Rational Runge–Kutta methods are not suitable for stiff systems of ODEs *

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Abstract: The present paper shows that rational RK-methods are not very appropriate to solve stiff differential equations. The CA₀-stability (i.e. componentwise contractivity) is defined and the non-existence of CA₀-stable rational RK-methods is demonstrated. Furthermore it is shown that the stepsizes which can be expected when solving a stiff differential system with a rational or with an explicit linear RK-method are of the same order of magnitude.

Keywords: Rational Runge-Kutta method, stiff ODEs, A-stability

1. Introduction

We consider the system of differential equations

$$y' = f(y), \quad y(x_0) = y_0,$$
 (1.1)

where $y_1, y_0, f(y)$ are elements of \mathbb{R}^n (or \mathbb{C}^n). For solving this initial value problem numerically, Wambecq [5] has proposed rational Runge-Kutta methods. These are nonlinear methods defined by

$$y_{1} = y_{0} + \sum_{i=1}^{s} \sum_{j=1}^{i} w_{ij} \frac{g_{i}g_{j}}{\sum_{k=1}^{s} b_{k}g_{k}},$$

$$g_{i} = hf\left(y_{0} + \sum_{j=1}^{i-1} a_{ij}g_{j}\right), \quad i = 1, \dots, s,$$
(1.2)

where h is the stepsize and a_{ij} , w_{ij} , b_k are real parameters. With (a, b) the scalar product of two

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vectors a and b, the product-quotient ab/d is defined for complex or real vectors in the following way:

$$\frac{ab}{d} = \frac{a \operatorname{Re}(b, d) + b \operatorname{Re}(d, a) - d \operatorname{Re}(a, b)}{(d, d)}.$$
(1.3)

Further, the conditions

$$\sum_{k=1}^{3} b_k g_k \neq 0 \tag{1.4}$$

and

$$\sum_{i=1}^{s} b_i = 1$$
 (1.5)

will be assumed. (1.4) ensures that the productquotient (1.3) is well defined and (1.5) is chosen in order to eliminate the ambiguity of the multiplicative constant in numerator and denominator of (1.2). Moreover, throughout this paper, method (1.2) will be supposed to be of order ≥ 1 , i.e. (see [5])

$$\sum_{i=1}^{s} \sum_{j=1}^{t} w_{ij} = 1.$$
 (1.6)

The methods of type (1.2) have been introduced for the numerical solution of stiff differential systems. Due to the fact that they are explicit and do not require the computation and the storage of the Jacobian of f, they are easy implementable and seem to be of great interest.

The aim of this work is to emphasize that in fact these methods are not very appropriate to solve stiff systems of differential equations.

For this purpose, we first motivate the introduction of a new stability criterion, called CA_0 stability (i.e. componentwise contractivity, see Section 2). Then, in Section 3, we show that the stepsizes which can be expected when solving a stiff differential system with a rational or with an explicit linear RK-method are of the same order of magnitude. In Section 4 we prove the non-existence of CA₀-stable rational RK-methods of type (1.2). Finally, in Section 5, we show that 2-stage methods of type (1.2) possess the componentwise contractivity property only for non-stiff problems.

2. The CA₀-stability

In [2] Hairer showed that the stability behaviour of method (1.2) for the linear equation

$$y' = Ay, \quad y(x_0) = y_0,$$
 (2.1)

where A is assumed to be a constant $n \times n$ matrix reducible to a diagonal form by a unitary transformation, is equivalent to its behaviour for the diagonal system

$$y' = \Lambda y, \quad y(x_0) = y_0, \quad \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n).$$

(2.2)

Due to the nonlinearity, applying (1.2) to the system (2.2), we get

$$y_1 = Ry_0,$$

 $R = \text{diag}(r_1, \dots, r_n) = I + \text{diag}(q_1, \dots, q_n),$ (2.3)

where the q_i are rational functions depending on all the $z_j \coloneqq h\lambda_j$ and on the initial vector y_0 , i.e. (with $z = (z_1, \dots, z_n)^T$) we have

$$q_i = q_i(z; y_0), \qquad R = R(z; y_0).$$
 (2.4)

This fact shows that we cannot restrict the stability analysis to a scalar test equation and has lead Hairer to define the concept of A-stability in the following way:

Definition 2.1. A subset D of the complex plane C is called a *stability region* of the method (1.2) if and only if in every dimension n the application of (1.2) to a system (2.2) with $h\lambda_i \in D$, i = 1, ..., n, and an arbitrary initial vector $y_0 \in \mathbb{C}^n$ yields a numerical solution y_1 satisfying $||y_1|| \leq ||y_0||$ (in the Euclidean norm).

