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The Order of B-Convergence of Algebraically Stable Runge-Kutta Methods

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In [6] it was shown that for a class of semi-linear problems many high order Runge-Kutta methods have order of optimal B -convergence one higher than the stage order. In this paper we show that for the more general class of nonlinear dissipative problems such a result holds only for a small class of Runge-Kutta methods and that such methods have at most classical order 3.

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1. INTRODUCTION

Consider the numerical solution of a stiff initial value problem

$$U'(t) = f(t, U(t)) \quad (t \geq 0), \quad U(0) = u_0, \quad (1.1)$$

with $f: \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ and $u_0 \in \mathbb{R}^m$, by the Runge-Kutta method

$$u_{n+1} = u_n + h \sum_{i=1}^s b_i f(t_n + c_i h, y_i), \quad (1.2a)$$

$$y_i = u_n + h \sum_{j=1}^s a_{ij} f(t_n + c_j h, y_j) \quad (1 \leq i \leq s). \quad (1.2b)$$

The real parameters a_{ij}, b_i, c_i determine the method, s is the number of stages and $h > 0$ is the stepsize. The vectors u_n approximate $U(t)$ at $t_n = nh$ ($n \geq 1$).

Let $|\cdot|$ represent some norm on \mathbb{R}^m . In this paper we will be concerned with bounds for the global error of the form

$$|U(t_n) - u_n| \leq \gamma(t_n) \|U\|_{\bar{p}}^{\bar{p}} h^p \quad (\text{for } n \geq 1, 0 < h \leq \bar{h}) \quad (1.3)$$

where $\|U\|_{\bar{p}}^{\bar{p}} = \max\{|U^{(j)}(t)|: 0 \leq t \leq t_n, 1 \leq j \leq \bar{p}\}$, and where $\bar{p} \in \mathbb{N}, \bar{h} > 0$ and $\gamma: (0, \infty) \rightarrow (0, \infty)$ are not affected by stiffness (see [13] and [16]). Let \mathcal{P} be a class of initial value problems given by (1.1). A Runge-Kutta method given by (1.2) is said to be *convergent of order p on \mathcal{P}* if there exist $\bar{p} \in \mathbb{N}, \bar{h} > 0$ and $\gamma: (0, \infty) \rightarrow (0, \infty)$ such that (1.3) holds whenever $U \in C^{(\bar{p})}([0, \infty))$ is a solution of a problem in \mathcal{P} and the u_n are computed from (1.2). Here it is essential that (1.3) should hold uniformly on the class \mathcal{P} , not only for each problem individually.

Usually a method is said to have order p if it is convergent with order p on the class of problems where f satisfies a Lipschitz condition with a prescribed Lipschitz constant. We will refer to this as the

classical order.

In this note we consider the class of dissipative problems given by (1.1) where $m \in \mathbb{N}$, the norm $|\cdot|$ on \mathbb{R}^m is generated by an inner product $\langle \cdot, \cdot \rangle$, $u_0 \in \mathbb{R}^m$ and $f: \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ is a continuous function satisfying

$$\langle f(t, \tilde{u}) - f(t, u), \tilde{u} - u \rangle \leq 0 \quad (\text{for all } t \in \mathbb{R} \text{ and } \tilde{u}, u \in \mathbb{R}^m). \quad (1.4)$$

As in [13] convergence on this class of problems will be called *B-convergence*.

REMARK 1.1. Most well known Runge-Kutta methods satisfy $c_i \in [0, 1]$ (for $i = 1, 2, \dots, s$). For those methods which have some abscissas outside $[0, 1]$ the above definition of convergence on classes of problems should be slightly modified by taking in (1.3) $\|U\|_h^{\overline{p}} = \max\{|U^{(j)}(t)|: ch \leq t \leq t_{n-1} + \overline{ch}, 1 \leq j \leq \overline{p}\}$, where $\underline{c} = \min\{0, c_1, c_2, \dots, c_s\}$ and $\overline{c} = \max\{1, c_1, c_2, \dots, c_s\}$. If one the c_i is negative we thus assume that the solution U of (1.1) can be extended in a smooth way on a small interval to the left of the origin.

