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Resolvent conditions and bounds on the powers of matrices, with relevance to numerical stability of initial value problems

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Abstract

We deal with the problem of establishing upper bounds for the norm of the *n*th power of square matrices. This problem is of central importance in the stability analysis of numerical methods for solving (linear) initial value problems for ordinary, partial or delay differential equations. A review is presented of upper bounds which were obtained in the literature under the resolvent condition occurring in the Kreiss matrix theorem, as well as under variants of that condition. Moreover, we prove new bounds, under resolvent conditions which generalize some of the reviewed ones. The paper concludes by applying one of the new upper bounds in a stability analysis of the trapezoidal rule for delay differential equations.

Keywords: Resolvent conditions; Stability analysis; Error growth; Numerical method; Discretization; Initial value problem; Delay differential equation; Trapezoidal rule

1. Introduction

1.1. The purpose of the paper

This paper is concerned with the analysis of numerical methods for the solution of (linear) initial value problems. Most methods in current use are applied in a step-by-step fashion so as to obtain numerical approximations corresponding to consecutive discrete values t_n of the time variable t. A crucial question about these methods is whether they behave *stably* or not. Here we use the term stable to designate the situation where any (numerical) errors, introduced at some stage of the calculations, are propagated mildly — i.e., do not blow up unduly in the subsequent applications of the numerical method.

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Fourier transformations, and the corresponding famous Von Neumann condition for stability, are classical tools for assessing a priori the stability of methods for solving (partial) differential equations. However, in many practical cases these tools fail to be relevant for analysing stability: e.g., for pseudo-spectral methods applied to initial-boundary value problems, and for finite volume or finite element methods based on unstructured grids.

Recently, progress was made in analysing stability without using Fourier transformation techniques. Conditions for stability were studied which are related to the so-called *resolvent condition of Kreiss*. These conditions apply in some cases where Fourier techniques fail. Moreover, due to the framework in which the conditions are formulated, applications are possible in the solution of ordinary and partial differential equations as well as of delay differential equations. The purpose of the present paper is threefold: we shall review various (recent) results related to the Kreiss resolvent condition; furthermore, we shall present a substantial generalization of some of the reviewed material; finally, we apply our generalization in deriving a new stability estimate in the numerical solution of delay differential equations.

1.2. Organization of the paper

Section 2 is still introductory in nature. In Section 2.1 we relate the stability analysis of numerical processes specified by square matrices B to the problem of deriving upper bounds on the norm $\|B^n\|$ (for $n=1,2,3,\ldots$). Further, in Section 2.2 we recall that the eigenvalues of B can be an unreliable guide to stability.

Section 3 gives a review of various upper bounds for $\|B^n\|$ obtained in the literature. In Section 3.1 we review two bounds for $\|B^n\|$ which are valid under the resolvent condition of Kreiss. The sharpness of these bounds is discussed in Section 3.2. In Section 3.3 we review some stronger versions as well as weaker versions of the Kreiss condition and corresponding bounds for $\|B^n\|$.

Section 4 deals with a quite general resolvent condition, which generalizes some of the conditions reviewed in Section 3. In Section 4.1 we formulate this resolvent condition, and we give a lemma on the arc length of the image, under a rational function, of a subarc of a circle in the complex plane. In Section 4.2 we prove Theorem 4.2 making use of this lemma. Theorem 4.2 gives upper bounds for $\|B^n\|$ under the general resolvent condition. Most of these bounds are new. Section 4.3 shortly discusses how the estimates for $\|B^n\|$, given in Theorem 4.2, depend on certain parameters. Moreover, a short discussion is given of the sharpness of these estimates.

In Section 5 we use one of the new estimates of $\|B^n\|$, given by Theorem 4.2, in a stability analysis of the trapezoidal rule applied to delay differential equations.

2. Stability analysis of linear numerical processes

2.1. Relating stability to bounds on $\|B^n\|$

We deal with an abstract numerical process of the form

$$u_n = Bu_{n-1} + b_n \quad (n=1,2,3,\ldots). \tag{2.1}$$

Here b_n denote given vectors in the s-dimensional complex space $\mathbb{C}^s$, and B denotes a given complex $s \times s$ matrix. Further, the vectors $u_n \in \mathbb{C}^s$ (for $n \geqslant 1$) are computed by applying (2.1), starting from a given $u_0 \in \mathbb{C}^s$.

Recurrence relations of the form (2.1) arise in the numerical solution of initial value problems for linear (ordinary, partial or delay) differential equations. The vectors u_n then provide numerical approximations to the solution of the problem under consideration. For instance, finite difference schemes for solving initial-boundary value problems in linear partial differential equations can be written in the form (2.1), as soon as the time step is constant and the space steps as well as the coefficients in the differential equation only depend on the space variables. In this situation, the dimension s is related to the space steps, and will tend to infinity if the steps approach zero. For actual numerical processes, written in the form (2.1), see e.g. [5] and the Sections 2.2, 5.1 of the present paper.

Suppose the numerical computations based on (2.1) were performed using a slightly perturbed starting vector $\tilde{u}_0$ instead of u_0. For $n \geqslant 1$, we then would obtain approximations $\tilde{u}_n$, instead of u_n, satisfying the recurrence relation $\tilde{u}_n = B\tilde{u}_{n-1} + b_n$ $(n = 1, 2, 3, \ldots)$. In the stability analysis of (2.1) the crucial question is whether, for $n \geqslant 1$, the *propagated errors* $v_n = \tilde{u}_n - u_n$ can be bounded suitably in terms of the *initial error* $v_0 = \tilde{u}_0 - u_0$. One may thus be looking for bounds of the form

$$|v_n| \leqslant M \cdot |v_0| \quad (n \geqslant 1). \tag{2.2}$$

Here M denotes a constant of moderate size. Further, $|\cdot|$ stands for a norm on $\mathbb{C}^s$ which is considered suitable for measuring error vectors; e.g. the familiar l_p-norm for vectors $x \in \mathbb{C}^s$, with components ξ_i, defined by

$$|x|_p = \left(\sum_{i=1}^{s} |\xi_i|^p \right)^{1/p} \quad (\text{if } 1 \leqslant p < \infty), \qquad |x|_p = \max_{1 \leqslant i \leqslant s} |\xi_i| \quad (\text{if } p = \infty).$$

By subtracting the recurrence relations satisfied by $\tilde{u}_n$ and by u_n from each other, we find $v_n = Bv_{n-1} = B^n v_0$. By defining, for $s \times s$ matrices A,

$$\|A\| = \max\{|Ax|/|x|: 0 \neq x \in \mathbb{C}^s\}, \tag{2.3}$$

we thus see that the stability analysis of process (2.1) amounts to deriving bounds on $\|B^n\|$. The following bound (2.4) would match (2.2):

$$\|B^n\| \leqslant M \quad (n \geqslant 1). \tag{2.4}$$

In this paper we shall deal with the general problem of deriving suitable upper bounds on $\|B^n\|$.

