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An Algebraic Characterization of B-convergent Runge-Kutta Methods *

Willem H. Hundsdorfer [1] and Josef Schneid [2]

[1] Centre for Mathematics and Computer Science, P.O. Box 4079, 1009 AB Amsterdam, The Netherlands

[2] Institut für Angewandte und Numerische Mathematik, Technical University of Vienna, Wiedner Hauptstrasse 8–10, A-1040 Vienna, Austria

Summary. In the analysis of discretization methods for stiff intial value problems, stability questions have received most part of the attention in the past. B-stability and the equivalent criterion algebraic stability are well known concepts for Runge-Kutta methods applied to dissipative problems. However, for the derivation of B-convergence results – error bounds which are not affected by stiffness – it is not sufficient in many cases to require B-stability alone. In this paper, necessary and sufficient conditions for B-convergence are determined.

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1. Introduction

The core of the concept of B-convergence is the derivation of stiffness-independent bounds for the global discretization errors of Runge-Kutta methods applied to nonlinear initial value problems [12]. The theory is based on a well known class of testproblems $\mathscr{F}_\mu$, introduced by Dahlquist [7], where $\mu \in \mathbb{R}$ is a measure of dissipation. The main object of this paper is to determine necessary and sufficient conditions for having B-convergence on $\mathscr{F}_\mu$ in terms of algebraic relations for the coefficients of the Runge-Kutta methods.

Sufficient conditions were presented already by Frank et al. [13, 14]; they showed that if the method is algebraically stable and also satisfies a slightly different algebraic condition – known as "diagonal stability" in matrix theory [1, 2] – then it is B-convergent on $\mathscr{F}_\mu$ for arbitrary $\mu \in \mathbb{R}$. In this paper it will be proved that for $\mu \geqq 0$ these two conditions are necessary as well, under some mild apriori assumptions on the method. This result shows that there

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can be a different behaviour of methods when applied to dissipative problems ($\mu=0$) or to strictly dissipative problems ($\mu<0$), as it is known from the work of Spijker, Dekker, Kraaijevanger and Schneid [21, 10, 20] that for $\mu<0$ algebraic stability on its own is already sufficient, and also necessary, for B-convergence on $\mathscr{F}_\mu$.

After some preliminaries in Sect. 2, the results on the algebraic characterization of B-convergence will be presented in Sect. 3. In order to prove these results, an algebraic criterion for the internal stability concept BS-stability is needed; this will be given in Sect. 4.

2. Preliminaries

2.1 The Class $\mathscr{F}_\mu$

In this paper stiff nonlinear initial value problems

(2.1 a) $$y'(t)=f(t, y(t)) \quad (\text{for } 0 \leqq t \leqq 1),$$

(2.1 b) $$y(0)=y_0$$

are considered, where $f\colon [0,1]\times\mathbb{C}^m\to\mathbb{C}^m$ and $y_0\in\mathbb{C}^m$ are given. We shall be concerned with error bounds for numerical approximations measured in the Euclidean norm $|u|=(u,u)^{1/2}$ where $(u,v)=u^*v$ denotes the standard inner product on $\mathbb{C}^m$ for arbitrary $m\in\mathbb{N}$.

It will be assumed that the function f satisfies a one-sided Lipschitz condition

(2.2) $$\operatorname{Re}(f(t,u)-f(t,v), u-v)\leqq\mu|\mu-v|^2 \quad (\text{for all } t\in[0,1] \text{ and } u, v\in\mathbb{C}^m),$$

with a constant $\mu\in\mathbb{R}$, the one-sided Lipschitz constant. The class of all functions $f\colon [0,1]\times\mathbb{C}^m\to\mathbb{C}^m$ with $m\in\mathbb{N}$ which satisfy (2.2) will be denoted by $\mathscr{F}_\mu$. For continuous functions f the condition (2.2) is equivalent with stability of the differential equation (2.1 a), in the sense that for any two solutions $\tilde{y}$ and y,

(2.3) $$|\tilde{y}(t+h)-y(t+h)|\leqq e^{\mu h}|\tilde{y}(t)-y(t)| \quad (\text{for } 0\leqq t\leqq t+h\leqq 1),$$

as can be seen from [11; Sect. 1.2], for example. If $\mu=0$ (or $\mu<0$) the initial value problem (2.1) is said to be (strictly) dissipative. The conventional Lipschitz constant L of $f\in\mathscr{F}_\mu$ may be arbitrarily large, which makes the class $\mathscr{F}_\mu$ useful as a test class for the analysis of numerical schemes for stiff nonlinear problems.

