x) - sb(i\,\Delta x), \quad i = 2, 3, \dots, s-1,\\ &\alpha_{s,s-1} = 2s^2 a(s\,\Delta x) - sb(s\,\Delta x),\\ &a_{i,i} = -2s^2 a(i\,\Delta x) + sb(i\,\Delta x) + c(i\,\Delta x), \quad i = 1, 2, \dots, s,\\ &\alpha_{i,i+1} = s^2 a(i\,\Delta x), \quad i = 1, 2, \dots, s-1,\\ &\alpha_{i,j} = 0 \quad \text{for } |i-j| > 1\end{aligned}\right\} \tag{2.4}$$

and with function φ defined by

$$\varphi(z) = [1 + (1-\theta)z]/[1 - \theta z]. \tag{2.5}$$

3. Stability

Suppose the numerical calculations based on (2.1) would be performed using a perturbed starting vector $\tilde{u}_0$, instead of u_0. We then would obtain approximations that we denote by $\tilde{u}_n$.

For instance $\tilde{u}_0$ may stand for a finite-digit representation in a computer of the true u_0 and the $\tilde{u}_n$ then stand for the numerical approximations obtained in the presence of the rounding error $v_0 = \tilde{u}_0 - u_0$.

In the stability analysis of (2.1) the crucial question is whether the difference $v_n = \tilde{u}_n - u_n$ (for $n \geqslant 1$) can be bounded suitably in terms of the perturbation $v_0 = \tilde{u}_0 - u_0$. Since $v_n = \tilde{u}_n - u_n = (\varphi(hA)\tilde{u}_{n-1} + p_n) - (\varphi(hA)u_{n-1} + p_n)$ we have

$$v_n = \varphi(hA)v_{n-1}, \quad n = 1, 2, 3, \ldots . \tag{3.1}$$

The stability analysis of (2.1) thus amounts to investigating the possible growth of vectors v_n satisfying the recurrence relation (3.1).

Let $\| \xi \|$ denote an arbitrary norm for $\xi \in \mathbb{R}^s$. We shall be concerned with three kinds of stability, characterized by the following inequalities.

$$\| v_n \| \leqslant \gamma n^q \| v_0 \| \quad \text{whenever } n \geqslant 1 \text{ and } v_0, v_1, v_2, \ldots \text{ satisfy (3.1)}, \tag{3.2}$$

$$\| v_n \| \leqslant \gamma \| v_0 \| \quad \text{whenever } n \geqslant 1 \text{ and } v_0, v_1, v_2, \ldots \text{ satisfy (3.1)}, \tag{3.3}$$

$$\| v_n \| \leqslant \| v_0 \| \quad \text{whenever } n \geqslant 1 \text{ and } v_0, v_1, v_2, \ldots \text{ satisfy (3.1)}. \tag{3.4}$$

Here γ, q denote positive constants. The properties (3.2), (3.3), (3.4) are called *weak stability, strong stability* and *contractivity*, respectively. In the following we focus on these properties with $\| \xi \| = | \xi |$ where $| \xi |$ denotes the *maximum norm*,

$$| \xi | = \max_i | \xi_i | \quad \text{for } \xi = (\xi_1, \xi_2, \ldots, \xi_s)^{\mathrm{T}} \in \mathbb{R}^s.$$

4. Stability analysis using the eigenvalues of *A*

An obvious manner to assess the stability of the process (2.1) is to use the eigenvalues of the matrix $\varphi(hA)$. Note that μ is an eigenvalue of the latter matrix if and only if $\mu = \varphi(h\lambda)$ where λ is an eigenvalue of A. In order to guarantee a mild growth, like (3.3), of the v_n satisfying (3.1) one might thus arrive at the requirement that $h > 0$ be chosen in such a way that $| \varphi(h\lambda) | < 1$ (for all eigenvalues λ of A).

We define the *stability region* S of the function φ by

$$S = \{ z \mid z \in \mathbb{C} \text{ is a regular point of } \varphi \text{ and } | \varphi(z) | \leqslant 1 \}.$$

Since $| \varphi(z) | <$ if and only if z belongs to the interior of S (denoted by int(S)), the above requirement can be cast into the form

$$h\lambda \in \operatorname{int}(S) \quad \text{for all eigenvalues } \lambda \text{ of } A. \tag{4.1}$$

This condition is notorious for being very *unreliable* (see e.g. [10,17,21,30]). The point is that (4.1) implies (3.3) indeed, but unfortunately γ depends on hA and can be extremely large for given h and A. So under condition (4.1) we can formally have strong stability but from a practical point of view mere instability.