It is well known (see [4], [9], for example) that stability of the Runge-Kutta method for all dissipative problems is guaranteed by algebraic stability

$$BA + A^T B - bb^T \geq 0 \quad \text{and } B > 0, \quad (1.5)$$

where $A = (a_{ij})$ and $B = \text{diag}(b_1, b_2, \dots, b_s)$ are $s \times s$ matrices, $b = (b_1, b_2, \dots, b_s)^T$, and > 0 (≥ 0) refers to positive (semi-) definiteness. Furthermore, if there exists a diagonal matrix $D > 0$ such that

$$DA + A^T D > 0 \quad (1.6)$$

then the scheme given by (1.2) is not too sensitive for perturbations on the internal stages (1.2b) and the internal vectors y_i are uniquely determined by (1.2b) (see [8], [10] and [12]).

It is now well known that stiffness has a significant impact on the accuracy of a Runge-Kutta method. In their fundamental paper [13] FRANK, SCHNEID and UEBERHUBER proved *B-convergence* with order q for those methods satisfying the stability conditions (1.5), (1.6), where q is the *stage order* of the method, which is the largest integer such that the following two simplifying order conditions hold,

$$B(q): b^T c^{j-1} = 1/j \quad (j = 1, 2, \dots, q),$$

$$C(q): A c^{j-1} = c^j/j \quad (j = 1, 2, \dots, q)$$

with $c^j = (c_1^j, c_2^j, \dots, c_s^j)^T$. However, in recent numerical experiments (see [10], [17]) the order of *B-convergence* appeared to be $q + 1$. This phenomenon has been analyzed in [6] for semi-linear problems $U'(t) = QU(t) + g(t, U(t))$ where the stiffness is contained in the linear part and g satisfies a Lipschitz condition. (As we recently discovered similar results were already given in [7] for some linear problems). For many methods, with notable exception of the Gauss methods with $s \geq 2$ (see [11] and [15]), the order of convergence on this class of semi-linear problems can be shown to be $q + 1$. This is due to cancellation and damping out of the local errors which are of order $q + 1$ themselves.

In this note we prove that for the more general class of nonlinear, dissipative problems such an order $q + 1$ result only holds for some special methods, and that the order of *B-convergence* is usually equal to the stage order. The counterexample which will be used to prove this result has a Jacobian $D_u f(t, u)$ whose eigenvalues are not only very large in modulus, but are also extremely rapidly varying along the solution $U(t)$. This is the cause for the discrepancy between our results and the before mentioned numerical experiments, which were performed on problems with smoothly varying eigenvalues.

2. BOUNDS FOR THE ORDER OF B -CONVERGENCE

2.1. The convergence results

In this section we consider a fixed Runge-Kutta method (1.2) which satisfies (1.5), (1.6), and we let q be its stage order. Let $d = (d_1, d_2, \dots, d_s)^T \in \mathbb{R}^s$ and $d_0 \in \mathbb{R}$ be defined by

$$d = \frac{1}{q!} \left(\frac{1}{q+1} c^{q+1} - Ac^q \right), \quad d_0 = \frac{1}{q!} \left(\frac{1}{q+1} - b^T c^q \right). \quad (2.1)$$

We state the following results, which will be proved in the next section.

THEOREM 2.1. *Assume $c_i - c_j$ is not an integer for $1 \leq i < j \leq s$, and the order of B -convergence of method (1.2) is $q + 1$. Then $d_0 = 0$ and all components of d are equal.*

THEOREM 2.2. *Assume $d_0 = 0$ and all components of d are equal. Then method (1.2) (satisfying (1.5), (1.6)) is B -convergent with order $q + 1$.*

Since we know from [13] that the order of B -convergence equals at least the stage order, these theorems provide us with an if and only if result in case $c_i - c_j \notin \mathbb{Z}$ (for $i \neq j$). This latter condition does not hold for the methods based for example on Lobatto quadrature. For such methods $c_s - c_1 = 1$, and the situation seems to be more complicated.

