On Error Growth Functions of Runge-Kutta Methods

E. Hairer* and M. Zennaro†

Abstract

This paper studies estimates of the form $\|y_1 - \widehat{y}_1\| \le \varphi(h\nu)\|y_0 - \widehat{y}_0\|$, where $y_1, \widehat{y}_1$ are the numerical solutions of a Runge-Kutta method applied to a stiff differential equation satisfying a one-sided Lipschitz condition (with constant ν). An explicit formula for the optimal function $\varphi(x)$ is given, and it is shown to be superexponential, i.e., $\varphi(x_1)\varphi(x_2) \le \varphi(x_1 + x_2)$ if x_1 and x_2 have the same sign. As a consequence, results on asymptotic stability are obtained. Furthermore, upper bounds for $\varphi(x)$ are presented that can be easily computed from the coefficients of the method.

Key words. Runge-Kutta methods, error growth functions, stiff differential equations, B-stability, asymptotic stability, superexponential functions.

1 Introduction

For the numerical solution of systems of ordinary differential equations

$$y' = f(t, y), \qquad y(t_0) = y_0 \tag{1.1}$$

*Dept. de mathématiques, Université de Genève, CH-1211 Genève 24, Switzerland, hairer@divsun.unige.ch

†Dipartimento di Scienze Matematiche, Università di Trieste, 34100 Trieste, Italy, zennaro@univ.trieste.it. The work of this author was supported by the Italian M.U.R.S.T. with funds 40% and 60%

(where $f : \mathbb{R} \times \mathbb{C}^n \to \mathbb{C}^n$) we consider Runge-Kutta methods defined by

$$\begin{aligned} g_i &= y_0 + h \sum_{j=1}^{s} a_{ij} f(t_0 + c_j h, g_j), \qquad i = 1, \ldots, s, \\ y_1 &= y_0 + h \sum_{i=1}^{s} b_i f(t_0 + c_i h, g_i). \end{aligned} \tag{1.2}$$

Here h is the step size (it may be adapted during the integration), s the number of stages, and c_i, a_{ij}, b_j are the coefficients determining the method. We refer the reader to the books of Butcher [3], Dekker & Verwer [4], and Hairer & Wanner [6] for a discussion of such methods.

In order to understand the behaviour of these methods when applied to stiff differential equations, several stability and contractivity concepts have been introduced. Let us briefly recall their definitions as far as they will be needed in this paper.

A-stability. This concept is based on the linear scalar autonomous test equation $y' = \lambda y$ with λ being a complex number. The numerical solution (given by (1.2)) is $y_1 = R(z) y_0$, where $z = h\lambda$, and

$$R(z) = 1 + z b^T (I - zA)^{-1} \mathbb{1} \tag{1.3}$$

is the so-called *stability function* of the method. Here we have used the matrix notation $b = (b_1, \ldots, b_s)^T$, $A = (a_{ij})_{i,j=1}^{s}$ for the coefficients of the method, and $\mathbb{1} = (1, \ldots, 1)^T$. The method (1.2) is called *A-stable* if

$$|R(z)| \le 1 \quad \text{whenever} \quad \Re z \le 0. \tag{1.4}$$

AN-stability. If one applies method (1.2) to the non-autonomous problem $y' = \lambda(t) y$, the numerical solution can be written as $y_1 = K(z_1, \ldots, z_s) y_0$, where $z_j = h\lambda(t_0 + c_j h)$, and the so-called *AN-stability function* $K(z_1, \ldots, z_s)$ is given by

$$K(z_1, \ldots, z_s) = 1 + b^T Z (I - AZ)^{-1} \mathbb{1} \tag{1.5}$$

with $Z = \mathrm{diag}(z_1, \ldots, z_s)$. The Runge-Kutta method is called *AN-stable* if

$$|K(z_1, \ldots, z_s)| \le 1 \quad \text{whenever} \quad \Re z_i \le 0 \quad \text{and} \quad z_j = z_k \text{ if } c_j = c_k. \tag{1.6}$$

B-stability. If the differential equation (1.1) satisfies the one-sided Lipschitz condition

$$\Re \langle f(t, y) - f(t, \widehat{y}), y - \widehat{y} \rangle \le 0, \tag{1.7}$$

the distance of two solutions is a non-increasing function of time. If for all such problems and for all step sizes $h > 0$ the numerical solutions $y_1, \widehat{y}_1$ corresponding to two different initial values $y_0, \widehat{y}_0$ satisfy

$$\|y_1 - \widehat{y}_1\| \leq \|y_0 - \widehat{y}_0\|, \tag{1.8}$$

then the method is called *B-stable*. The norm used corresponds to the inner product employed in (1.7).

Error Growth Function. If the differential equation satisfies

$$\Re\langle f(t,y) - f(t,\widehat{y}), y - \widehat{y}\rangle \leq \nu\|y - \widehat{y}\|^2, \tag{1.9}$$

for some real ν (positive or negative), then a simple application of the Gronwall Lemma shows that

$$\|y(t) - \widehat{y}(t)\| \leq e^{\nu(t-t_0)}\|y_0 - \widehat{y}_0\| \qquad \text{for} \quad t \geq t_0. \tag{1.10}$$

In this situation we are interested in obtaining analogous estimates for the numerical solution. In particular we are interested in the smallest value $\varphi(h\nu)$, such that the difference of any two numerical solutions satisfies

$$\|y_1 - \widehat{y}_1\| \leq \varphi(h\nu)\|y_0 - \widehat{y}_0\| \tag{1.11}$$

for all differential equations (1.1) satisfying (1.9). This function, introduced by Burrage & Butcher [1], is called the *error growth function* of the Runge-Kutta method. Interesting results concerning this function can be found in [2]. In particular, it is explained how upper bounds of $\varphi(h\nu)$ can be obtained.