We illustrate the above point by problem (2.2) with

$$a(x) = 1, \qquad b(x) = -1000, \qquad c(x) = 0. \tag{4.2}$$

Let $A = (\alpha_{ij})$ and φ be defined by (2.4), (2.5) with $s = 20$, $\theta = 0.25$. From [26] it follows that the eigenvalues λ of A are different from each other and satisfy $-26514 < \lambda < 0$. The stability region of φ equals

$$S = \{ z \mid z \in \mathbb{C} \text{ with } |z+2| \leqslant 2 \}. \tag{4.3}$$

Since $(15 \times 10^{-5}) \times 26514 < 4$, condition (4.1) is fulfilled with $h = 15 \times 10^{-5}$. However, a straightforward numerical computation reveals that, with this stepsize and with the maximum norm, the smallest γ for which (3.3) holds equals $\gamma \simeq 2 \times 10^{12}$. We also refer to [10] for interesting examples with (2.2), (4.2), (3.3) where $\gamma > K^s$, for some $K > 1$, while (4.1) is fulfilled.

From the above it is clear that the concept of a stability region can fail in assessing the stability of numerical processes if it is used in the naive way (4.1). More reliable ways to apply stability regions include the use of the concept of the spectrum of a family of matrices (see [6,17]) and the use of an upper bound for the entries of the matrix A. The latter possibility will be discussed in the Sections 6, 7.

5. General sufficient conditions for weak stability

In this section we study weak stability for the process

$$u_n = \varphi_n(h_n A) u_{n-1} + p_n, \quad n = 1, 2, 3, \ldots, \tag{5.1}$$

which is a bit more general than (2.1). With $h_n > 0$ we denote variable steps and with φ_n variable rational functions of the type described in Section 2. Processes (5.1) arise when one wants to adapt the stepsize or the method locally to the probable smoothness of the true solution that is approximated. For instance, in (2.3) one might change Δt or θ depending on the behaviour of $f(t)$.

Analogously to (3.1) we consider

$$v_n = \varphi_n(h_n A) v_{n-1}, \quad n = 1, 2, 3, \ldots . \tag{5.2}$$

We deal with an arbitrary norm $\| \xi \|$ in $\mathbb{R}^s$ and define the corresponding matrix norm by

$$\| T \| = \max\{ \| T\xi \| : \xi \in \mathbb{R}^s \text{ with } \| \xi \| = 1 \},$$

for all square matrices T of order s. The matrix A in (5.1) is assumed to satisfy a so-called *circle condition*

$$\| A + \rho \| \leqslant \rho \tag{5.3}$$

where ρ is a positive real constant.

For studying the stability of (5.1) it is convenient to introduce the disk

$$D(\rho) = \{ z \mid z \in \mathbb{C} \text{ and } |z + \rho| \leqslant \rho \} \tag{5.4}$$

and to define functions ψ_n by

$$\psi_n(z) = \varphi_n(h_n z) \cdots \varphi_2(h_2 z) \varphi_1(h_1 z), \quad n \geqslant 1. \tag{5.5}$$

We list three conditions that are essential in the following theorem,

$$\psi_n \text{ has no removable singularities or poles in } D(\rho) \quad \text{for } n \geqslant 1, \tag{5.6}$$

$$| \psi_n(z) | \leqslant K \quad \text{for } z \in D(\rho), \quad n \geqslant 1, \tag{5.7}$$

$$\left| \frac{\mathrm{d}}{\mathrm{d}z} \psi_n(z) \right| \leqslant Ln \quad \text{for } z \in D(\rho), \quad n \geqslant 1. \tag{5.8}$$

Theorem 5.1. *Let K, L, ρ be given positive constants. Assume A satisfies* (5.3) *and φ_n, h_n are such that* (5.5)–(5.8) *are fulfilled. Then all matrices $\varphi_n(h_nA)$ exist and all v_n with* (5.2) *satisfy*

$$\| v_n \| \leqslant (2K + L\rho)\sqrt{n}\, \| v_0 \|, \quad n \geqslant 1. \tag{5.9}$$

Proof. Let $n \geqslant 1$ be given and write $\varphi_n = P/Q$ with P and Q as in Section 2. It follows from (5.6) that the polynomial Q is nonzero in the disk $D(h_n\rho)$. Since, by (5.3), all eigenvalues of the matrix h_nA are contained in this disk, the matrix $Q(h_nA)$ is regular so that $\varphi_n(h_nA)$ exists.