2.2. Eigenvalue conditions

In this subsection we review some simple conditions for (2.4) formulated in terms of the *eigenvalues* λ of the matrix B. We denote the *spectral radius* of B by

$$r(B) = \max\{|\lambda|: \lambda \text{ is an eigenvalue of } B\}.$$

It follows from the Jordan canonical form of B (see, e.g., [8]) that an M with property (2.4) exists if and only if

$$\begin{aligned} &r(B) \leqslant 1, \text{ and any Jordan block corresponding to an} \\ &\quad \text{eigenvalue } \lambda \text{ of } B, \text{ with } |\lambda| = 1, \text{ has order } 1. \end{aligned} \tag{2.5}$$

However, it was noticed already long ago (see, e.g., [16]) that the eigenvalue condition (2.5) can be a very misleading guide to stability. The fact is, that under condition (2.5) the smallest M satisfying (2.4) can be prohibitively large. This phenomenon occurs in practice, even under the subsequent condition (2.6), which is stronger than (2.5).

$$r(B) < 1. \tag{2.6}$$

An instructive example, illustrating that (2.5), (2.6) are unreliable, is provided by the $s \times s$ bidiagonal matrix

$$B = \begin{pmatrix} \lambda_1 & & & \\ 2 & \lambda_2 & & \\ & \ddots & \ddots & \\ & & 2 & \lambda_s \end{pmatrix}. \tag{2.7}$$

We consider the situation where s is large and all $|\lambda_i| < 1$, so that (2.6) holds.

For any $s \times s$ matrix A and $1 \leqslant p \leqslant \infty$, we use the notation

$$\|A\|_p = \max\{|Ax|_p/|x|_p\colon 0 \neq x \in \mathbb{C}^s\}. \tag{2.8}$$

It is easy to see that, for $1 \leqslant p \leqslant \infty$, the matrix B defined by (2.7) satisfies

$$\|B^n\|_p \geqslant 2^n \quad (n = 1, 2, \ldots, s-1). \tag{2.9}$$

For moderately large values of s, say $s \approx 100$, we have $\|B^{s-1}\|_p \gtrsim 10^{30}$, so that actually instability manifests itself although (2.6) is fulfilled.

We note that matrices of the form (2.7) exist which may be thought of as arising in the numerical solution of initial-boundary value problems, e.g.,

$$u_t(x,t) + u_x(x,t) = u(x,t), \quad u(0,t) = 0, \quad u(x,0) = f(x),$$

where $0 \leqslant x \leqslant 1$, $t \geqslant 0$ and f is a given function. Consider the difference scheme

$$\frac{1}{\Delta t}(u_{m,n} - u_{m,n-1}) + \frac{1}{\Delta x}(u_{m,n-1} - u_{m-1,n-1}) = u_{m,n-1},$$

where $\Delta t > 0$, $\Delta x = 1/s < 1$, $m = 1, 2, \ldots, s$ and $n = 1, 2, 3, \ldots$. We define $u_{0,n-1} = 0$ and $u_{m,0} = f(m\Delta x)$, so that $u_{m,n}$ approximates $u(m\Delta x, n\Delta t)$. Clearly, when $\Delta t/\Delta x = 2$, the vectors u_n with components $u_{m,n}$ $(1 \leqslant m \leqslant s)$ satisfy $u_n = Bu_{n-1}$ where B is of the form (2.7) with $\lambda_i = -1 + \Delta t \in (-1, 1)$. Further, since $\Delta x = 1/s$ it is natural to focus on large values of s.

The above example (2.7) shows that under the general conditions (2.5), (2.6) the size of M in (2.4) is not under control and errors can grow exponentially — see (2.9). In the rest of this paper we focus on reliable conditions on arbitrary $s \times s$ matrices B under which such disastrous error growth cannot take place.

3. Stability estimates and resolvent conditions from the literature

3.1. The resolvent condition of Kreiss

Throughout this Subsection 3.1 we assume, unless stated otherwise, that $\|\cdot\|$ is a matrix norm induced by an arbitrary vector norm in $\mathbb{C}^s$, according to (2.3).

We shall relate property (2.4) (with moderate M) to the condition that

$$r(B) \leqslant 1 \quad \text{and} \quad \|(\zeta I - B)^{-1}\| \leqslant \frac{L}{|\zeta| - 1} \quad \text{for all } \zeta \in \mathbb{C} \text{ with } |\zeta| > 1. \tag{3.1}$$

Here I denotes the $s \times s$ identity matrix, and L is a real constant. One usually calls $(\zeta I - B)^{-1}$ the *resolvent* of B at ζ, and we shall refer to (3.1) as the *Kreiss resolvent condition*. We use the latter terminology because (3.1) was used, with $\|\cdot\| = \|\cdot\|_2$, by Kreiss [10] in formulating what nowadays is called the Kreiss matrix theorem. In many cases of practical interest it is easier to verify (3.1) than (2.4).