The results of this paper would remain valid if only real initial value problems, with $f\colon [0,1]\times\mathbb{R}^m\to\mathbb{R}^m$, $y_0\in\mathbb{R}^m$, were considered. Although a restriction to real problems is more natural, working in the complex space $\mathbb{C}^m$ has the advantage that some proofs are easier to formulate. Any problem in $\mathbb{C}^m$ can always be written as a real one with dimension $2m$, by identifying $\mathbb{C}$ with $\mathbb{R}^2$ in the usual way. We also note that arbitrary inner products $\langle\cdot,\cdot\rangle$ on $\mathbb{C}^m$ might be considered as well; the restriction to the Euclidean inner product has only been made for notational convenience.

2.2 The Implicit Runge-Kutta Methods

For the numerical solution of initial value problems (2.1) we consider implicit Runge-Kutta methods. Let $h>0$ be the stepsize and $t_n=nh$ for $n=0, 1, 2, \ldots$ and $nh \leqq 1$. Approximations y_n to $y(t_n)$ are computed from the scheme

$$y_n=y_{n-1}+h\sum_{i=1}^{s} b_i f(t_{n-1}+c_i h, Y_i^n), \tag{2.4a}$$

$$Y_i^n=y_{n-1}+h\sum_{j=1}^{s} a_{ij} f(t_{n-1}+c_j h, Y_j^n) \qquad (1\leqq i\leqq s). \tag{2.4b}$$

Here, $s\in\mathbb{N}$ is the number of stages and a_{ij}, b_i, c_i are real parameters defining the method. For convenience it will be assumed that all $c_i\in[0,1]$; otherwise, some of the definitions would need modification (for example, the function $f(t, y)$ then had to be defined for values t outside the integration interval $[0, 1]$). Almost all well known Runge-Kutta methods are such that the abscissas c_i are different; such methods are called *nonconfluent*.

Consider the $s\times s$ matrices $A=(a_{ij})$, $B=\operatorname{diag}(b_1, \ldots, b_s)$, and the vector $b=(b_1, \ldots, b_s)^T\in\mathbb{R}^s$. The Runge-Kutta method (2.4) is said to be *algebraically stable* if

$$B \quad \text{and} \quad BA+A^T B-bb^T \quad \text{are positive semi-definite.} \tag{2.5}$$

This algebraic condition, introduced in [3] and [5], is known to be equivalent for nonconfluent methods to the following unconditional contractivity property, called *B-stability*,

$$|\tilde{y}_n-y_n|\leqq|\tilde{y}_{n-1}-y_{n-1}| \quad (\text{for all } h>0 \text{ and } f\in\mathscr{F}_0) \tag{2.6}$$

for any two sequences of approximations computed by the Runge-Kutta scheme (2.4) with different starting values y_0 and $\tilde{y}_0$. Note that (2.6) is the discrete analogue of (2.3) for $\mu=0$.

In order to treat also the effect of perturbations of the internal stages (2.4b), a slightly different algebraic condition was considered in [13],

(2.7) there is a diagonal matrix D such that
D and $DA+A^T D$ are positive definite.

Both conditions (2.5) and (2.7) will turn out to be essential for having error bounds independent of the stiffness. For important classes of Runge-Kutta methods it is known whether (2.5) and (2.7) are valid, see [9, 11, 13] (cf. also Sect. 3.3).