Using the Taylor expansion $\psi_n(z) = \sum_{j=0}^{\infty} c_j(z+\rho)^j$ (for $z \in D(\rho)$), we have for any integer $m \geqslant 0$ (cf. [7])

$$\| \psi_n(A) \| \leqslant \sum_{j=0}^{m} |c_j| \| A + \rho \|^j + \sum_{j=m+1}^{\infty} |c_j| \| A + \rho \|^j.$$

From (5.3), the Cauchy–Schwartz inequality and Parseval's formula we get

$$\begin{aligned} \| \psi_n(A) \| &\leqslant \sqrt{m+1} \left(\sum_{j=0}^{m} c_j^2 \rho^{2j} \right)^{1/2} + \left(\sum_{j=m+1}^{\infty} \rho^2/j^2 \right)^{1/2} \left(\sum_{j=m+1}^{\infty} j^2 c_j^2 \rho^{2j-2} \right)^{1/2} \\ &\leqslant \sqrt{m+1}\, K + \rho \left(\sum_{j=m+1}^{\infty} j^{-2} \right)^{1/2} nL. \end{aligned}$$

Since

$$\sum_{j=m+1}^{\infty} j^{-2} \leqslant \int_m^{\infty} x^{-2}\, \mathrm{d}x = m^{-1},$$

we can choose $m = n$ to obtain

$$\| \psi_n(A) \| \leqslant (2K + L\rho)\sqrt{n}. \quad \square$$

In order to apply Theorem 5.1 one has to verify whether (5.8) is fulfilled. For this purpose the following lemma can be helpful, in which we deal with the simpler conditions

$$| \psi_n(z) | \leqslant M^n \quad \text{for } |z + \rho| \leqslant \rho + \epsilon, \quad n \geqslant 1, \tag{5.10}$$

$$\psi_n \text{ is a polynomial of degree} \leqslant mn, \quad n \geqslant 1. \tag{5.11}$$

Lemma 5.2. *Let K, ρ be given positive constants. Assume φ_n, h_n are such that* (5.5), (5.6), (5.7) *are fulfilled.*

(a) *If* (5.11) *holds for some integer m, then* (5.10) *is fulfilled for some M and $\epsilon > 0$.*

(b) *If* (5.10) *holds for some M and $\epsilon > 0$, then* (5.8) *is fulfilled for some constant L.*

Proof. (a) Assume (5.11) and let $n \geqslant 1$ be given. We expand $\psi_n(z)$ about $z = -\rho$,

$$\psi_n(z) = \sum_{j=0}^{mn} c_j(z+\rho)^j.$$

From the Cauchy integral formula (see e.g. [8, p.2]) one obtains immediately $|c_j| \leqslant k\rho^{-j}$ for all j. Hence, with $\epsilon = \rho$, we have for $|z + \rho| \leqslant \rho + \epsilon$ the inequality

$$| \psi_n(z) | \leqslant \sum_{j=0}^{mn} K2^j \leqslant (K2^{m+1})^n,$$

and (5.10) is satisfied with $M = K2^{m+1}$ and $\epsilon = \rho$.

(b) Assume now, to prove the second part of the lemma, that (5.10) is satisfied and let $n \geqslant 1$. Using the Taylor expansion

$$\psi_n(z) = \sum_{j=0}^{\infty} c_j(z+\rho)^j$$

one obtains from the Cauchy integral formula

$$|c_j| \leqslant M^n(\epsilon+\rho)^{-j} \quad \text{for } j=0, 1, 2, \dots . \tag{5.12}$$

Take an integer $m \geqslant 0$ so large that

$$\left(M\rho^m(\epsilon+\rho)^{-m}\right)^n \leqslant K\epsilon\rho^{-1} \quad \text{for all } n \geqslant 1. \tag{5.13}$$

Then we have for all $z \in D(\rho)$

$$\left|\sum_{j=mn+1}^{\infty} c_j(z+\rho)^j\right| \leqslant \sum_{j=mn+1}^{\infty} M^n\rho^j(\epsilon+\rho)^{-j} \leqslant K.$$

In view of (5.7) this implies that the polynomial

$$p(z) = \sum_{j=0}^{mn} c_j(z+\rho)^j$$

is bounded by $2K$ (for $z \in D(\rho)$). An application of Bernstein's theorem (cf. [8, p. 195]) then gives

$$\left|\frac{\mathrm{d}}{\mathrm{d}z}p(z)\right| \leqslant 2K\rho^{-1}mn \quad \text{for } z \in D(\rho). \tag{5.14}$$

Inequalities (5.12) and (5.13) also give, for $z \in D(\rho)$,

$$\begin{aligned}\left|\frac{\mathrm{d}}{\mathrm{d}z}\psi_n(z) - \frac{\mathrm{d}}{\mathrm{d}z}p(z)\right| &= \left|\sum_{j=mn+1}^{\infty} jc_j(z+\rho)^{j-1}\right| \leqslant M^n \sum_{j=mn+1}^{\infty} j(\epsilon+\rho)^{-j}\rho^{j-1} \\ &= \epsilon^{-2}(\rho+\epsilon(mn+1))\left(M\rho^m(\epsilon+\rho)^{-m}\right)^n \\ &\leqslant K\left(\epsilon^{-1}+(mn+1)\rho^{-1}\right).\end{aligned}$$

Combining this result with (5.14) we arrive at (5.8) with $L = K(\epsilon^{-1} + (3m+1)\rho^{-1})$. □

Remark 5.3. Theorem 5.1 is closely related to the material in [19, p. 3].