2.2. Proof of the convergence results

Let $e = (1, 1, \dots, 1)^T \in \mathbb{R}^s$ and

$$K(Z) = 1 + b^T Z (I - AZ)^{-1} e, \quad (2.2)$$

$$L(Z) = d_0 + b^T Z (I - AZ)^{-1} d \quad (2.3)$$

for $Z = \text{diag}(\zeta_1, \zeta_2, \dots, \zeta_s)$ with $\zeta_i \in \mathbb{C}$. It is known (see, for example [4], [9]), that (1.5) holds iff $|K(Z)| \leq 1$ for all $Z = \text{diag}(\zeta_j)$ with $\text{Re} \zeta_j \leq 0$ ($1 \leq j \leq s$). Further we have

LEMMA 2.3. *$(1 - K(Z))^{-1} L(Z)$ is uniformly bounded for $Z = \text{diag}(\zeta_j)$ with $\text{Re} \zeta_j \leq 0$ ($1 \leq j \leq s$) iff $d_0 = 0$ and $d = ve$ for some $v \in \mathbb{R}$.*

PROOF. Let δ be a small positive parameter, and assume that $|\zeta_j| \leq \delta$ (for $j = 1, 2, \dots, s$). Then

$$1 - K(Z) = -b^T Z e + O(\delta^2),$$

$$L(Z) = d_0 + b^T Z d + O(\delta^2).$$

Obviously, $d_0 = 0$ is necessary for $(1 - K(Z))^{-1} L(Z)$ to be bounded. Assume $1 \leq j < k \leq s$ and consider the choice $\zeta_l = 0$ (for $l \neq j, k$), $\zeta_j = ib_k \delta$ and $\zeta_k = -ib_j \delta$. Then

$$b^T Z e = 0, \quad b^T Z d = i\delta b_j b_k (d_j - d_k),$$

and since (1.5) implies $b_j b_k > 0$ the necessity of $d_j = d_k$ also follows.

On the other hand, if $d_0 = 0$ and $d = ve$ we have $(1 - K(Z))^{-1} L(Z) \equiv -v$. \square

We now consider the test problem

$$U'(t) = \lambda(t)[U(t) - g(t)] + g'(t), \quad U(0) = g(0) \quad (2.4)$$

where $g: \mathbb{R} \rightarrow \mathbb{C}$ and $\lambda: \mathbb{R} \rightarrow \mathbb{C}$ is such that $\text{Re} \lambda(t) \leq 0$ (for all t). This complex scalar problem can be converted to a real, dissipative problem by identifying \mathbb{C} with \mathbb{R}^2 in the usual way. The solution of (2.4) is $U(t) = g(t)$ (for all t).

Let $Z_n = \text{diag}(z_1^{(n)}, z_2^{(n)}, \dots, z_s^{(n)})$, $z_i^{(n)} = h\lambda(t_n + c_i h)$ ($1 \leq i \leq s, n \geq 0$). Besides (1.2) we consider

$$U(t_{n+1}) = U(t_n) + h \sum_{i=1}^s b_i f(t_n + c_i h, Y_i) + \rho_n, \quad (2.5a)$$

$$Y_i = U(t_n) + h \sum_{j=1}^s a_{ij} f(t_n + c_j h, Y_j) + r_i^{(n)} \quad (1 \leq i \leq s) \quad (2.5b)$$

with $Y_i = U(t_n + c_i h)$. The ρ_n and $r_i^{(n)}$ are local (residual) errors. Subtraction of (1.2) from (2.5) leads to the following recursion for the global errors $\epsilon_n = U(t_n) - u_n$

$$\epsilon_{n+1} = K(Z_n)\epsilon_n + b^T Z_n (I - AZ_n)^{-1} r_n + \rho_n \quad (2.6)$$

where $r_n = (r_1^{(n)}, r_2^{(n)}, \dots, r_s^{(n)})^T$. By a Taylor series expansion it follows that