If (2.4) holds, then $r(B) \leqslant 1$. Moreover, a power series expansion of the resolvent, for $|\zeta| > 1$, then yields

$$\|(\zeta I - B)^{-1}\| = |\zeta|^{-1} \left\| \sum_{n=0}^{\infty} (\zeta^{-1} B)^n \right\| \leqslant |\zeta|^{-1} (1 - |\zeta^{-1}|)^{-1} \max\{1, M\}.$$

It follows that (2.4) implies (3.1), with $L = \max\{1, M\}$. For the case where $\|\cdot\| = \|\cdot\|_2$, Kreiss [10] succeeded in proving that conversely (3.1) implies (2.4) with $M = M_{L,s}$ only depending on L and s.

In the following we shall be interested in the case where s is large. Therefore, it is important to understand how $M_{L,s}$ depends on s. The original proof of Kreiss does not provide a sharp value for $M_{L,s}$, and many subsequent authors studied the size of this quantity; see [31] for a historical survey. Eventually, for arbitrary matrix norms (2.3), the following theorem was obtained — for its proof see, e.g., [5, pp. 208, 209].

Theorem 3.1. *For any real constant L and any $s \times s$ matrix B satisfying* (3.1), *we have*

$$\|B^n\| \leqslant \mathrm{e} L s \quad (n \geqslant 1,\ s \geqslant 1), \tag{3.2a}$$

$$\|B^n\| \leqslant \mathrm{e} L (n+1) \quad (n \geqslant 1,\ s \geqslant 1). \tag{3.2b}$$

According to this theorem, under the Kreiss resolvent condition, the size of $\|B^n\|$ is rather well under control. Exponential error growth cannot occur — at the worst there may be weak instability in that the propagated errors increase linearly with n or s.

For applications of the above theorem (and its predecessors), one may consult [5,7,10,15,17,18,23, 25]; for diverse theoretical issues related to the theorem, we refer to [5,13,14,26,29].

3.2. The sharpness of the stability estimates (3.2)

In this subsection we discuss the sharpness of the estimates (3.2) for the interesting case where $\|\cdot\| = \|\cdot\|_\infty$. We focus on this norm because of the following three reasons: there exist rather complete results about the sharpness of (3.2) for the norm $\|\cdot\|_\infty$; moreover, important practical situations exist where $\|(\zeta I - B)^{-1}\|_\infty$ can rather easily be estimated; finally, error estimates in terms of the l_∞-norm allow of a useful and easy interpretation. For sharpness results pertinent to other norms, we refer to [5,12,24].

It is known that $s \times s$ matrices B_s exist, satisfying (3.1) with $\|\cdot\| = \|\cdot\|_\infty$ and with some finite $L = L_s$ (for $s = 1, 2, 3, \ldots$), such that the quotient $\|(B_s)^{s-1}\|_\infty/(sL_s)$ tends to e when $s \to \infty$ (see [5, Corollary 2.3]). It follows that the estimates given in Theorem 3.1 are sharp in that the constant e, occurring in the right-hand members of (3.2a) and (3.2b), cannot be replaced by any smaller constant.

Unfortunately, the values L_s, in the above counterexample, tend to ∞ when $s \to \infty$. Therefore, the nice sharpness result just mentioned is related to the fact that the estimates in Theorem 3.1 are required to follow from (3.1) simultaneously for *all possible values* of L. The above counterexample fails to be relevant to the important question in how far the stability estimates (3.2a) and (3.2b) are also best possible, when L is an arbitrary but *fixed* constant. In fact, for $\|\cdot\| = \|\cdot\|_\infty$ and $L = 1$, these estimates can substantially be improved: in this situation the resolvent condition (3.1) is known to imply $\|B^n\|_\infty \leqslant 1$ $(n \geqslant 1,\ s \geqslant 1)$ — see, e.g., [5, Theorem 2.6].

The important problem arises as to whether the upper bounds (3.2a) and (3.2b) can be improved, for all fixed values L, to bounds on $\|B^n\|_\infty$ which do not grow, or which grow (much) slower than linearly with s or n.

This problem was solved by Kraaijevanger [9]. He succeeded in constructing $s \times s$ matrices B_s satisfying (3.1), with $\|\cdot\| = \|\cdot\|_\infty$ and $L = \pi + 1$, such that

$$\|(B_s)^n\|_\infty = 2s - 1 = 2n - 1 \quad \text{(whenever } n = s \geqslant 1\text{).} \tag{3.3}$$

In view of (3.3), we conclude that the upper bounds (3.2a) and (3.2b) cannot be improved, for all fixed values L, into bounds which grow slower than linearly with s or n.

3.3. Variants to the Kreiss resolvent condition

Throughout this subsection we assume again, unless specified otherwise, that $\|\cdot\|$ is a matrix norm induced by an arbitrary vector norm in $\mathbb{C}^s$, according to (2.3). We shall deal with two *stronger* versions of condition (3.1) as well as two *weaker* versions.

In view of the conclusion at the end of Section 3.2, the question poses itself of whether bounds on $\|B^n\|$ which grow slower than linearly with s or n can still be established under conditions that are slightly *stronger* than (3.1) (and fulfilled in cases of practical interest). Below we review shortly two conclusions, obtained in the literature, pertinent to this question. For additional results, see [3,13,22].

Consider for arbitrary $s \times s$ matrices B the condition that

$$r(B) \leqslant 1 \quad \text{and} \quad \|(\zeta I - B)^{-m}\| \leqslant \frac{L}{(|\zeta| - 1)^m} \quad \text{for } |\zeta| > 1 \quad \text{and} \quad m = 1, 2, 3, \ldots. \tag{3.4a}$$

Clearly, this so-called *Hille-Yosida* or *iterated resolvent condition* implies (3.1). Unlike (3.1), condition (3.4a) implies the stability estimate

$$\|B^n\| \leqslant Ln!(\mathrm{e}/n)^n \leqslant \mathrm{e}L\sqrt{n} \quad (n \geqslant 1,\ s \geqslant 1). \tag{3.4b}$$

This estimate was obtained by various authors. It follows for instance easily from the material in [2, p. 41] in combination with [11], or directly from [13].