Remark 5.4. Theorem 5.1 combined with Lemma 5.2 shows that (5.5), (5.6), (5.7), (5.10) imply an estimate of type (5.9). This fact is closely related to the material in [30, pp. 385, 386].

Remark 5.5. Similarly Theorem 5.1 and Lemma 5.2 show that (5.5), (5.6), (5.7), (5.11) imply (5.9). This is related to a stability estimate in [31, pp. 289, 290].

6. Weak and strong stability with respect to the maximum norm

6.1. Weak stability

From now on we confine our considerations to the maximum norm (cf. the end of Section 3). We study the recurrence relation (3.1) for matrices $A = (\alpha_{ij})$ satisfying

$$A = (\alpha_{ij}) \text{ is a real } s \times s \text{ matrix}, \quad s \geqslant 1, \tag{6.1a}$$

$$|\alpha_{i1}| + \cdots + |\alpha_{i,i-1}| + \alpha_{ii} + |\alpha_{i,i+1}| + \cdots + |\alpha_{i,s}| \leqslant 0, \quad 1 \leqslant i \leqslant s, \tag{6.1b}$$

$$|\alpha_{i1}| + |\alpha_{i2}| + \cdots + |\alpha_{is}| \leqslant \alpha, \quad 1 \leqslant i \leqslant s \tag{6.1c}$$

where α is a given positive constant.

It is easily verified that the matrix A defined by (2.4) satisfies (6.1) with

$$\alpha = \sup_x \{4s^2 a(x) - 2sb(x) - c(x)\}. \tag{6.2}$$

Let φ be as in Section 2 and $D(\rho)$ as in (5.4). Since $\varphi(0) = \varphi'(0) = 1$ there is a positive ρ for which $D(\rho)$ is contained in the stability region S. We define the *stability radius* $r \in (0, \infty]$ by

$$r = \sup\{\rho \mid \rho > 0 \text{ and } D(\rho) \text{ is contained in } S\}.$$

The relevance of r to the stability of (2.1) is obvious from the following theorem.

Theorem 6.1. *Let h, α be given with $0 < h < \infty$, $0 < \alpha < \infty$. Then the following statements* (A.1) *and* (A.2) *are equivalent.*

(A.1) $h \leqslant 2r\alpha^{-1}$,

(A.2) $\varphi(hA)$ *exists and* (3.1) *implies* $|v_n| \leqslant \gamma n^{1/2} |v_0|$ (*for all* s, A *satisfying* (6.1) *and all* $n \geqslant 1$, $v_0 \in \mathbb{R}^s$). *Here γ is a constant independent of s, A, n, v_0.*

The above theorem is an easy consequence of the Theorems 2.1 and 4.1 in [30]. We present a proof of the implication (A.1) ⇒ (A.2) that is a bit simpler than the corresponding proof in [30] and, moreover, provides an expression for γ in (A.2),

$$\gamma = 2 + \tfrac{1}{2}\alpha h \cdot \operatorname{Max}\{|\varphi'(z)|: z \in D(\tfrac{1}{2}\alpha h)\}. \tag{6.3}$$

Proof of (A.2), (6.3). For all matrices T of order s we denote by $\|T\|$ the matrix norm corresponding to the maximum norm in $\mathbb{R}^s$.

Let A, s satisfy (6.1). Applying Theorem 2.1 of [30] it follows that A satisfies the circle condition (5.3) with $\rho = \frac{1}{2}\alpha$.

For h, $\alpha \in (0, \infty)$ satisfying assumption (A.1) we thus have $h\rho \leqslant r$ and therefore $D(h\rho) \subset D(r)$ (where $D(r)$ stands for $\{z \mid \operatorname{Re} z \leqslant 0\}$ if $r = \infty$). In view of $D(r) \subset S$ there follows

$$D(h\rho) \subset S \quad \text{with } \rho = \tfrac{1}{2}\alpha. \tag{6.4}$$

We shall apply Theorem 5.1 with $\|\xi\| = |\xi|$, $\varphi_n = \varphi$, $h_n = h$. Clearly (5.5) holds with $\psi_n(z) = [\varphi(hz)]^n$. Since all $z \in D(\rho)$ satisfy $hz \in D(h\rho)$, we see from (6.4) that (5.6), (5.7), (5.8) hold with

$$K = 1, \qquad L = h \cdot \operatorname{Max}\{|\varphi'(z)|: z \in D(h\rho)\}.$$

Theorem 5.1 thus proves (A.2) with γ as in (6.3). □

The stability result (A.2) has an obvious advantage over the strong stability estimate (3.3) valid under condition (4.1). In (3.3) the factor γ can blow up (as $s \to \infty$), while the γ in (A.2) is independent of the individual s, A satisfying (6.1). The latter γ can even be chosen independently of h, α. For $r < \infty$ this is evident from (6.3), (A.1) while for $r = \infty$ the proof is more difficult (see [2]).