Remark 2.1. For any given Runge-Kutta method it is straightforward to check whether (2.5) is satisfied. Some necessary and sufficient conditions for (2.7) to hold can be found in [1] and [2]. For example, it is known that (2.7) implies that all principles minors of A are positive, and this is also sufficient in case $s=2$. If A is triangular, then (2.7) holds iff all $a_{ii}>0$. Furthermore, (2.7) implies that for any principal submatrix A' of A and any positive diagonal matrix D', all eigenvalues of $D'A'$ have a positive real part. □

Let $c^k=(c_1^k, \ldots, c_s^k)^T \in \mathbb{R}^s$ for $k \in \mathbb{N}$ and $c^0=e=(1, \ldots, 1)^T$. The *stage order* q of the Runge-Kutta method is defined to be the largest integer such that

$$kb^T c^{k-1}=1 \quad \text{and} \quad kAc^{k-1}=c^k \quad \text{for } k=1,2,\ldots,q. \tag{2.8}$$

Values of q for various classes of Runge-Kutta methods can be found in [11, 14]; usually, the stage order is at least one.

Algebraically stable methods having some $b_i=0$ are known to be *reducible* (in the sense of Dahlquist and Jeltsch [8]), which means that some of the stages in (2.4b) can be omitted without changing the numerical results. It is obviously no severe restriction to consider only irreducible methods.

Finally, we note that for implicit Runge-Kutta methods the internal vectors Y_i^n are defined as the solution of the nontrivial system of algebraic equations (2.4b). If (2.7) is satisfied then this system has a unique solution for all $f \in \mathscr{F}_\mu$ (under a mild stepsize restriction if $\mu>0$), see [6, 11]. More general conditions can be found in [18]. Throughout this paper it will be tacitly assumed that there is a unique solution for all appropriate stepsizes h.

2.3 *B-convergence*

We shall be concerned with bounds for the global discretization errors which only depend on the smoothness and stability of the exact solution. Let $p>0$ and $\mu \in \mathbb{R}$. The Runge-Kutta method (2.4) is called *B-convergent of order p on* $\mathscr{F}_\mu$ if for any initial value problem (2.1) with $f \in \mathscr{F}_\mu$ there is an error bound

$$|y(t_n)-y_n| \leqq Ch^p \quad (\text{for } 0<h \leqq H,\ 0 \leqq t_n \leqq 1), \tag{2.9}$$

where the error constant C only depends on μ and on certain bounds $M_j=\max\{|y^{(j)}(t)|: 0 \leqq t \leqq 1\}$ for derivatives of the exact solution, and the maximal stepsize H only depends on μ. If this holds for some $p>0$ the method will simply be called B-convergent on $\mathscr{F}_\mu$.

Stiff initial value problems have large Lipschitz constants L – which are, by definition, prohibited to enter C – together with relatively smooth, stable solutions. So, for any given initial value problem (2.1) with $f \in \mathscr{F}_\mu$, the estimate (2.9) legitimates the adaptation of the stepsize to the smoothness of the solution only.

The above definition of B-convergence, with C depending exclusively on μ and some of the M_j, is a strong one, and is also called *optimal* B-convergence. A weaker form is obtained if C is allowed to depend as well on some of the quantities $K_{ij}=\max\{|\partial^{i+j} f(t, y(t))/\partial t^i \partial y^j|: 0 \leqq t \leqq 1\}$, though not on K_{01} as this bound is proportional to the Lipschitz constant L. Usually, this weaker form has the effect that the order p in (2.9) can be raised by one, see [14]. A second alternative would be to allow C to depend on the dimension m of the initial value problem. This, however, makes no difference in general (see Sect. 3.3), i.e., from a bound depending on m it can be concluded for most methods that a bound valid uniformly in m also exists.

3. Characterization of B-convergence

In this section a characterization of B-convergence on $\mathscr{F}_\mu$ for Runge-Kutta methods will be given in terms of the algebraic conditions (2.5) (algebraic stability) and (2.7). The cases $\mu<0$ and $\mu\geqq 0$ are considered separately. The results for $\mu<0$ are based on [10, 20, 21]; they are included here only for completeness.