A still better stability estimate can be established under the following condition (3.5a), which was introduced in [28].

$$r(B) \leqslant 1 \quad \text{and} \quad \|(\zeta I - B)^{-1}\| \leqslant \frac{L}{|\zeta - 1|} \quad \text{for } |\zeta| > 1. \tag{3.5a}$$

Since $|\zeta - 1|^{-1} \leqslant (|\zeta| - 1)^{-1}$, also this condition implies (3.1). Moreover, as was shown in [3], condition (3.5a) implies the inequality

$$\|B^n\| \leqslant \mathrm{e}L^2/2 \quad (n \geqslant 1,\ s \geqslant 1), \tag{3.5b}$$

the right-hand member of which does not grow with n or s. We refer to the paper just mentioned for an application of (3.5b) in proving numerical stability for a class of Runge–Kutta methods in the numerical solution of initial-boundary value problems for parabolic partial differential equations.

Clearly, in order to apply the general stability estimates (3.2), (3.4b) or (3.5b) in any practical situation, one has to check whether the corresponding resolvent conditions are actually fulfilled. Sometimes this may be difficult, and there are cases where one cannot even prove (3.1) (see, e.g., Section 5.2). Therefore, it is an important issue of whether estimates similar to (3.2a) and (3.2b) still hold under resolvent conditions which are *weaker* than (3.1). Below we mention two results pertinent to this issue.

Consider, for arbitrary $s \times s$ matrices B and a given constant $\delta > 0$, the condition that

$$r(B) \leqslant 1 \quad \text{and} \quad \|(\zeta I - B)^{-1}\| \leqslant L \frac{|\zeta|^{\delta \cdot s}}{|\zeta| - 1} \quad \text{for } |\zeta| > 1. \tag{3.6a}$$

This weaker version of (3.1) is known to imply that

$$\|B^n\| \leqslant \mathrm{e}L[\delta s + \min\{s, n+1\}] \quad (n \geqslant 1,\ s \geqslant 1); \tag{3.6b}$$

see [21] for a proof and an application of (3.6b). We conclude that under condition (3.6a), similarly as under the stronger condition (3.1), the norm $\|B^n\|$ cannot grow faster than linearly with s.

A further weaker version of (3.1), considered in the literature, requires that, for a given fixed value $\alpha > 0$, the $s \times s$ matrix B satisfies

$$r(B) \leqslant 1 \quad \text{and} \quad \|(\zeta I - B)^{-1}\| \leqslant L \frac{|\zeta|^{\alpha}}{(|\zeta| - 1)^{1+\alpha}} \quad \text{for } |\zeta| > 1 \tag{3.7a}$$

(cf. [6,17,27]). Under this condition the norm of the resolvent is allowed to grow (when $|\zeta| \to 1+$) like $(|\zeta| - 1)^{-1-\alpha}$, which is faster than in the situation (3.1). In [6] it was shown that, under condition (3.7a),

$$\|B^n\| \leqslant \mathrm{e}L(n+1)^{1+\alpha} \quad (n \geqslant 1,\ s \geqslant 1). \tag{3.7b}$$

Further, by the arguments in [27], condition (3.7a) is seen to imply, for the case where $\|\cdot\| = \|\cdot\|_2$, that

$$\|B^n\| \leqslant cLs(n+1)^{\alpha} \quad (n \geqslant 1,\ s \geqslant 1), \tag{3.7c}$$

where $c = 32\,\mathrm{e}^{1+\alpha}/\pi$.

We conclude this section by noting that slightly modified versions of (3.1), (3.5a), (3.6a), (3.7a) were considered in the literature as well: most of the papers mentioned above also deal with the situation where the inequality for the norm of the resolvent is required to hold only for $1 < |\zeta| < \rho$ — where ρ is a finite constant — rather than for all ζ with $|\zeta| > 1$. In this situation upper bounds for $\|B^n\|$ were proved which equal the original bounds, specified in (3.2), (3.5b), (3.6b), (3.7b) and (3.7c), respectively, multiplied by a factor γ only depending on ρ (and α). For the special case (3.5b), the corresponding factor γ is exceptionally simple in that $\gamma = 1$ for any ρ with $1 < \rho < \infty$: it can be proved that $\|B^n\| \leqslant \mathrm{e}L^2/2 \quad (n \geqslant 1,\ s \geqslant 1)$ whenever $r(B) \leqslant 1$ and $\|(\zeta I - B)^{-1}\| \leqslant L|\zeta - 1|^{-1}$ $(1 < |\zeta| < \rho)$.

4. Stability estimates under a general resolvent condition

4.1. Preliminaries

Throughout this Section 4 we assume, unless specified otherwise, that $\|\cdot\|$ is an arbitrary norm on the vector space of all complex $s \times s$ matrices (i.e., $\|A\| > 0$ for $A \neq 0$, and $\|A + B\| \leqslant \|A\| + \|B\|$, $\|\lambda \cdot A\| = |\lambda| \cdot \|A\|$ for all $\lambda \in \mathbb{C}$ and all $s \times s$ matrices A, B).

We shall present upper bounds for $\|B^n\|$, under the following general resolvent condition:

$$r(B) \leqslant 1 \quad \text{and} \quad \|(\zeta I - B)^{-1}\| \leqslant \frac{L}{(|\zeta| - 1)^k |\zeta - 1|^l} \quad (1 < |\zeta| < \rho). \tag{4.1}$$

Here L is a positive constant, k and l are nonnegative fixed integers with $k + l \geqslant 1$, and $1 < \rho \leqslant \infty$. Clearly, condition (4.1) generalizes some of the resolvent conditions reviewed in Section 3.

In deriving our upper bounds for $\|B^n\|$, we shall make use of

Lemma 4.1. *Let $\alpha \leqslant \beta \leqslant \alpha + 2\pi$, $r > 0$, and let Γ denote the subarc of a circle given by $\zeta = r\mathrm{e}^{\mathrm{i}t}$ $(\alpha \leqslant t \leqslant \beta)$. Assume $R(\zeta) = P(\zeta)/Q(\zeta)$, where $P(\zeta)$, $Q(\zeta)$ are polynomials of a degree not exceeding s, with $Q(\zeta) \neq 0$ on Γ. Then*

$$\int_\Gamma |R'(\zeta)|\,|\mathrm{d}\zeta| \leqslant \pi s \,\mathrm{diam}\, R(\Gamma) \leqslant 2\pi s \max_\Gamma |R(\zeta)|. \tag{4.2}$$

In (4.2) we denote by $\mathrm{diam}\, R(\Gamma)$ the diameter of the set $\{R(r\mathrm{e}^{\mathrm{i}t})\colon \alpha \leqslant t \leqslant \beta\}$. We note that this lemma allows of a simple geometrical interpretation since the integral in (4.2) equals the arc length of the image, under (the mapping) R, of Γ. A version of this lemma with $\beta = \alpha + 2\pi$ was already proved in [20] and in [31]. The more general Lemma 4.1 is no consequence of that version. But, property (4.2), for the general case $\alpha \leqslant \beta \leqslant \alpha + 2\pi$, can easily be proved by a straightforward adaptation of the arguments used in [20]. We omit the details.