The question arises whether Theorem 6.1 remains valid if the factor $\sqrt{n}$ in (A.2) would be omitted. Unfortunately, the answer to this question is negative. A counterexample is provided by $\varphi(z) = 1 + z - \frac{1}{4}z^3$ (which has a stability radius $r = 1$), $h = 1$, $\alpha = 2$, $A = (\alpha_{ij})$ with $\alpha_{ii} = -1$, $\alpha_{i,i+1} = 1$, $\alpha_{ij} = 0$ ($j < i$ or $j > i + 1$). It can be seen that here the factor $\sqrt{n}$ cannot be omitted, by expanding $\{\varphi(hA)\}^n$ in a Taylor series (similarly as in the subsequent proof of Theorem 6.2) and by applying Theorem 3 of [31] to the function $f(t) = \varphi(-1 + \exp[\mathrm{i}t])$.

6.2. Strong stability

In the counterexample at the end of Section 6.1 we have $h = 1 = 2r\alpha^{-1}$ so that equality holds in (A.1). The subsequent theorem shows that in case of strict inequality in (A.1) there is strong stability with a suitable factor γ.

Theorem 6.2. *Let h, α be given with $0 < h < \infty$, $0 < \alpha < \infty$, $h < 2r\alpha^{-1}$. Then* (3.1) *implies $|v_n| \leqslant \gamma |v_0|$ (for all s, A satisfying* (6.1) *and all $n \geqslant 1$, $v_0 \in \mathbb{R}^s$). Here $\gamma = \Gamma(h\alpha)$ with a function $\Gamma(t)$ satisfying $\Gamma(t) \leqslant \Gamma(t') < \infty$ (for $0 < t \leqslant t' < 2r$).*

Proof. (1) Let h, α be as in the theorem and let A, s satisfy (6.1). Using the same notations and arguments as in the proof in Section 6.1 we arrive again at the circle condition (5.3) and at (6.4).

Defining the Taylor coefficients c_{nj} by

$$\{\varphi(h\rho(-1+z))\}^n = c_{n0} + c_{n1}z + c_{n2}z^2 + \cdots \quad \text{for } |z| \leqslant 1,$$

we have

$$\begin{aligned}\{\varphi(hA)\}^n &= \{\varphi(h\rho[-1 + (1 + \rho^{-1}A)])\}^n \\ &= c_{n0} + c_{n1}(1 + \rho^{-1}A) + c_{n2}(1 + \rho^{-1}A)^2 + \cdots\end{aligned}$$

(cf. [7]). Consequently,

$$\|\{\varphi(hA)\}^n\| \leqslant |c_{n0}| + |c_{n1}| + |c_{n2}| + \cdots, \quad n \geqslant 1. \tag{6.5}$$

Introducing $f(t) = \varphi(h\rho(-1 + \exp[\mathrm{i}t]))$ we have the expressions

$$c_{nj} = \frac{1}{2\pi}\int_{-\pi}^{\pi} \{f(t)\}^n \,\mathrm{e}^{-\mathrm{i}jt}\,\mathrm{d}t, \qquad n \geqslant 1, \quad j \geqslant 0. \tag{6.6}$$

(2) In order to bound the right-hand member in (6.5) we look somewhat closer at the function f.

Writing $\lambda = \varphi''(0)$ we have, for any $R > 0$, the relation

$$\varphi(R(-1 + \exp[\mathrm{i}t])) = \exp\{\mathrm{i}Rt - \tfrac{1}{2}R(-R + 1 + \lambda R)t^2 + \mathcal{O}(t^3)\} \quad \text{for } t \to 0.$$

If $r < \infty$, we have $|\varphi(z)| \leqslant 1$ (for $z \in D(r)$) and, by choosing $R = r$, there follows $(-r + 1 + \lambda r) \geqslant 0$ so that $\lambda \geqslant 1 - 1/r$. If $r = \infty$, we arrive in a similar way at $\lambda \geqslant 1$.

Applying the above relation once more, but now with $R = h\rho$, we see that

$$f(t) = \exp\{ih\rho t - \beta t^2 + \mathcal{O}(t^3)\} \quad \text{for } t \to 0$$

with $\beta = \frac{1}{2}h\rho(1 + (\lambda - 1)h\rho)$. The above lower bounds for λ imply $\beta > 0$. Since also $|f(t)| < 1$ (for $0 < |t| \leqslant \pi$) we can apply a stability result that is well known in the numerical solution of partial differential equations (see e.g. the corollary in [31, p. 278]). It follows that there is a constant γ such that the c_{nj}, given by (6.6), satisfy $|c_{n0}| + |c_{n1}| + |c_{n2}| + \cdots \leqslant \gamma$ (for al $n \geqslant 1$). We define $\Gamma(h\alpha)$ to be the smallest γ for which the inequality $\|\{\varphi(hA)\}^n\| \leqslant \gamma$ (for all $n \geqslant 1$ and s, A satisfying (6.1)) is valid. □