Definition 2.2. A method (1.2) is A_0 -stable if and only if $\{x \in \mathbb{R} \mid x \leq 0\}$ is a stability region, *A*-stable if and only if $\{z \in \mathbb{C} \mid \text{Re}(z) \leq 0\}$ is a stability region.

Within this frame, a complete characterization of the A-stability of methods (1.2) with s = 2 has been given by Calvo and Mar-Quemada [1]. For instance, they have proved that the method

$$y_{1} = y_{0} + \frac{g_{1}g_{1}}{2g_{1} - g_{2}},$$

$$g_{1} = hf(y_{0}), \qquad g_{2} = hf(y_{0} + g_{1}),$$
(2.5)

is A-stable.

But, due to the dependence of R in y_0 , the property

$$\|R(z; y_0) y_0\| \le \|y_0\| \tag{2.6}$$

is not sufficient to ensure

$$\|R(z; y_0)\| \le 1. \tag{2.7}$$

To illustrate this, we consider (2.5) applied to the two-dimensional system

$$y' = \Lambda y, \qquad y_0 = (1, 10^{-\mu})^{\mathrm{T}},$$

 $\Lambda = \mathrm{diag}(-1, \lambda_2), \qquad (2.8)$

with stepsize h = 1. As a first example, we take $\lambda_2 = -4$ and $\mu = 1$. This leads to the numerical solution $y_1 = (0.59, 0.11)^T$, i.e. $r_1 = 0.59$ and $r_2 = 1.1$. The second example is obtained by setting $\lambda_2 = -10^6$ and $\mu = 7$. In this case we obtain $y_1 = (0.999998, 0.999995, 10^{-5})^T$, $r_1 = 0.999998$ and $r_2 = 99.9995$. Besides the fact that (2.7) is not satisfied though the method is A-stable, we observe here that the component of the solution corresponding to the smallest eigenvalue (i.e. λ_2) is increasing instead of decreasing faster as the other component as is the case for the exact solution.

The major consequence of this lack of componentwise contractivity is that the numerical solution of (2.2) can possess completely wrong components despite of the A-stability of the applied method. However this bad property can not only be 'catastrophic' for the accuracy of the numerical solution but also for the automatic error estimate and consequently for the automatic stepsize adjustment, since the usual algorithms are based on the components of the local truncation error and of the solution y_1 .

For these reasons, we think it is crucial that a nonlinear method possesses the componentwise contractivity property.

Definition 2.3. A method (1.2) is called CA_0 -stable if and only if in every dimension *n* the application of (1.2) to a system $y' = \Lambda y$, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ with $h\lambda_i \in \{x \in \mathbb{R} \mid x \leq 0\}$ and an arbitrary initial vector $y_0 \in \mathbb{C}^n$ yields rational functions r_i satisfying $|r_i| \leq 1, i = 1, \dots, n$.

Observe that CA_0 -stability implies A_0 -stability.

3. Numerical behaviour

Before we study the CA_0 -stability of rational RK-methods, we want to point out some experimental results.

For the numerical tests, we have used the 2-stage A₀-stable method of order 2 embedded in a method of order 3 given by Hairer [2] and the A-stable method (2.5) of order 1 embedded in a method of order 2 (a method which has been derived in the same way as Hairer's method). Though it has no influence on the next developments, we have to remark here that the embedding used in these two cases was not very appropriate because of the different behaviour of the stability functions $R(h\lambda)$; y_0) and $\tilde{R}(h\lambda; y_0)$ (computed for $y' = \lambda y$) when $h\lambda$ tends to infinity. The algorithm used for the automatic stepsize control is described in [2]. All the computations have been done on the IBM 370-168 of the University of Heidelberg using double precision arithmetic.