4.2. Formulation and proof of general stability estimates

The following theorem summarizes our upper bounds for $\|B^n\|$, under the resolvent condition (4.1).

Theorem 4.2. *There is a constant γ depending only on k, l, ρ such that, for all $n \geqslant 1$, $s \geqslant 1$ and for each $s \times s$ matrix B satisfying* (4.1),

$$\|B^n\| \leqslant \gamma L n^{k-1} \min\{s, n\} \quad (\textit{if } k \geqslant 1,\ l = 0), \tag{4.3a}$$

$$\|B^n\| \leqslant \gamma L n^{k} \min\{\log(s+1), \log(n+1)\} \quad (\textit{if } k \geqslant 0,\ l = 1), \tag{4.3b}$$

$$\|B^n\| \leqslant \gamma L n^{k+l-1} \quad (\textit{if } k \geqslant 0,\ l \geqslant 2). \tag{4.3c}$$

Clearly, the bound (4.3a) is closely related to the estimates (3.2) and (3.7b), (3.7c) (with $\alpha = k-1$). The proof below of (4.3a) will consist in a straightforward application of arguments used earlier in the literature. It will rely among other things on Lemma 4.1 with $\beta = \alpha + 2\pi$.

To the best of our knowledge, the estimates (4.3b) and (4.3c) are new. Our proof of (4.3b) will require an application of Lemma 4.1 with $\beta < \alpha + 2\pi$.

Proof of Theorem 4.2. (1) Let $n \geqslant 1$, $s \geqslant 1$ and let the $s \times s$ matrix B satisfy (4.1). We shall use the Dunford–Taylor representation (see, e.g., [19, Chapter 10])

$$B^n = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \zeta^n (\zeta I - B)^{-1} \,\mathrm{d}\zeta,$$

where Γ is the positively oriented circle $|\zeta| = r$ with $r = \min\{\rho, 1 + 1/(n+1)\}$.

By a well known corollary to the Hahn–Banach theorem (see, e.g., [19, Chapter 3]), there is a linear mapping F from the vector space of all complex $s \times s$ matrices to $\mathbb{C}$, with $F(B^n) = \|B^n\|$ and $|F(A)| \leqslant \|A\|$ for all $s \times s$ matrices A. Consequently,

$$\|B^n\| = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \zeta^n R(\zeta) \,\mathrm{d}\zeta, \tag{4.4a}$$

where $R(\zeta) = F((\zeta I - B)^{-1})$ and

$$|R(\zeta)| \leqslant L(|\zeta| - 1)^{-k} |\zeta - 1|^{-l} \quad \text{for } 1 < |\zeta| \leqslant \rho.$$

(2) Let $l = 0$. Similarly as in [12], [5, pp. 208, 209] we perform a partial integration so as to obtain from (4.4a)

$$\|B^n\| = \frac{-1}{2\pi \mathrm{i}(n+1)} \int_\Gamma \zeta^{n+1} R'(\zeta) \,\mathrm{d}\zeta \leqslant \frac{r^{n+1}}{2\pi(n+1)} \int_\Gamma |R'(\zeta)| \,|\mathrm{d}\zeta|. \tag{4.4b}$$

By still using arguments similar to those in the above references, one can see that $R(\zeta) = P(\zeta)/Q(\zeta)$, where $P(\zeta)$, $Q(\zeta)$ are polynomials of a degree not exceeding s. Furthermore, for $|\zeta| = r$, we have $Q(\zeta) \neq 0$. Consequently, we can conclude from (4.4a), (4.4b) and Lemma 4.1 (with $\beta = \alpha + 2\pi$) that

$$\|B^n\| \leqslant \frac{r^{n+1}}{(n+1)(r-1)^k} L \min\{s, n+1\}.$$

This inequality implies the relations (4.5a) and (4.5b), which in their turn prove (4.3a):

$$\|B^n\| \leqslant \mathrm{e} L (n+1)^{k-1} \min\{s, n+1\} \quad \text{if } n+1 \geqslant (\rho - 1)^{-1}, \tag{4.5a}$$

$$\|B^n\| \leqslant \frac{L \rho^{n+1}}{(n+1)(\rho-1)^k} \min\{s, n+1\} \quad \text{if } n+1 < (\rho - 1)^{-1}. \tag{4.5b}$$

(3) Let $l=1$. We decompose the circle Γ into two subarcs Γ_0 and Γ_1, where Γ_0 is given by $\zeta = re^{it}$ $(-\delta \leqslant t \leqslant \delta)$, and Γ_1 by $\zeta = re^{it}$ $(\delta \leqslant t \leqslant 2\pi - \delta)$. Here δ is a value with $0 \leqslant \delta \leqslant \pi$ to be specified below. Putting $\zeta_0 = re^{i\delta}$, we obtain from (4.4a), by partial integration, the representation

$$\|B^n\| = \frac{1}{2\pi i}\int_{\Gamma_0} \zeta^n R(\zeta)\,d\zeta + \frac{-1}{2\pi i(n+1)}\int_{\Gamma_1} \zeta^{n+1}R'(\zeta)\,d\zeta$$
$$+ \frac{1}{2\pi i(n+1)}(\bar{\zeta}_0^{n+1}R(\bar{\zeta}_0) - \zeta_0^{n+1}R(\zeta_0)).$$

We denote the three successive terms in the right-hand member of the last equality by I_0, I_1, I_2, respectively.