$$\rho_n = d_0 h^{q+1} U^{(q+1)}(t_n) + h^{q+2} R_0^{(n)}, \quad (2.7a)$$

$$r_n = dh^{q+1} U^{(q+1)}(t_n) + h^{q+2} R_n \quad (2.7b)$$

where $R_n = (R_1^{(n)}, R_2^{(n)}, \dots, R_s^{(n)})^T \in \mathbb{C}^s$ and $|R_i^{(n)}| \leq c \max_{0 \leq \theta \leq 1} |U^{(q+2)}(t_n + \theta c_i h)|$ ($0 \leq i \leq s; c_0 := 1$) for some $c > 0$ which only depends on the coefficients of the method. With these relations we now can prove the theorems of section 2.1.

Proof of theorem 2.1. Assume either $d_0 \neq 0$ or some components of d differ. Then, in view of lemma 2.3, we can choose for any $C > 0$ a matrix $Z = \text{diag}(\zeta_1, \zeta_2, \dots, \zeta_s)$ with $\text{Re} \zeta_j < 0$ ($1 \leq j \leq s$) and $|(1 - K(Z))^{-1} L(Z)| > C$. By the algebraic stability condition we know $|K(Z)| < 1$.

Let $h > 0$ be a stepsize. Consider testproblem (2.4) with $g(t) = t^{q+1}/(q+1)!$ and $\lambda: \mathbb{R} \rightarrow \mathbb{C}$ such that $\text{Re} \lambda(t) \leq 0$ (for all t) and $h\lambda(t_n + c_i h) = \zeta_i$ (for $1 \leq i \leq s$ and all $n \geq 0$) with the ζ_i as above. (The problem thus depends on the stepsize). From (2.6), (2.7) it follows that the global errors satisfy

$$\epsilon_n = K(Z)\epsilon_{n-1} + h^{q+1} L(Z),$$

from which we obtain

$$\epsilon_n = (1 - K(Z))^n (1 - K(Z))^{-1} L(Z) h^{q+1}.$$

Now let $h \downarrow 0$ while $t_n = nh$ and the ζ_j are fixed. Then

$$h^{-(q+1)} |\epsilon_n| \rightarrow |(1 - K(Z))^{-1} L(Z)| > C.$$

Since C can be taken arbitrarily large, the order is not $q+1$. \square

Proof of theorem 2.2. This proof is a rather straightforward generalization of an idea used by KRAAIJEVANGER [15] for the implicit midpoint rule. We only present the proof for the testproblem (2.4) which contains already all essential difficulties.

Assume $d_0 = 0$ and $d = \nu e$ for some $\nu \in \mathbb{R}$. By (2.6), (2.7) we have

$$\epsilon_{n+1} = K(Z_n)\epsilon_n + L(Z_n)h^{q+1}U^{(q+1)}(t_n) + \sigma_n$$

where

$$\sigma_n = h^{q+2}(b^T Z_n (I - AZ_n)^{-1} R_n + R_0^{(n)}).$$

From (1.6) we can conclude that all elements of the transposed vector $b^T Z (I - AZ)^{-1}$ are uniformly bounded for $Z = \text{diag}(\zeta_j)$, $\text{Re} \zeta_i \leq 0$ (BS-stability [12], [14; lemma 2.4.3]). Therefore

$$|\sigma_n| \leq \gamma_1 h^{q+2} \|U\|_{n+1}^{(q+2)}$$

for some $\gamma_1 > 0$ which only depends on the coefficients of the method. Define for all $n \geq 0$

$$\hat{\epsilon}_n = \epsilon_n + \nu h^{q+1} U^{(q+1)}(t_n).$$

Since, by our assumption, $L(Z_n) = -\nu(1 - K(Z_n))$ it follows that

$$\hat{\epsilon}_{n+1} = K(Z_n)\hat{\epsilon}_n + \hat{\sigma}_n$$

with

$$\hat{\sigma}_n = \sigma_n + \nu h^{q+1} (U^{(q+1)}(t_{n+1}) - U^{(q+1)}(t_n)),$$