The problems used in most of the tests we have done are the pure diffusion (c = 0) and the diffusion-convection (c = 25) problem (Hindmarsh-Byrne [3])

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - c \cdot \frac{\partial u}{\partial x}, \quad 0 \le x \le 1, t \ge 0,$$
$$u(0, t) = 1, \qquad \frac{\partial u}{\partial x}(1, t) = 0, \quad t > 0,$$
$$u(x, 0) = 0, \quad 0 < x < 1.$$
(3.1)

The stepsizes chosen by these programs are always very small and comparable with the steplengths which would have been chosen by a program using an explicit linear RK-method. The only exception we have found is when the stationary solution has nearly been attained and these observations completely agree with the results of Hairer–Wanner mentioned in [2].

To explain these small stepsizes, consider the system

$$y' = \Lambda y, \qquad \Lambda = \operatorname{diag}(\lambda_1, \lambda_2),$$

with $\lambda_1, \lambda_2 \in \mathbb{R}$ and $\lambda_1 \ll \lambda_2 < 0$ (3.2)

and let $(y_i)_{i \ge 1}$ be the sequence of numerical solution obtained from $y_0 \in \mathbb{R}^2$ by iteration of a rational RK-method with a fixed stepsize *h*. Observe that the sequence of quotient y_{2i}/y_{1i} can converge to a constant value which can be interpreted as a

fix-point of the iteration

$$\frac{y_{2,i+1}}{y_{1,i+1}} = \frac{r_2(h\lambda_1, h\lambda_2; y_{1i}, y_{2i})}{r_1(h\lambda_1, h\lambda_2; y_{1i}, y_{2i})} \cdot \frac{y_{2i}}{y_{1i}},$$
(3.3)

where r_1 and r_2 are the stability functions of the method (see Section 2) and the quotient

$$\frac{r_2(h\lambda_1, h\lambda_2; y_{1i}, y_{2i})}{r_1(h\lambda_1, h\lambda_2; y_{1i}, y_{2i})}$$
(3.4)

in fact only depends of $h\lambda_1$, $h\lambda_2$ and of the quotient $(y_{2i}/y_{1i})^2$ (see Section 5). In consequence, after a minimum number of iterations, the two components of the numerical solution converge to zero with the same rate of convergence $(y_{2i}/y_{1i} = \text{const.})$. (Observe that this is not the case for the true solution!). This implies that the two components of the numerical solution at each iteration play a role in the estimation of the error until we can neglect them.

Thus, for reasons of accuracy, the steplength is forced to stay small. We remark that we have here an inconvenience comparable to the condition

$$h|\lambda_i| < \text{const}, \quad i = 1, \dots, n, \tag{3.5}$$

which forces $h\lambda_i$ to stay in the stability region in the case of an explicit linear RK-method.

It seems that a possibility to eliminate this inconvenience is to rescale at each step the system we integrate, i.e. to replace y by Dy where D is a diagonal matrix such that all the components of Dy_0 are of the same order of magnitude (unless the null ones). But now the problem is that the reduction to diagonal form by a unitary transformation of a scaled (non-diagonal) problem yields a non scaled problem in general. And, consequently, we cannot reduce the stability analysis of this algorithm to diagonal scaled systems.

4. Rational RK-methods are not CA₀-stable

For reason of convenience, we now shall use the matrix

$$Z \coloneqq \operatorname{diag}(z_1, \dots, z_n) = h\Lambda \tag{4.1}$$

instead of the vector z.

Using this notation, we have:

Lemma 4.1. The application of (1.2) to the problem (2.2) yields the following expressions for the vectors

$$g_i \text{ and } b \coloneqq \sum_{i=1}^{s} b_i g_i:$$

$$g_i = P_i(Z) y_0, \quad b = P(Z) y_0, \quad (4.2)$$

where

$$P_{i}(Z) = \sum_{j=1}^{i} \Phi_{j}^{i} Z^{j}, \quad i = 1, \dots, s,$$

$$P(Z) = \sum_{j=1}^{s} \Phi_{j} Z^{j},$$
(4.3)

and

$$\Phi_{j}^{i} = \begin{cases} 1 & \text{for } j = 1 \text{ and } i = 1, \dots, s, \\ \sum_{l_{1}, l_{2}, \dots, l_{j-1}} a_{il_{1}} a_{l_{1}l_{2}} \dots a_{l_{j-2}l_{j-1}} \\ \text{for } j = 2, \dots, s \text{ and } i = j, \dots, s, \\ 0 & \text{otherwise}, \end{cases}$$

$$(4.4)$$

$$\Phi_j = \sum_{i=1}^s b_i \Phi_j^i$$
(4.5)

(with $a_{ij} = 0$ for j > i).