We define $y = 2\delta[\pi(r-1)]^{-1}$ and assume that $y \geqslant 4$. We have

$$|I_0| \leqslant \frac{Lr^{n+1}}{\pi(r-1)^k}\int_0^{\delta} \frac{dt}{\sqrt{(r-1)^2 + (2t/\pi)^2}} = \frac{Lr^{n+1}\log(y + \sqrt{1+y^2})}{2(r-1)^k}$$
$$\leqslant \frac{Lr^{n+1}}{(r-1)^k}[1/2 + \log(y/2)].$$

By applying (among other things) Lemma 4.1, with $\alpha = \delta$, $\beta = 2\pi - \delta$, we also have

$$|I_1| \leqslant Ks, \ |I_2| \leqslant K/\pi \quad \text{where } K = \frac{Lr^{n+1}}{(r-1)^{k+1}(n+1)\sqrt{1+y^2}}.$$

We first choose $\delta = \pi$. We have $\|B^n\| = |I_0|$ and $y = 2(r-1)^{-1} \geqslant 4$ so that $\|B^n\| \leqslant Lr^{n+1}(r-1)^{-k}\{1 + \log[(r-1)^{-1}]\}$.

Next, we assume that $s < n$ and we choose $\delta = \pi(s+1)/(n+1)$. We now have $y = 2(s+1)[(r-1)(n+1)]^{-1} \geqslant 2(s+1) \geqslant 4$. Combining the inequality $\|B^n\| \leqslant |I_0| + |I_1| + |I_2|$ and our upper bounds for $|I_0|$, $|I_1|$, $|I_2|$ we arrive at the estimate $\|B^n\| \leqslant Lr^{n+1}(r-1)^{-k}\{1 + \log[(r-1)^{-1}(s+1)/(n+1)]\}$.

The two bounds for $\|B^n\|$ just obtained are equivalent to

$$\|B^n\| \leqslant \frac{r^{n+1}}{(r-1)^k} L\left\{1 + \log\left[\frac{\min\{s+1, n+1\}}{(n+1)(r-1)}\right]\right\}.$$

This inequality implies the relations (4.6a) and (4.6b), which in their turn prove (4.3b):

$$\|B^n\| \leqslant eL(n+1)^k[1 + \log(1 + \min\{s,n\})] \quad \text{if } n+1 \geqslant (\rho-1)^{-1}, \tag{4.6a}$$

$$\|B^n\| \leqslant \frac{L\rho^{n+1}}{(\rho-1)^k}\left\{1 + \log\left[\frac{1+\min\{s,n\}}{(n+1)(\rho-1)}\right]\right\} \quad \text{if } n+1 < (\rho-1)^{-1}. \tag{4.6b}$$

(4) Let $l \geqslant 2$. In order to prove (4.3c), we use (4.4a) so as to obtain

$$\|B^n\| \leqslant \frac{Lr^{n+1}}{\pi(r-1)^{k+l}} J \quad \text{with } J = \int_0^{\pi} \frac{dt}{(1 + (\mu t)^2)^{l/2}} \quad \text{and} \quad \mu = \frac{2}{\pi(r-1)}.$$

Introducing the variable x by the relation $\mu t = (e^x - e^{-x})/2$, we have

$$J \leqslant 2^{l-1}\mu^{-1}\int_0^\infty (e^x + e^{-x})^{1-l}\,dx \leqslant 2^{l-1}\mu^{-1}(l-1)^{-1}\left[\frac{2}{e^x + e^{-x}}\right].$$

Combining this estimate of J and the above bound for $\|B^n\|$, one obtains the relations (4.7a) and (4.7b), which in their turn prove (4.3c):

$$\|B^n\| \leqslant \frac{2^{l-2}e}{l-1}L(n+1)^{k+l-1} \quad \text{if } n+1 \geqslant (\rho-1)^{-1}, \tag{4.7a}$$

$$\|B^n\| \leqslant \frac{2^{l-2}}{l-1}\frac{L\rho^{n+1}}{(\rho-1)^{k+l-1}} \quad \text{if } n+1 < (\rho-1)^{-1}. \qquad \square \tag{4.7b}$$

4.3. Remarks in connection with Theorem 4.2

The estimates (4.3) in Theorem 4.2 have deliberately been formulated concisely without indicating how γ may depend on the parameters k, l, ρ. Bounds for $\|B^n\|$ in which the dependence on these parameters is explicit can be obtained from (4.5)–(4.7). As an illustration we mention that (4.5) can be used in proving, for $k \geqslant 1$, $l = 0$ and any $s \times s$ matrix B satisfying (4.1), that

$$\|B^n\| \leqslant cL(n+1)^{k-1}\min\{s, n+1\} \quad (n \geqslant 1, s \geqslant 1),$$

where $c = e$ (for $\rho \geqslant 3/2$), $c = \max\{e, \rho^2 2^{-k}(\rho-1)^{-k}\}$ (for $1 < \rho < 3/2$). We note that this bound can be applied in the situation (3.7a) (with $\alpha = k-1$), so as to yield (3.7c) with a smaller value for c than the one given in Section 3.3.

We conclude this section by a short discussion of the sharpness of the stability estimates, given in Theorem 4.2, for the important case $\|\cdot\| = \|\cdot\|_\infty$. We focus on the question of whether these estimates can be improved, for all fixed L and ρ, to bounds on $\|B^n\|_\infty$ which grow slower with n or s than the bounds in (4.3).

Kraaijevanger's result (3.3) makes clear that, when $k = 1$, $l = 0$, the estimate in (4.3a) cannot be improved, for all L, ρ, into a bound of the form $\|B^n\|_\infty \leqslant c\min\{\phi(s), \psi(n)\}$, where $c = c(\rho, L)$ only depends on ρ, L and either $\phi(s)$ or $\psi(n)$ grows slower than linearly with s or with n, respectively. On the other hand, an essential improvement over the estimate in (4.3b) is possible when $k=0$, $l=1$: in Section 3.3 we have seen that in this case $\|B^n\| \leqslant c$ with $c = eL^2/2$.