We illustrate the above theorem by problem (2.2), (4.2). Consider, as in Section 4, the matrix (2.4) with $s = 20$. From (6.2) we obtain $\alpha = 41\,600$. Choosing φ as in (2.5) with $\theta = 0.25$ we see from (4.3) that the stability radius equals $r = 2$. Since $(9 \times 10^{-5}) \times 41\,600 < 4$, the stepsize restriction of Theorem 6.2 is fulfilled with $h = 9 \times 10^{-5}$. For this stepsize the theorem thus guarantees strong stability with factor $\gamma = \Gamma(t)$, $t = h\alpha \simeq 3.7 < 4$. A straightforward numerical computation reveals that, in this example, there is strong stability with $\gamma \simeq 2.3$, which is well in agreement with the theorem.

A further interesting example is provided by (2.5) with $\theta = 0.5$. In this case $r = \infty$, so that, by Theorem 6.2, there is *strong* stability with factor $\gamma = \Gamma(\alpha h)$ for *any* $\alpha > 0$, $h > 0$. This result seems not to follow easily from the related material in [2], [19] or [30].

7. Time dependent problems

7.1. Weak stability

We consider the generalized version of (2.1),

$$u_n = \varphi(hA_n)u_{n-1} + p_n, \quad n = 1, 2, 3, \ldots . \tag{7.1}$$

Here A_n are $s \times s$ matrices of type (6.1). Processes of the form (7.1) occur in the numerical solution of linear differential equations with coefficients depending on (the time) t. For instance, if the functions a, b, c in (2.2) would also depend on t, we would arrive at a process (7.1).

The question arises whether the stability radius r is also relevant to the stability of (7.1) Analogously to (3.1) we consider

$$v_n = \varphi(hA_n)v_{n-1}, \quad n = 1, 2, 3, \ldots . \tag{7.2}$$

In order to answer the above question we define the quantity $R \in [0, \infty]$ by

$$R = \sup\{\rho \mid \rho = 0, \text{ or } 0 < \rho < \infty \text{ and } \varphi \text{ absolutely monotonic on } [-\rho, 0]\}$$

(a function is called absolutely monotonic on an interval if the values of the function and all its derivatives are finite and $\geqslant 0$ on that interval).

Theorem 7.1. *Let h, α be given with $0 < h < \infty$, $0 < \alpha < \infty$. Then the following statements* (B.1) *and* (B.2) *are equivalent.*

(B.1) $h \leqslant 2R\alpha^{-1}$,

(B.2) *$\varphi(hA_n)$ exists and* (7.2) *implies $|v_n| \leqslant \gamma n^q |v_0|$ (for all s, A_n satisfying* (6.1) *and all $n \geqslant 1$, $v_0 \in \mathbb{R}^s$). Here γ, q are constants independent of s, A_n, n, v_0.*

Proof. First of all, we relate requirement (6.1) to the circle notation (5.3) as in the proof in Section 6.1.

Next, (B.1) can be seen to imply (B.2) with $\gamma = 1$, $q = 0$ by applying [27, section 3] or [30, theorem 5.1]. Cf. also [28].

Finally, (B.1) can be proved from (B.2) by applying the material in [29, pp. 660, 661]. □

This theorem shows that already weak stability with arbitrary exponent q implies the stepsize restriction $h \leqslant 2R\alpha^{-1}$. The above question can now be settled by comparing R with r.

The definition of R implies that, for any $\rho \in (0, R)$, the Taylor coefficients $c_k = (k!)^{-1}\varphi^{(k)}(-\rho)$ satisfy $c_k \geqslant 0$ and

$$c_0 + c_1\rho + c_2\rho^2 + \cdots = \varphi(0) = 1.$$

Consequently, the disk $D(\rho)$ (cf. (5.4)) is contained in the stability region S. It follows that $R \leqslant r$. Hence restriction (B.1) is at least as strong as (A.1) in Theorem 6.1. In many cases $R < r$ so that (B.1) is stronger than (A.1) (cf. the next section).

7.2. *Contractivity*

We turn to a relation generalizing the recurrence relations (3.1), (5.2), (7.2),

$$v_n = \varphi_n(h_n A_n) v_{n-1}, \quad n = 1, 2, 3, \ldots . \tag{7.3}$$

Here A_n are matrices satisfying (6.1) while h_n, φ_n are as in Section 5.

To each function φ_n there corresponds a quantity R as defined in section 7.1. In view of the dependence on n it will be denoted by R_n.

The following theorem has a structure similar to the Theorems 6.1, 7.1. It has a wider scope than the latter theorems in that the general relation (7.3) is treated. On the other hand, the stepsize restriction of the theorem only follows from a contractivity property (which is stronger than a stability property of the type occurring in Theorem 6.1 or 7.1).