Proof. The result is obtained by a simple induction argument. \Box

Remark. The readers who are familiar with the trees introduced by Butcher in the case of linear methods will observe that Φ_j is simply the polynomial of degree 1 in b_i and j-1 in a_{ik} associated with the only tree of order j without ramifications.

From now on, we shall suppose Z real.

We have already seen in Section 2 that the numerical solution of (2.2) obtained by the use of (1.2) is of the form

$$y_1 = R(Z; y_0) y_0,$$
 (4.6)

where

$$R = \text{diag}(r_1, \dots, r_n)$$

with $r_i(Z; y_0) = 1 + q_i(Z; y_0).$ (4.7)

Lemma 4.2. The rational function $q_j(Z; y_0)$ defined in (4.7) is given by

$$q_j(Z; y_0) = \frac{N_j(Z; y_0)}{D(Z; y_0)}, \qquad (4.8)$$

where

$$N_{j}(Z; y_{0}) = \sum_{K=1}^{s} \left(\sum_{L=2}^{2s} \alpha_{KL}(Z^{L}y_{0}, y_{0}) \right) z_{j}^{K}, \quad (4.9)$$

$$D(Z; y_0) = (P(Z)y_0, P(Z)y_0), \qquad (4.10)$$

and

$$\alpha_{KL} = \sum_{M=1}^{s} \Phi_{L-M} \left(\sum_{i=1}^{s} \sum_{j=1}^{s} w_{ij} \left(\Phi_{K}^{i} \Phi_{M}^{j} + \Phi_{M}^{i} \Phi_{K}^{j} \right) \right) - \Phi_{K} \sum_{M=1}^{s} \sum_{i=1}^{s} \sum_{j=1}^{s} w_{ij} \Phi_{M}^{i} \Phi_{L-M}^{j}$$
(with $w_{ij} = 0$ for $j > i$).
(4.11)

Proof. Simple calculations taking into account Lemma 4.1.

This allow us to prove the main result:

Theorem 4.3. There exists no CA_0 -stable rational RK-methods of type (1.2).

Proof. Choosing n = 2 and $y_0 = (0, 1)^T$, (4.9) and (4.10) become:

$$N_1(Z; y_0) = \sum_{K=1}^{s} \left(\sum_{L=2}^{2s} \alpha_{KL} z_2^L \right) z_1^K$$
(4.12)

and

$$D(Z; y_0) = \left(\sum_{j=1}^{s} \Phi_j z_2^{j}\right)^2.$$
 (4.13)

Suppose now that the method is CA₀-stable. This implies that

$$-2D(Z; y_0) \leq N_1(Z; y_0) \leq 0$$

for all real negative z_1 and z_2 . (4.14)

But since, for our particular choice, $D(Z; y_0)$ is independent of z_1 and $N_1(Z; y_0)$ is a polynomial in z_1 without constant term, (4.14) is equivalent to

$$N_1(Z; y_0) = 0 \quad \forall z_1 \le 0, \, \forall z_2 \le 0.$$
 (4.15)

Therefore we must have (see (4.12)):

$$\alpha_{KL} = 0 \quad \forall K, L. \tag{4.16}$$

Observing now that, because of (1.5) and (1.6), $\alpha_{12} = 1$ (4.17)

we have obtained the contradiction. \Box

5. 2-stage rational RK-methods and CA₀-stability

In this section we want to show that 2-stage rational RK-methods are componentwise contrac-

tive only when the problem to be integrated is non-stiff. For this study, we need the following general result:

Proposition 5.1. Let Z be a real diagonal $n \times n$ matrix and $y_0 \in \mathbb{R}^n \setminus \{0\}$. Let P_{kj} be the permutation matrix which exchange the kth and jth columns (or rows). Then

$$q_k(Z; y_0) = q_j(P_{kj}ZP_{kj}; P_{kj}y_0).$$

Proof. This result is easily seen by combining (1.2) with (4.2) and (4.3) or from (4.9), (4.10) and (4.3).