3.1 The Case $\mu<0$

Theorem 3.1. *Let $\mu<0$, and assume that the Runge-Kutta method has stage order $q\geqq 1$ and its coefficient matrix A is nonsingular. Then*

$$(2.5) \Rightarrow B\text{-convergence on } \mathscr{F}_\mu.$$

Theorem 3.2. *Let $\mu\in\mathbb{R}$ be arbitrary, and assume that the abscissas of the Runge-Kutta method satisfy $c_i-c_j\notin\mathbb{Z}$ if $i\neq j$. Then*

$$B\text{-convergence on } \mathscr{F}_\mu \Rightarrow (2.5).$$

Theorem 3.2 can be proved by a counterexample, based on material of [3, 5] (see [10, 20], for example). A proof of Theorem 3.1 can be found in [21], where it was shown that the order p of B-convergence is at least $q-1/2$. This was improved in [10], where an order q result was derived under the assumption of irreducibility and $1-b^TA^{-1}e\in(-1, 1)$ (note that (2.5) implies $1-b^TA^{-1}e\in[-1, 1]$). In [20] it was shown that also in case $1-b^TA^{-1}e=-1$ the order is at least q.

By combining the above theorems we obtain the following result.

Corollary 3.3. *Let $\mu<0$, and assume that the Runge-Kutta method has stage order $q\geqq 1$, A is non-singular, and $c_i-c_j\notin\mathbb{Z}$ if $i\neq j$. Then*

$$B\text{-convergence on } \mathscr{F}_\mu \Leftrightarrow (2.5).$$

3.2 The Case $\mu\geqq 0$

Theorem 3.4. *Let $\mu\in\mathbb{R}$ be arbitrary, and assume that the Runge-Kutta method has stage order $q\geqq 1$. Then*

$$(2.5) \text{ and } (2.7) \Rightarrow B\text{-convergence on } \mathscr{F}_\mu.$$

Theorem 3.5. *Let $\mu \geqq 0$, and assume that the Runge-Kutta method is such that $b_i \neq 0$ for all i and $c_i - c_j \neq 0$ if $i \neq j$. Assume in addition that the j-th row of A is nonzero in case $c_j = 0$. Then*

$$B\text{-convergence on } \mathscr{F}_\mu \Rightarrow (2.7).$$

The proof of Theorem 3.5 will be given in Sect. 4.3. Theorem 3.4 is due to [14], where it was also shown that the order of B-convergence p is at least q. This is not necessarily the maximal order. The implicit midpoint rule, for example, has stage order $q=1$ and is known to be B-convergent on $\mathscr{F}_\mu$ with order $p=2$ for any $\mu \in \mathbb{R}$ (see [17]). By considering local errors $|y(t_1) - y_1|$ it can be seen that we always have $p \leqq q+1$ for irreducible methods. There are, apart from the implicit midpoint rule, some special methods where the order $q+1$ is achieved (see [4]), but generally it is only known that $p \in [q, q+1]$.

By a combination of Theorems 3.2, 3.4 and 3.5, we arrive at a characterization of B-convergence on $\mathscr{F}_\mu$, $\mu \geqq 0$, for methods which are irreducible in the sense of [8]. The proof will be given in Sect. 4.3.

Corollary 3.6. *Let $\mu \geqq 0$, and assume that the Runge-Kutta method is irreducible, it has stage order $q \geqq 1$, and $c_i - c_j \notin \mathbb{Z}$ if $i \neq j$. Then*

$$B\text{-convergence on } \mathscr{F}_\mu \Leftrightarrow (2.5) \text{ and } (2.7).$$

3.3 Consequences and Remarks

For most well known classes of algebraically stable Runge-Kutta methods (see [11]) it can be determined with the above theorems whether they are B-convergent on $\mathscr{F}_\mu$. The Gauss methods, as well as the Radau IA and IIA methods and the two-stage Lobatto IIIC method satisfy (2.5) and (2.7), and thus they are B-convergent on $\mathscr{F}_\mu$ for any $\mu \in \mathbb{R}$ (see [14]). All algebraically stable, irreducible, diagonally implicit Runge-Kutta methods have $a_{ii} > 0$ for all i, and hence (2.7) also holds, see Remark 2.1. Lobatto IIIC methods with more than two stages are also algebraically stable, but violate (2.7) (see [9]), and so it follows from Theorems 3.1, 3.5 that these methods are B-convergent on $\mathscr{F}_\mu$ if and only if $\mu < 0$.