Theorem 7.2. *Let h_n, α be given with $0 < h_n < \infty$, $0 < \alpha < \infty$. Then the following statements* (C.1) *and* (C.2) *are equivalent.*

(C.1) $h_n \leqslant 2R_n\alpha^{-1}$ (*for* $n = 1, 2, 3, \ldots$),

(C.2) $\varphi_n(h_n A_n)$ *exists and* (7.3) *implies* $|v_n| \leqslant |v_0|$ (*for all* s, A_n *satisfying* (6.1) *and all* $n \geqslant 1$, $v_0 \in \mathbb{R}^s$).

Proof. Requirement (6.1) is related to (5.3) as in the proofs given above.

(C.1) implies (C.2) by [27; section 3] or [30; theorem 5.1].

Assume (C.2). In order to prove (C.1) we choose $A_1 = A_2 = \cdots = A_{n-1} = 0$. It follows that $\varphi_n(h_n A_n)$ exists and

$$|\varphi_n(h_n A_n) v_0| = |\varphi_n(h_n A_n) \cdots \varphi_2(h_2 A_2)\varphi_1(h_1 A_1) v_0| = |v_n| \leqslant |v_0|.$$

Consequently $\|\varphi_n(h_n A_n)\| \leqslant 1$ for all matrices A_n of order $s \geqslant 1$ with $\|A_n + \rho\| \leqslant \rho = \frac{1}{2}\alpha$. It follows that $h_n\alpha \leqslant 2R_n$ (cf. [27, section 3] or [30, theorem 5.1]). □

In view of the contractivity property (C.2) the quantity R_n is called the *contractivity radius* of φ_n.

We conclude this section with a numerical illustration. Consider again problem (2.2), (4.2) and the process (2.1) with matrix (2.4), $s = 20$, $\alpha = 41\,600$. For the rational function (2.5) with $\theta = 0.25$ the contractivity radius equals $R = \frac{4}{3}$. Since $(6 \times 10^{-5}) \times 41\,600 \leqslant \frac{8}{3}$, the stepsize restriction of Theorem 7.2 is fulfilled with $h = 6 \times 10^{-5}$. For this stepsize the theorem thus guarantees strong stability with factor $\gamma = 1$. A straightforward numerical computation shows that, with this stepsize, the smallest γ equals $\gamma \simeq 1$, indeed.

For a numerical illustration of the relevance of the contractivity radius R in hyperbolic problems we refer to [15,23].

8. Properties of the stability and contractivity radius

8.1. On the stability radius of explicit methods

In the following we review some results on the stability radius r (as defined in section 6.1) for functions φ of the type described in Section 2. Whereas section 8.2 deals with proper rational functions, we assume here that φ is a polynomial of (exact) degree m.

In [12] Jeltsch and Nevanlinna proved

$$r \leqslant m. \tag{8.1}$$

Further they showed that the maximum value $r = m$ is only attained by the polynomial $\varphi(z) = (1 + z/m)^m$, corresponding to (a cyclic application of) Euler's method (cf. e.g. [5]). For the proof of these results they made use of the theory of positive real functions. In [13] an alternative proof (of a more general result) was given by these authors which basically relies on maximum principles and order star techniques (cf. [33]). For a proof only based on order star techniques we refer to [32]. As was noted in [13], still another proof of the above results is easily obtained from Bernstein's inequality (cf. [8, p. 195]). We finally mention that it is also possible to give the proof by exploiting the well-known Courant–Friedrichs–Lewy condition for discretizations of hyperbolic partial differential equations, see [24].

We turn our attention to the recurrence relation (2.1) with $p_n = 0$. In order to compare different methods with each other, we should take into account the computational effort per step. In our case the computation of u_n from u_{n-1} requires m matrix-vector multiplications. Hence we should compare scaled stepsizes h/m and therefore also (cf. Theorems 6.1, 6.2) *scaled stability radii* $\tilde{r} = r/m$ (see also [13, p. 72]). It follows immediately from the results above that the maximum value for $\tilde{r}$ is equal to 1, and that this value is only attained by $\varphi(z) = (1 + z/m)^m$.

In order to have a high order of accuracy for the process (2.1) approximating the exact solution $U(t)$ of the ordinary differential equation in Section 2, it is necessary (cf. e.g. [5]) that

$$\varphi(z) = \exp(z) + \mathcal{O}(z^{p+1}) \quad \text{for } z \to 0 \tag{8.2}$$

for a large integer p. Note that it follows from our assumptions on φ in Section 2 that $p \geqslant 1$. For $p = 1$ we have seen that the scaled stability radius $\tilde{r}$ can attain the maximum value 1. For $p > 1$ no general analogous result seems to be available. However, for the Taylor polynomials

$$T_m(z) = 1 + z + z^2/2! + \cdots + z^m/(m!), \tag{8.3}$$

satisfying (8.2) with $p = m$, it was proved in [14] that the scaled stability radius $\tilde{r}_m$ tends to $(2\mathrm{e})^{-1}$ (for $m \to \infty$).