We shall now restrict our considerations to consistent 2-stage rational RK-methods, i.e. methods with s = 2, $b_1 + b_2 = 1$ and $w_{11} + w_{21} + w_{22} = 1$. Without restriction of the generality, we can suppose $a_{21} \neq 0$ (otherwise we have the explicit Euler method: 1-stage and linear!).

Only methods of the form

$$y_{1} = y_{0} + \frac{b_{1}b_{1}}{b_{1}g_{1} + b_{2}g_{2}},$$

$$g_{1} = hf(y_{0}), \qquad g_{2} = hf(y_{0} + a_{21}g_{1}) \qquad (5.1)$$

with $b_{1} + b_{2} = 1$ and $\Phi_{2} = b_{2}a_{21} \neq 0,$

can be CA₀-stable (since CA₀-stability implies A₀-stability, this is a consequence of [2, Proposition 4] for $b_2 \neq 0$; the case $b_2 = 0$ can be eliminated by showing that a necessary condition for CA₀-stability is then $w_{11} + w_{21} + w_{22} = 0$).

We shall also restrict the study of the stability of methods of the form (5.1) to two-dimensional differential systems of the form (2.2) (i.e. n = 2). In this case we get a rational function $q_1(Z; y_0)$ (or equivalently $r_1(Z; y_0)$) given by (see Lemma 4.2):

$$q_1(Z; y_0) = \frac{N_1(Z; y_0)}{D(Z; y_0)},$$
(5.2)

where

$$N_{1}(Z; y_{0}) = y_{10}^{2} z_{1}^{3} (1 + \Phi_{2} z_{1}) + y_{20}^{2} z_{1} z_{2}^{2} [1 + \Phi_{2} (2 z_{2} - z_{1})], \quad (5.3)$$

$$D(Z; y_0) = y_{10}^2 z_1^2 (1 + \Phi_2 z_1)^2 + y_{20}^2 z_2^2 (1 + \Phi_2 z_2)^2.$$
(5.4)

We have the following necessary condition for CA_0 -stability (i.e. the condition for scalar equations; compare with [2]):

Lemma 5.2. If (5.1) is CA_0 -stable, then $\Phi_2 \leq -\frac{1}{2}$.

The main result is now:

Theorem 5.3. Let n = 2, let α be a real positive number and

$$Z_{\alpha} = z_1 \begin{pmatrix} 1 & 0 \\ 0 & \alpha \end{pmatrix}.$$

Suppose $\Phi_2 \leq -\frac{1}{2}$. Then
(i) $r_1 \begin{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & z_2 \end{pmatrix}; y_0 \end{pmatrix} = 1$

for all $y_0 \in \mathbb{R}^2 \setminus \{0\}$ and all real $z_2 < 0$, (ii) $|r_1(Z_{\alpha}; y_0)| \leq 1$ for all $y_0 \in \mathbb{R}^2 \setminus \{0\}$ and all real $z_1 < 0$ if and only if $\alpha = 0$ or $\alpha \geq \frac{1}{2}$. Moreover, $|r_1(Z_{\alpha}; y_0)| > 1$ if $0 < \alpha < \frac{1}{2}$,

$$z_1 < [\Phi_2(1-2\alpha)]^{-1}$$

and

$$\alpha^2 y_{20}^2 > y_{10}^2 (1 + \Phi_2 z_1) / ((1 - 2\alpha) \Phi_2 z_1 - 1)$$

Before proving Theorem 5.3, we want to state its main consequence, Corollary 5.4 (also see Fig. 1).