The authors found that, somewhat surprisingly, a conclusion, similar to the one just mentioned for $k = 1$, $l = 0$, can be reached whenever $k \neq 0$ or $l \neq 1$. In fact, for each $k \geqslant 1$, the estimate in (4.3a) cannot be improved into a bound of the form $\|B^n\|_\infty \leqslant c(\rho, L, k)n^{k-1}\min\{\phi(s), \psi(n)\}$ with any functions $\phi(s)$, $\psi(n)$ as considered above. Further, for each $k \geqslant 1$, the estimate in (4.3b) cannot be improved into $\|B^n\|_\infty \leqslant c(\rho, L, k)n^k\min\{\phi(s), \psi(n)\}$ with either $\phi(s)$ or $\psi(n)$ growing slower than $\log(s+1)$ or $\log(n+1)$, respectively. Finally, for each $k \geqslant 0$ and $l \geqslant 2$, the estimate in (4.3c) cannot be improved into $\|B^n\|_\infty \leqslant c(\rho, L, k, l)\psi(n)$ with $\lim_{n\to\infty}\psi(n)/n^{k+l-1} = 0$. More details are given in [4].

5. Stability analysis in the numerical solution of delay differential equations

5.1. Applying the trapezoidal rule to a linear test problem

The above general considerations will be illustrated in the numerical solution of the initial value problem

$$Z'(t) = f(Z(t), Z(t-\tau)) \quad (t \geqslant 0), \qquad Z(t) = g(t) \quad (t \leqslant 0).$$

Here f, g are given functions, $\tau > 0$ is a fixed delay, and $Z(t)$ is unknown (for $t > 0$).

We focus on the following well-known version of the *trapezoidal rule*:

$$z_n = z_{n-1} + \frac{h}{2}[f(z_n, z_{n-s+1}) + f(z_{n-1}, z_{n-s})] \quad (n \geqslant 1). \tag{5.1}$$

Here s denotes an integer with $s \geqslant 2$, and $h = \tau/(s-1)$ is the so-called stepsize. Further, z_n are approximations to $Z(t)$ at the gridpoints $t = t_n = nh$. Putting $z_n = g(t_n)$ $(n \leqslant 0)$, one may compute successively approximations z_n (for $n = 1, 2, 3, \ldots$) from (5.1).

Many authors (see, e.g., [1,30,32]) studied the stability of numerical methods, for the above initial value problem, by analysing the behaviour of the methods in the solution of the following linear test problem:

$$Z'(t) = \lambda Z(t) + \mu Z(t-\tau) \quad (t \geqslant 0), \qquad Z(t) = g(t) \quad (t \leqslant 0).$$

Here λ, μ denote fixed complex coefficients, and $g(t)$, $Z(t) \in \mathbb{C}$.

Method (5.1), when applied to the test equation, reduces to the recurrence relation

$$z_n = az_{n-1} + bz_{n-s+1} + bz_{n-s} \quad (n \geqslant 1),$$

where $a = (2+x)(2-x)^{-1}$, $b = y(2-x)^{-1}$ and $x = h\lambda$, $y = h\mu$. This recurrence relation can be written in the form

$$u_n = Bu_{n-1} \quad (n \geqslant 1) \quad \text{where } u_n = (z_n, z_{n-1}, \ldots, z_{n-s+1})^{\mathrm{T}}.$$

Here the $s \times s$ companion matrix $B = (\beta_{ij})$ is defined, for $s \geqslant 3$, by $\beta_{ij} = a$ (if $i = j = 1$), $\beta_{ij} = b$ (if $i = 1$ and $j = s-1, s$), $\beta_{ij} = 1$ (if $1 \leqslant j = i-1 \leqslant s-1$), and $\beta_{ij} = 0$ otherwise. For $s = 2$, we have $\beta_{11} = a + b$, $\beta_{12} = b$, $\beta_{21} = 1$, $\beta_{22} = 0$. Clearly, B depends (only) on x, y and s. Accordingly, we shall write $B = B_s(x, y)$.

Following standard practice in dealing with the above test problem, we consider the so-called *stability region*

$$S = \{(x, y) \colon r(B_s(x, y)) < 1 \text{ for all } s \geqslant 2\}.$$

It is known that all pairs (x, y) with $\mathrm{Re}\, x < -|y|$ belong to S, and that all $(x, y) \in S$ satisfy $\mathrm{Re}\, x \leqslant -|y|$ (see, e.g., [30]).

But, as highlighted in Section 2, with regard to error propagation the crucial question is not of whether the spectral radius condition $r(B_s(x, y)) < 1$ is fulfilled, but of whether $\|B^n\|$ is of moderate size, where $B = B_s(x, y)$ and $\|\cdot\|$ is related to a suitable vector norm according to (2.3).

In the following we focus on estimating $\|B^n\|_\infty$ for $B = B_s(x, y)$, $n \geqslant 1$, $s \geqslant 2$, uniformly for all $(x, y) \in S$.

5.2. Obtaining stability results by using resolvents

In [21] it was proved that, corresponding to any given fixed $s \geqslant 2$, there exists no finite L such that $B = B_s(x, y)$ satisfies the Kreiss condition (3.1) (with $\|\cdot\| = \|\cdot\|_\infty$) uniformly for all $(x, y) \in S$. Since (2.4) implies (3.1) (with $L = \max\{1, M\}$, see Section 3.1), it follows that the quantity M_s, defined by

$$M_s = \sup\{\|B^n\|_\infty\colon n \geqslant 1,\ B = B_s(x, y),\ (x, y) \in S\},$$

satisfies

$$M_s = \infty \quad (\text{for } s = 2, 3, 4, \ldots).$$

In spite of this negative stability result, it is still possible to establish an upper bound for $\|B^n\|_\infty$ (uniformly for $B = B_s(x, y)$ with $(x, y) \in S$) which is only slightly weaker than (3.2). This bound can be obtained by a combination of Theorem 4.2 and the following lemma.