8.2. *On the stability radius of implicit methods*

In this section we assume that φ is as in Section 2 with degree of the numerator $P(z)$ equal to m and degree of the denominator $Q(z)$ equal to n. Whereas the stability radius r of polynomials is necessarily bounded by m (cf. (8.1)), it is possible for rational functions that $r = \infty$. In the latter case we call φ *A-acceptable* (cf. e.g. [5]). Even the so-called Padé approximations $\varphi(z) = \Phi_{m/n}(z)$, satisfying the order condition (8.2) with highest possible order $p = m + n$ (cf. [5]), are A-acceptable for many pairs (m, n). In fact, the Padé approximation $\Phi_{m/n}$ is A-acceptable if and only if $n - 2 \leqslant m \leqslant n$ (cf. [33]).

Contrary to the polynomial case it is for rational functions not obvious how to scale the stability radius. The computational effort per integration step essentially depends on the way one transforms the recurrence relation (2.1) into an algorithm. Here the presence of multiple and/or real poles in the function φ, or the special structure of the matrix A (such as bandstructure, symmetry, dimension) may play a significant role.

We finally mention that the function φ defined by (2.5) has a stability radius

$$r = \begin{cases} (1-2\theta)^{-1} & \text{if } 0 \leqslant \theta < \frac{1}{2}, \\ \infty & \text{if } \frac{1}{2} \leqslant \theta \leqslant 1. \end{cases}$$

8.3. *On the contractivity radius of explicit methods*

In this section we turn again to the case where φ is a polynomial of degree m satisfying the assumptions made in Section 2. In Section 7 the contractivity radius R has been defined and shown to satisfy the bound

$$R \leqslant r. \tag{8.4}$$

Together with (8.1) this leads to the bound $R \leqslant m$. A sharper bound was given in [15] where it was shown that (8.2) implies

$$R \leqslant m - p + 1. \tag{8.5}$$

Moreover it was proved in [15] that equality in (8.5) is possible if and only if $p \leqslant 2$ or $p \geqslant m - 1$.

Using arguments similar to those in section 8.1 it is better, for the purpose of comparison, to consider the *scaled contractivity radius* $\tilde{R} = R/m$. In view of (8.5) we have $\tilde{R} \leqslant 1$. Further, it easily follows from section 8.1 and (8.4) that equality holds only for the polynomial $\varphi(z) = (1 + z/m)^m$. This explains the negative results in [23], where it was attempted to break the barrier $\tilde{R} \leqslant 1$.

In [15] maximum values for $\tilde{R}$ and the corresponding polynomials were tabulated for $1 \leqslant p \leqslant m \leqslant 10$. For the Taylor polynomials (cf. (8.3)) it was proved that the saled contractivity radius $\tilde{R}_m$ equals $1/m$. Hence $\tilde{R}_m$ tends to zero (for $m \to \infty$), which is less favourable than the situation for the scaled stability radius $\tilde{r}_m$ (cf. section 8.1).

8.4. *On the contractivity radius of implicit methods*

Let the rational function φ be as in section 8.2. As in the polynomial case, the contractivity radius R satisfies the bound (8.4). Another bound for R, only depending on the poles of φ, can be found in [9]. Here the bound was obtained by using the decomposition of φ into partial fractions. From this bound it follows that for proper rational functions we have

$$\text{if } \varphi \text{ has no positive real poles then } R = 0. \tag{8.6}$$

On the other hand $R = \infty$ is also possible, as can be seen from the example given at the end of this section. Unfortunately, functions φ with $R = \infty$ are subject to an *order barrier* $p \leqslant 1$ (cf. (8.2)), which is an immediate consequence of a lemma due to Bolley and Crouzeix [1] (cf. also [27]). Results on optimization of R for given $p \geqslant 2$ and m, n with $m + n \geqslant p$ can be found in [27,9]. In [9] an algorithm was presented for the (numerical) computation of R for a given rational function φ. This algorithm was applied to the Padé approximations $\Phi_{m,n}$ for $0 \leqslant m,\ n \leqslant 11$. It was also proved in [9] that $R = 0$ for the Padé approximations $\Phi_{m/n}$ with $n = 2, 4, 6, \ldots$ by noting that these functions have no positive real poles (cf. (8.6)). This result rather contrasts with the situation for the stability radius r, as described in section 8.2.

For scaling of the contractivity radius we refer to the remark made in section 8.2 concerning scaling of the stability radius.

We conclude this section with the value R for the function φ defined by (2.5),

$$R = \begin{cases} (1-\theta)^{-1} & \text{if } 0 \leqslant \theta < 1, \\ \infty & \text{if } \theta = 1. \end{cases}$$

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