Corollary 5.4. Let n = 2, $\alpha > 0$ and

$$Z_{\alpha}=z_1\begin{pmatrix}1&0\\0&\alpha\end{pmatrix}.$$

Suppose $\Phi_2 \leq -\frac{1}{2}$. Then, with the notations of (4.1) and (4.6) we have:

(i) $||R(Z; y_0)|| = 1$ for all $y_0 \in \mathbb{R}^2 \setminus \{0\}$ and all



Fig. 1. The set described in Corollary 5.4 (tg $\gamma = \frac{1}{2}$).

diagonal matrices Z such that $z_1 \leq 0$, $z_2 \leq 0$ and $z_1 \cdot z_2 = 0$,

(ii) $||R(Z_{\alpha}; y_0)|| \leq 1$ for all $y_0 \in \mathbb{R}^2 \setminus \{0\}$ and all real $z_1 < 0$ if and only if $\frac{1}{2} \leq \alpha \leq 2$.

Proof. Simple application of Theorem 5.3 and Proposition 5.1. \Box

Thus for non-scalar two-dimensional problems of the form (2.2) with negative real eigenvalues λ_i , the method (5.1) is componentwise contractive for all h > 0 if and only if $\frac{1}{2} \leq \lambda_2/\lambda_1 \leq 2$, i.e. essentially when the problem is non-stiff.

We now give the proof of Theorem 5.3.

Proof of Theorem 5.3. From (4.6), (4.7), (5.2), (5.3) and (5.4) we easily obtain assertion (i) and assertion (ii) for the case $\alpha = 0$.

Now suppose $z_1 < 0$ and $\alpha > 0$. Then (5.3) and (5.4) become

$$N_{1}(Z_{\alpha}; y_{0}) = z_{1}^{3} \{ y_{10}^{2} (1 + \Phi_{2} z_{1}) + y_{20}^{2} \alpha^{2} [1 + \Phi_{2} (2\alpha - 1) z_{1}] \}, \quad (5.5)$$

$$D(Z_{\alpha}; y_0) = z_1^2 \left\{ y_{10}^2 (1 + \Phi_2 z_1)^2 + y_{20}^2 \alpha^2 (1 + \Phi_2 \alpha z_1)^2 \right\}$$
(5.6)

and we see, since $\Phi_2 \leq -\frac{1}{2}$:

 $q_1(Z_{\alpha}; y_0) \leq 0$

for all
$$y_0 \in \mathbb{R}^2 \setminus \{0\}$$
 and all $z_1 < 0$ if $\alpha \ge \frac{1}{2}$,
 $a_1(\mathbf{Z} : \mathbf{v}_1) \ge 0$

$$(q_1(Z_{\alpha}, y_0)) = 0$$

if $0 < \alpha < \frac{1}{2} < \alpha < [\Phi(1 - 2\alpha)]^{-1}$

and
$$\alpha^2 y_{20}^2 > y_{10}^2 (1 + \Phi_2 z_1) / ((1 - 2\alpha) \Phi_2 z_1 - 1).$$

It remains therefore to prove

$$q_1(Z_{\alpha}; y_0) \ge -2$$

for all $y_0 \in \mathbb{R}^2 \setminus \{0\}$ and all $z_1 < 0$ if $\alpha \ge \frac{1}{2}$.

But
$$q_1(Z_{\alpha}; y_0) \ge -2$$
 is equivalent to

$$y_{10}^{2}(1 + \Phi_{2}z_{1})[2 + (1 + 2\Phi_{2})z_{1}] + y_{20}^{2}\alpha^{2}[2 + (4\Phi_{2}\alpha + 1)z_{1} + (2\Phi_{2}\alpha^{2} + 2\alpha - 1)\Phi_{2}z_{1}^{2}] \ge 0.$$

Since $z_1 < 0$, $\alpha \ge \frac{1}{2}$ and $\Phi_2 \le -\frac{1}{2}$, we have $(1 + \Phi_2 z_1) [2 + (1 + 2\Phi_2) z_1] > 0$, $4\Phi_2 \alpha + 1 \le 0$ and $2\Phi_2 \alpha^2 + 2\alpha - 1 \le 0$, which completes the proof. \Box

To conclude, we mention that, for two-dimensional problems of the form (2.2) with negative real eigenvalues, a 3-stage method (1.2) is componentwise contractible for all h > 0 only if λ_2/λ_1 belongs to $[\frac{1}{2}, 2]$ (i.e. again when the problem is non-stiff). The proof, though more technical, is similar to the proof given in this section for 2-stage methods and is available in [4].

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