$$|\hat{\sigma}_n| \leq \gamma_2 h^{q+2} \|U\|_{t_{n+1}}^{(q+2)}$$

for some $\gamma_2 > 0$, again only depending on the coefficients of the method. By using $|K(Z_n)| \leq 1$ we obtain in a standard way

$$|\hat{\epsilon}_n| \leq \gamma_2 t_n h^{q+1} \|U\|_{t_n}^{(q+2)} \quad (\text{for all } n \geq 0),$$

and since $|\hat{\epsilon}_n - \epsilon_n| \leq \nu h^{q+1} \|U\|_{t_n}^{(q+1)}$ the order $q+1$ result follows. \square

3. EXAMPLES

In this section we examine those Runge-Kutta methods satisfying (1.5) and (1.6) which have an order of B -convergence one more than the stage order q . We saw in section 2 that such methods should satisfy $C(q)$ and $B(q+1)$ with

$$\frac{1}{q!} \left(\frac{1}{q+1} c^{q+1} - A c^q \right) = \nu e, \quad \nu \neq 0. \quad (3.1)$$

We first note that for any Runge-Kutta method satisfying $C(q), B(q+1)$ and (3.1) a classical order of $q+2$ is not attainable, since a necessary condition for a method to have order $q+2$ is

$$b^T (A c^q - c^{q+1} / (q+1)) = 0,$$

which from (3.1) is equivalent to

$$\nu b^T e = 0.$$

This is impossible since $\nu \neq 0$ and $b^T e = 1$. In addition one can show that, if $s \geq 2$, (3.1) cannot hold for $q=s$ so that the maximum classical order of an s -stage Runge-Kutta method satisfying (3.1) is s , in which case $C(s-1)$ and $B(s)$ hold.

Furthermore if we now require such methods to satisfy (1.5) and (1.6) we can obtain further restrictions on the maximum classical order. Burrage [3] has shown that if a Runge-Kutta method satisfying $B(2)$ and $C(q)$ is algebraically stable then its classical order must be $2q-1$. Thus we can conclude

THEOREM 3.1 *Any Runge-Kutta method satisfying (1.5), (1.6), $d_0=0, d=\nu e, \nu \neq 0$ has classical order at most 3.*

We conclude this paper with three examples of methods which satisfy the conditions of Theorem 3.1. Since the maximum classical order is at most 3 we will study only those methods which satisfy $C(s-1)$ and $B(s)$ for $s=2$ and $s=3$. Furthermore, we will restrict our attention to either diagonally implicit or singly-implicit methods since these methods are more important in terms of cheap implementation than other classes of Runge-Kutta methods.

EXAMPLE 1. It is easy to show (see BURRAGE [3], for example) that the family of algebraically stable two-stage DIRKs with classical order 2 is given by

$$\begin{array}{c|cc} \lambda & \lambda & \\ 1-\lambda & 1-2\lambda & \lambda \\ \hline & 1/2 & 1/2 \end{array} \quad , \lambda \geq 1/4.$$

If $\lambda=1/4$ or $\lambda=1/2$ then (3.1) holds and the order of B -convergence is 2. We observe that this can also be concluded from KRAAIJEVANGER [15] since the method with $\lambda=1/2$ reduces to the implicit midpoint rule and the method with $\lambda=1/4$ can be considered as consisting of two implicit midpoint rule steps. If $\lambda=(k+1)/2$ where k is a positive integer we can not apply Theorem 2.1 and so we can only conclude from our results that the order of B -convergences is at least one.