Lemma 5.1. *Let* $\mathrm{Re}\, x \leqslant -|y|$. *Then the matrix* $B = B_s(x, y)$ *satisfies*

$$r(B) \leqslant 1 \quad \textit{and} \quad \|(\zeta I - B)^{-1}\|_\infty \leqslant \frac{11}{(|\zeta| - 1)|\zeta + 1|} \quad (\text{for } 1 < |\zeta| < \tfrac{3}{2}). \tag{5.2}$$

Proof. Let $x, y \in \mathbb{C}$, with $\mathrm{Re}\, x \leqslant -|y|$, and let $s \geqslant 2$, $B = B_s(x, y)$. The polynomial $P(\zeta) = \det(\zeta I - B)$ can be written in the form

$$P(\zeta) = (\zeta - a)\zeta^{s-1} - (\zeta + 1)b.$$

Let $\zeta \in \mathbb{C}$, with $|\zeta| > 1$. In [21, pp. 243, 244] it was shown that the spectral radius $r(B) \geqslant 1$, and that

$$\|(\zeta I - B)^{-1}\|_\infty \leqslant 2\left\{\frac{1}{|\zeta| - 1} + \frac{|\zeta|^{s-1}}{|P(\zeta)|}\right\}.$$

We write ζ in the form

$$\zeta = \frac{2 + z}{2 - z} \quad \text{with} \quad \mathrm{Re}\, z > 0,\ z \neq 2.$$

By straightforward calculations it can be seen that

$$\zeta - a = \frac{4(z - x)}{(2 - z)(2 - x)}, \qquad (\zeta + 1)b = \frac{4y}{(2 - z)(2 - x)},$$

$$|\zeta|^2 - 1 = \frac{8\mathrm{Re}\, z}{|2 - z|^2}, \qquad |\zeta + 1| = \frac{4}{|2 - z|}.$$

These equalities imply that

$$\frac{|P(\zeta)|}{|\zeta|^{s-1}} \geqslant |\zeta|^{-1}\{|(\zeta - a)\zeta| - |(\zeta + 1)b|\} \geqslant \frac{4(|(z - x)\zeta| + \mathrm{Re}\, x)}{|\zeta(2 - z)(2 - x)|}.$$

Since $\mathrm{Re}\, z - \mathrm{Re}\, x \leqslant |z - x|$, we have

$$\begin{aligned} |(z - x)\zeta| + \mathrm{Re}\, x &\geqslant |z - x|(|\zeta| - 1) + \mathrm{Re}\, z \\ &\geqslant (|\zeta| - 1)\big||2 - x| - |2 - z|\big| + \tfrac{1}{8}(|\zeta|^2 - 1)|2 - z|^2. \end{aligned}$$

Combining this bound for $|(z-x)\zeta|+\mathrm{Re}\,x$ with the above lower bound for $|P(\zeta)|/|\zeta|^{s-1}$, we obtain

$$\begin{aligned}\frac{|P(\zeta)|}{|\zeta|^{s-1}} &\geqslant \frac{|\zeta|-1}{|\zeta|}\left[\left|1-\left|\frac{2-z}{2-x}\right|\right|\cdot|\zeta+1|+\frac{1}{2}(|\zeta|+1)\left|\frac{2-z}{2-x}\right|\right]\\ &\geqslant \frac{|\zeta|-1}{|\zeta|}\left[\left||\zeta+1|-\frac{4}{|2-x|}\right|+\frac{2}{|2-x|}\right]\\ &\geqslant \frac{|\zeta|-1}{|\zeta|}\max\left\{\frac{2}{|2-x|},\frac{|\zeta+1|}{2}\right\}.\end{aligned}$$

In view of the above upper bound for $\|(\zeta I-B)^{-1}\|_\infty$, we arrive at

$$\|(\zeta I-B)^{-1}\|_\infty \leqslant 2\left[1+|\zeta|\min\left\{\frac{|2-x|}{2},\frac{2}{|\zeta+1|}\right\}\right](|\zeta|-1)^{-1}.$$

We conclude that, for $|\zeta|>1$,

$$\|(\zeta I-B)^{-1}\|_\infty \leqslant (2|\zeta+1|+4|\zeta|)|\zeta+1|^{-1}(|\zeta|-1)^{-1}.$$

This implies (5.2). □

The following neat stability result for the trapezoidal rule can now easily be proved.

Theorem 5.2. *There is a constant c such that $B=B_s(x,y)$ satisfies*

$$\|B^n\|_\infty \leqslant cn\min\{\log(s+1),\log(n+1)\} \quad (n\geqslant 1, s\geqslant 2),$$

uniformly for all $(x,y)\in S$.

Proof. Lemma 5.1 shows that the matrix $-B$ satisfies (4.1) with $\|\cdot\|=\|\cdot\|_\infty$ and $k=l=1$, $L=11$, $\rho=3/2$. In view of Theorem 4.2, we have $\|B^n\|_\infty=\|(-B)^n\|_\infty\leqslant cn\min\{\log(s+1),\log(n+1)\}$ with $c=11\gamma$. Here γ is constant. □

We note that the upper bound for $\|B^n\|_\infty$ given by the above theorem can be interpreted as a stability result of the form

$$|\tilde z_n - z_n| \leqslant \phi(s,n)\max\{|\tilde z_0-z_0|,|\tilde z_{-1}-z_{-1}|,\dots,|\tilde z_{-s+1}-z_{-s+1}|\},$$

valid for any two sequences z_n, $\tilde z_n$, computed from (5.1) with $f(\xi,\eta)=\lambda\xi+\mu\eta$ and $\mathrm{Re}\,\lambda\leqslant-|\mu|$. Here $\phi(s,n)=cn\min\{\log(s+1),\log(n+1)\}$ is growing only slightly faster than linearly with n, so that a mild error propagation is present.

Finally, we note that, in line with the first paragraph of Section 4.3, a fully explicit upper bound for $\|B^n\|_\infty$ can be obtained as well. From (4.6a) and Lemma 5.1, we easily obtain, for $B=B_s(x,y)$ and all $(x,y)\in S$,

$$\|B^n\|_\infty \leqslant 11\mathrm{e}(n+1)[1+\min\{\log(s+1),\log(n+1)\} \quad (n\geqslant 1, s\geqslant 2).$$

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