There are some methods, such as the Lobatto IIIA schemes, which are not algebraically stable and do not satisfy (2.7), but which have $c_1 = 0$, $c_s = 1$ and $e_1^T A = 0$. Theorems 3.2 and 3.5 cannot be applied to show that these methods are not B-convergent; in fact, the trapezoidal rule, which is a Lobatto IIIA method, is B-convergent on $\mathscr{F}_\mu$ for any $\mu \in \mathbb{R}$ (see [17]). On the other hand, Theorem 3.2 does not apply either to the Lobatto IIIB methods, while it follows from the material presented in [19] that these methods are *not* B-convergent on $\mathscr{F}_\mu$ for any $\mu \in \mathbb{R}$; note that Theorem 3.5 is applicable but only gives this result for $\mu \geqq 0$.

For *variable* stepsizes the condition in Theorem 3.2 can be relaxed to $c_i - c_j \neq 0$ (nonconfluency), see [10]. Thus, the Lobatto IIIA methods are not B-convergent on $\mathscr{F}_\mu$ with arbitrary variable stepsizes, for any $\mu \in \mathbb{R}$. In [10] it was also shown that Theorem 3.1 remains valid for variable stepsizes, and the same holds for Theorem 3.4, as can be easily seen by an inspection of its proof as given in [14] or [11].

Theorem 3.5 would already be valid if only initial value problems with dimension $m=s$ were considered (see Sect. 4.2, 4.3). The proof of Theorem 3.2 is even based on a scalar counterexample. It follows that for Runge-Kutta methods satisfying the assumptions of these theorems, B-convergence uniformly in m – which we consider – follows already from B-convergence where m is allowed to enter the constants C and H in (2.9).

4. Characterization of *BS*-stability

In this section an algebraic characterization of the internal stability concept BS-stability will be given. It will turn out that this provides a tool for a simple proof of Theorem 3.5.

4.1 BS-stability

Consider along with one Runge-Kutta step (2.4) a perturbed step

(4.1 a) $$\tilde{y}_n = y_{n-1} + h\sum_{i=1}^{s} b_i f(t_{n-1}+c_i h, \tilde{Y}_i^n) + w_0,$$

(4.1 b) $$\tilde{Y}_i^n = y_{n-1} + h\sum_{j=1}^{s} a_{ij} f(t_{n-1}+c_j h, \tilde{Y}_j^n) + w_i \qquad (1\leqq i\leqq s).$$

The perturbations $w_j\in\mathbb{C}^m$ may represent errors caused by inexactly solving the algebraic equations (2.4 b), but also local discretization errors may be represented this way. Let $w=(w_1^T, \ldots, w_s^T)^T\in\mathbb{C}^{ms}$. The Runge-Kutta method is called *BS-stable on* $\mathscr{F}_\mu$ if there exists a uniform bound for the difference between (2.4 a) and (4.1 a) of the type

(4.2) $$|\tilde{y}_n - y_n| \leqq C(|w_0|+|w|) \qquad (\text{for all } h\in(0, H] \text{ and } f\in\mathscr{F}_\mu)$$

with C, $H>0$ only depending on μ. It is known from [13] that the algebraic condition (2.7) is sufficient to have BS-stability on $\mathscr{F}_\mu$ for arbitrary $\mu\geqq 0$. We will show that this condition is, in general, also necessary.

In order to prove this result some notations are needed. The i-th row $(a_{i1}, \ldots, a_{is})^T$ of A will be denoted by a_i^T. For a given $m\in\mathbb{N}$, let $\mathbf{A}=A\otimes I$, $\mathbf{b}^T=b^T\otimes I$ and $\mathbf{a}_i^T=a_i^T\otimes I$, where I is the $m\times m$ identity matrix and $\otimes$ denotes the Kronecker product; further, $\mathbf{I}$ will stand for the $sm\times sm$ identity matrix. Vectors $u\in\mathbb{C}^{sm}$ will be partitioned as $(u_1^T, \ldots, u_s^T)^T$ with $u_j\in\mathbb{C}^m$ $(1\leqq j\leqq s)$, and for all components u_j we define the scaled counterparts $\hat{u}_j$ by

$$\hat{u}_j = |u_j|^{-1} u_j \quad \text{if } u_j \neq 0, \quad \text{and} \quad \hat{u}_j = 0 \quad \text{if } u_j = 0.$$