EXAMPLE 2. The family of 2-stage singly-implicit methods satisfying $C(1)$ and $B(2)$ is given by (see [1])

$$\begin{array}{c|cc} c_1 & \begin{bmatrix} 1 & c_1 \\ 1 & c_2 \end{bmatrix} & \begin{bmatrix} 0 & -\lambda^2 \\ 1 & 2\lambda \end{bmatrix} & \begin{bmatrix} 1 & c_1 \\ 1 & c_2 \end{bmatrix}^{-1} \\ c_2 & & & \\ \hline & \frac{c_2-1/2}{c_2-c_1} & \frac{1/2-c_1}{c_2-c_1} & \end{array} , c_1 \neq c_2. \quad (3.2)$$

From [3] and [10; sect. 5.10] it follows that (1.5), (1.6) are fulfilled iff

$$\lambda \geq 1/4, \quad c_1 c_2 - \frac{1}{2}(c_1 + c_2) + \lambda^2 - \lambda + \frac{1}{2} = 0.$$

If, in addition, $c_2 + c_1 = 4\lambda$ then (3.1) is satisfied with $q=1$ and $\nu=3(\lambda^2 - \lambda + 1/6)/2$. Thus if

$$\lambda \geq 1/4, \quad c_1 = 2\lambda \pm (5\lambda^2 - 3\lambda + 1/2)^{1/2}, \quad c_2 = 4\lambda - c_1 \quad (3.3)$$

then the family of methods given by (3.2) is algebraically stable with order of B -convergence 2. We note that in the case $\lambda=(3+\sqrt{3})/6$ the stage order is 2, but the order of B -convergence is still only 2.

EXAMPLE 3. The family of 3-stage singly-implicit methods of order 3 satisfying $C(2)$ and $B(3)$ is given by (see [1])

$$\begin{array}{c|ccc} c_1 & \begin{bmatrix} 1 & c_1 & c_1^2 \\ 1 & c_2 & c_2^2 \\ 1 & c_3 & c_3^2 \end{bmatrix} & \begin{bmatrix} 0 & 0 & 2\lambda^3 \\ 1 & 0 & -6\lambda^2 \\ 0 & \frac{1}{2} & 3\lambda \end{bmatrix} & \begin{bmatrix} 1 & c_1 & c_1^2 \\ 1 & c_2 & c_2^2 \\ 1 & c_3 & c_3^2 \end{bmatrix}^{-1} \\ c_2 & & & \\ c_3 & & & \\ \hline & b_1 & b_2 & b_3 \end{array} , c_1 \neq c_2 \neq c_3 \quad (3.4)$$

where

$$b_1 = \frac{c_2 c_3 - (c_2 + c_3)/2 + 1/3}{(c_1 - c_2)(c_1 - c_3)}, \quad b_2 = \frac{c_1 c_3 - (c_1 + c_3)/2 + 1/3}{(c_2 - c_1)(c_2 - c_3)}, \quad b_3 = 1 - b_1 - b_2.$$

From [3] and [10; sect. 5.10] it can be seen that the conditions (1.5), (1.6) hold if

$$\begin{aligned} g_1 &= -2\lambda^3 + 3\lambda^2 - \lambda + 1/12 \geq 0, \\ x_1 &= 4\lambda^3/3 - 3\lambda^2 + 6\lambda/5 - 1/9 - 12\lambda^2 g_1 + 6\lambda g_2 \geq 0, \\ x_2 &= \lambda^3 - 2\lambda^2 + 3\lambda/4 - 1/15 + g_2/2 + 3\lambda g_1, \\ g_1 x_1 &> x_2^2, \\ g_2 &\geq 12g_1^2 + 2g_1 - 1/180 \end{aligned}$$

where

$$g_1 = \int_0^1 p(x) dx, \quad g_2 = \int_0^1 xp(x) dx + (c_1 + c_2 + c_3)g_1, \quad p(x) = \prod_{j=1}^3 (c_j - x).$$

If, in addition

$$c_1 + c_2 = 9\lambda - c_3, \quad c_1 c_2 = 18\lambda^2 - 9\lambda c_3 + c_3^2, \quad c_3^3 - 9\lambda c_3^2 + 18\lambda^2 c_3 = 6\lambda^3 + 4g_1 \quad (3.5)$$

then (3.1) holds with $q=2$ and $\nu=2g_1/3$.

Some numerical computations show that the family of methods given by (3.4) and (3.5) is algebraically stable with order of B -convergence 3 if

$$\lambda \in [-.3518, .9458].$$

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