Finally, $\mathscr{D}_0$ stands for the set of block-diagonal matrices $\mathbf{Z}=\operatorname{diag}(Z_1, \ldots, Z_s)$ where all Z_j are $m\times m$ matrices with $m\in\mathbb{N}$ and $\operatorname{Re}(v, Z_j v)\leqq 0$ for all $v\in\mathbb{C}^m$, $1\leqq j\leqq s$.

It is known, see [16], that for nonconfluent Runge-Kutta methods *BS*-stability on $\mathscr{F}_0$ is equivalent with the existence of a positive constant C such that

$$(4.3)\qquad |\mathbf{b}^T\mathbf{Z}(\mathbf{I}-\mathbf{A}\mathbf{Z})^{-1}w|\leqq C|w| \quad (\text{for all } w\in\mathbb{C}^{sm} \text{ and } \mathbf{Z}\in\mathscr{D}_0).$$

Lemma 4.1. *Suppose the Runge-Kutta method is BS-stable on* $\mathscr{F}_0$, *and* $c_i-c_j\neq 0$ *if* $i\neq j$. *Then, for any sequence* $\{u^n\}$ *in* $\mathbb{C}^{sm}$ *with* $m\in\mathbb{N}$ *and* $\mathbf{b}^T u^n\neq 0$, *there is an index* j, $1\leqq j\leqq s$, *such that*

$$(4.4)\qquad \limsup_{n\to\infty} |\mathbf{b}^T u^n|^{-1}\operatorname{Re}(\hat{u}_j^n, \mathbf{a}_j^T u^n)>0.$$

Proof. Suppose the condition in the lemma does not hold, i.e. there are $u^n\in\mathbb{C}^{sm}$ with $\mathbf{b}^T u^n\neq 0$ such that

$$(4.5)\qquad \limsup_{n\to\infty} |\mathbf{b}^T u^n|^{-1}\operatorname{Re}(\hat{u}_j^n, \mathbf{a}_j^T u^n)\leqq 0 \quad (1\leqq j\leqq s).$$

We may assume that $|\mathbf{b}^T u^n|=1$; this is only a matter of scaling.

Define the vectors $p^n\in\mathbb{C}^{sm}$ by

$$p_j^n=\mathbf{a}_j^T u^n+r_j^n,\qquad r_j^n=-[\operatorname{Re}(\hat{u}_j^n, \mathbf{a}_j^T u^n)]^+\,\hat{u}_j^n \quad (1\leqq j\leqq s),$$

where $\alpha^+=\max\{\alpha, 0\}$. By this construction we have $\operatorname{Re}(p_j^n, u_j^n)\leqq 0$ $(1\leqq j\leqq s)$, and $|r_j^n|\to 0$ $(1\leqq j\leqq s,\ n\to\infty)$. Hence, there are $u^n, p^n\in\mathbb{C}^{sm}$ such that

$$(4.6)\qquad \operatorname{Re}(p_j^n, u_j^n)\leqq 0 \quad (1\leqq j\leqq s),\qquad |\mathbf{b}^T u^n|=1 \quad\text{and}\quad |p^n-\mathbf{A}u^n|\to 0 \quad (n\to\infty).$$

Next, we slightly modify the vectors p^n; define $q^n\in\mathbb{C}^{sm}$ by

$$q_j^n=-n^{-1}\hat{u}_j^n \quad\text{if } p_j^n=0, u_j^n\neq 0, \quad\text{and}\quad q_j^n=p_j^n \quad\text{otherwise.}$$

Then $q_j^n=0$ only if $u_j^n=0$, while we still have $\operatorname{Re}(q_j^n, u_n^j)\leqq 0$ $(1\leqq j\leqq s)$. By applying Lemma 2.4.7 of [15] it now follows that $u^n=\mathbf{Z}^n q^n$ for some $\mathbf{Z}^n\in\mathscr{D}_0$. Since $|p^n-q^n|\to 0$ $(n\to\infty)$, we see from (4.6) that there exist $q^n\in\mathbb{C}^{sm}$, $\mathbf{Z}^n\in\mathscr{D}_0$ such that

$$(4.7)\qquad |\mathbf{b}^T\mathbf{Z}^n q^n|=1,\qquad |(\mathbf{I}-\mathbf{A}\mathbf{Z}^n)\,q^n|\to 0 \quad (n\to\infty).$$

Finally, setting $w^n=(\mathbf{I}-\mathbf{A}\mathbf{Z}^n)\,q^n$, we obtain

$$(4.8)\qquad |\mathbf{b}^T\mathbf{Z}^n(\mathbf{I}-\mathbf{A}\mathbf{Z}^n)^{-1}w^n|=1 \quad\text{while } |w^n|\to 0 \quad (n\to\infty),$$

which is a contradiction to (4.3). □

Lemma 4.2. *Suppose the Runge Kutta method is BS-stable on* $\mathscr{F}_0$, $c_i-c_j\neq 0$ *if* $i\neq j$, *and* $b_j\neq 0$ *for all* j. *Then, for any real nonzero vector* $v\in\mathbb{R}^{sm}$ *there is an index* j, $1\leqq j\leqq s$, *such that* $(v_j, \mathbf{a}_j^T v)>0$.

Proof. Let $v \in \mathbb{R}^{sm}$, $v \neq 0$, and let $w \in \mathbb{R}^{sm}$ be such that $\mathbf{b}^T w \neq 0$ and $w_j = 0$ whenever $v_j = 0$ (such a w exists since all b_j are nonzero). We apply Lemma 4.1 to $u^n = v + i\lambda^n w \in \mathbb{C}^{sm}$ where $\lambda^n \in \mathbb{R}$, $\lambda^n \to 0$. Note that $v_j = 0$ implies $u_j^n = 0$ for all n. It follows that there is an index j for which $v_j \neq 0$ and

$$\limsup_{\lambda \to 0} |\mathbf{b}^T v + i\lambda \mathbf{b}^T w|^{-1} \{(v_j, \mathbf{a}_j^T v) + \lambda^2 (w_j, \mathbf{a}_j^T w)\} > 0, \tag{4.9}$$

and this implies $(v_j, \mathbf{a}_j^T v) > 0$. □

Theorem 4.3. *Let $\mu \geqq 0$, and suppose the Runge-Kutta method is such that $c_i - c_j \neq 0$ if $i \neq j$, and $b_j \neq 0$ for all j. Then*

$$BS\text{-stability on } \mathscr{F}_\mu \iff (2.7).$$

Proof. We only have to demonstrate the necessity of (2.7); sufficiency is well known, see [13, 11]. Since $\mathscr{F}_0 \subset \mathscr{F}_\mu$ for $\mu \geqq 0$, it follows from Lemma 4.2 that BS-stability on $\mathscr{F}_\mu$ implies

$$\text{for any } v \in \mathbb{R}^{sm},\ v \neq 0, \text{ there is a } j \text{ such that } \sum_{k=1}^{s} a_{jk}(v_j, v_k) > 0. \tag{4.10}$$

Let, for arbitrary nonzero $v \in \mathbb{R}^{sm}$, $S(v)$ be the $s \times s$ matrix with entries $s_{jk}(v) = (v_j, v_k)$. The matrix $S(v)$ belongs to the class $\mathscr{S}_0$ of nonzero, symmetric, positive semi-definite $s \times s$ matrices. Moreover, any matrix $S \in \mathscr{S}_0$ can be decomposed as

$$S = W^T W = S(w)$$

for some $s \times s$ matrix $W = [w_1, \ldots, w_s]$ and with $w = (w_1^T, \ldots, w_s^T)^T \in \mathbb{R}^{ss}$ (for example, by Cholesky factorization). Thus, if $m \geqq s$ then

$$\{S(v) : v \in \mathbb{R}^{sm},\ v \neq 0\} = \mathscr{S}_0. \tag{4.11}$$

Since m in (4.10) is arbitrary (it may be chosen equal to s), we see that BS-stability on $\mathscr{F}_\mu$ implies

$$\text{for any } S \in \mathscr{S}_0 \text{ there is a } j \text{ such that } \sum_{k=1}^{s} a_{jk} s_{jk} > 0. \tag{4.12}$$

By observing that

$$\sum_{k=1}^{s} a_{jk} s_{jk} = \sum_{k=1}^{s} a_{jk} s_{kj} = (AS)_{jj},$$

it follows from Theorem 1 in [1] that (2.7) holds. □

4.2. Remarks

For any $v \in \mathbb{R}^{sm}$, $m \in \mathbb{N}$, there exists a $w \in \mathbb{R}^{ss}$ such that $S(v)=S(w)$ (see the proof of Theorem 4.3). Hence, the algebraic condition (2.7) would follow already from BS-stability on $\mathscr{F}_0$ if only initial value problems with dimension $m=s$ were considered. Note further that $|\mathbf{b}^T v|^2 = b^T S(v) b$ and $|v_j|^2 = e_j^T S(v) e_j$ $(1 \leqq j \leqq s)$.

With these observations it can also be shown that Lemma 4.1 can be extended: for nonconfluent Runge-Kutta methods BS-stability on $\mathscr{F}_0$ is *equivalent* to the condition given in Lemma 4.1. This can be proved by first showing that if the method is not BS-stable on $\mathscr{F}_0$, then there are $u^n \in \mathbb{C}^{sm_n}$ with $m_n \in \mathbb{N}$, $\mathbf{b}^T u^n \neq 0$ such that (4.5) holds (this is fairly straightforward; use (4.3)), and subsequently noting that we can take $m_n \leqq s$. This result allows a characterization of BS-stability on $\mathscr{F}_0$ also in case some of the weights b_j are zero.

In a similar way as in Sect. 4.1 an algebraic criterion can be derived for BSI-stability on $\mathscr{F}_\mu$, a concept which requires that the difference between the internal vectors $|\tilde{Y}_i^n - Y_i^n|$ in (2.4b), (4.1b) can be uniformly bounded by $C|w|$ for $0 < h \leqq H$, $f \in \mathscr{F}_\mu$, with C, $H > 0$ only depending on μ (cf. [13, 11]). This concept is related to the conditioning of the algebraic equations in the Runge-Kutta method, rather than to the effect of perturbations on the numerical approximations. In case A is nonsingular – or, more general, if A has no zero column – it can be shown that BSI-stability on $\mathscr{F}_\mu$ is equivalent with (2.7). The sufficiency of (2.7) was proved already in [13]; the fact that (2.7) is also necessary for nonconfluent methods with nonsingular matrix A generalizes a related result of [9].

4.3. Proofs of Theorem 3.5 and Corollary 3.6

In order to prove Theorem 3.5 we consider a Runge-Kutta method with $c_i - c_j \neq 0$ if $i \neq j$, $b_i \neq 0$ for all i, and $a_j^T \neq 0$ if $c_j = 0$. Suppose the method is B-convergent on $\mathscr{F}_\mu$ for some $\mu \geqq 0$. Then it follows in particular, by considering (2.9) with $n=1$ for arbitrary $f \in \mathscr{F}_\mu$, that the method is B-consistent on $\mathscr{F}_\mu$, and this was shown in [16] to be equivalent to BS-stability on $\mathscr{F}_\mu$ (for nonconfluent methods with $a_j^T \neq 0$ in case $c_j = 0$). Theorem 4.3 thus shows that the algebraic condition (2.7) is satisfied.

Next, for proving Corollary 3.6, consider an irreducible Runge-Kutta method with $c_i - c_j \in \mathbb{Z}$ if $i \neq j$. Assume this method to be B-convergent on $\mathscr{F}_\mu$ for some $\mu \geqq 0$. Then Theorem 3.2 implies that we have algebraic stability. For an irreducible, algebraically stable method all rows of A and all weights b_i are nonzero, as can be seen from the material presented in [8]. Theorem 3.5 now shows that (2.7) holds as well. Theorem 3.4 completes the proof of Corollary 3.6.

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