The aim of this paper is to get more insight into the error growth function. In Section 2 we discuss explicit formulas. A simple upper bound of $\varphi(h\nu)$ is given in Section 3. There we also consider error growth functions for problems satisfying a Lipschitz condition in addition to (1.9). For this restricted class of problems estimates with $\varphi(h\nu) < 1$ can be obtained also for methods whose stability function is of modulus one at infinity. In Section 4 we prove that the error growth function is *superexponential*. This allows us to obtain results on the asymptotic stability of the numerical solution (Section 5).

2 Study of Error Growth Functions

We are interested in the error growth functions for three classes of differential equations. The first class (we denote it by $\mathcal{F}_A$) consists of all linear systems with constant coefficients, whose logarithmic norm is bounded by ν:

$$y' = Cy, \qquad \mu(C) \leq \nu. \tag{2.1}$$

Recall that the logarithmic norm $\mu = \mu(C)$ is the smallest real number such that $\Re\langle v, Cv\rangle \leq \mu\langle v, v\rangle$ for all vectors v. We do not make any assumption on the dimension of the system. As second class $\mathcal{F}_K$, we consider scalar complex-valued nonlinear problems (1.1) satisfying the one-sided Lipschitz condition (1.9). Finally, we let $\mathcal{F}_B$ be the class of all nonlinear problems (1.1) satisfying the one-sided Lipschitz condition (1.9), without any restriction on the dimension of the system. Throughout this paper we assume that $f(t, y)$ is a continuous function.

Definition 2.1 *Let ν be a given real number and set $x = h\nu$, where h is the step size. We then denote by $\varphi_A(x)$, $\varphi_K(x)$ and $\varphi_B(x)$ the smallest numbers φ such that the difference of any two numerical solutions satisfies*

$$\|y_1 - \widehat{y}_1\| \leq \varphi\|y_0 - \widehat{y}_0\|$$

for all problems from the classes $\mathcal{F}_A$, $\mathcal{F}_K$ and $\mathcal{F}_B$, respectively. These functions are called error growth functions *corresponding to $\mathcal{F}_A$, $\mathcal{F}_K$ and $\mathcal{F}_B$.*

An explicit formula for $\varphi_A(x)$ is obtained from a Theorem of von Neumann (see [6], Section IV.11).

Theorem 2.1 *Let $R(z)$ be the stability function (1.3). Then it holds*

$$\varphi_A(x) = \sup_{\Re z \leq x} |R(z)|. \tag{2.2}$$

Formula (2.2) means that it is sufficient to consider scalar problems (2.1) for the computation of $\varphi_A(x)$. Since the class of scalar linear problems (2.1) is a subclass of $\mathcal{F}_K$, which again is a subclass of $\mathcal{F}_B$, it holds for all x that

$$\varphi_A(x) \leq \varphi_K(x) \leq \varphi_B(x). \tag{2.3}$$

Moreover, they are increasing functions of x.

Theorem 2.2 *The error growth function for scalar nonlinear problems satisfying (1.9) is given by*

$$\varphi_K(x) = \sup_{\Re z_1 \le x, \ldots, \Re z_s \le x} |K(z_1, \ldots, z_s)|, \tag{2.4}$$

where $K(z_1, \ldots, z_s)$ *is the AN-stability function (1.5).*

Proof. *Upper Bound.* Consider a scalar problem satisfying (1.9) and apply the method (1.2) with two different initial values $y_0, \widehat{y}_0$. Defining $z_i := h(f(t_0 + c_i h, g_i) - f(t_0 + c_i h, \widehat{g}_i))/(g_i - \widehat{g}_i)$ if the internal stages g_i and $\widehat{g}_i$ are different, and $z_i := h\nu = x$ if $g_i = \widehat{g}_i$, we see that the numerical solution satisfies $y_1 - \widehat{y}_1 = K(z_1, \ldots, z_s)(y_0 - \widehat{y}_0)$ with K given in (1.5). Hence, the right-hand expression of (2.4) is an upper bound of $\varphi_K(x)$.

Lower Bound. We first consider nonconfluent Runge-Kutta methods. For given $z_1, \ldots, z_s$ with $\Re z_j \le x$, we let $\lambda(t)$ be a continuous function satisfying $h\lambda(t_0 + c_j h) = z_j$ and $\Re\lambda(t) \le x/h$. Applying the Runge-Kutta method to $y' = \lambda(t)y$, we obtain $y_1 - \widehat{y}_1 = K(z_1, \ldots, z_s)(y_0 - \widehat{y}_0)$ and, consequently, $\varphi_K(x) \ge |K(z_1, \ldots, z_s)|$ for all z_j with $\Re z_j \le x$.

For confluent methods the proof is more complicated. Without loss of generality we assume the method to be irreducible. By extending the techniques of Hundsdorfer & Spijker [8] (see [6], Sect. IV.12, Proof of Theorem 12.18) one can show that, for given $z_1, \ldots, z_s$ (for which the matrix $I - AZ$ is invertible), there exists a continuous function $f : \mathbb{C} \to \mathbb{C}$ satisfying (1.9) such that the Runge-Kutta solutions y_1, g_i and $\widehat{y}_1, \widehat{g}_i$ corresponding to $y_0 = 0$, $\widehat{y}_0 = 1$, $h = 1$ satisfy

$$f(\widehat{g}_i) - f(g_i) = z_i(\widehat{g}_i - g_i) \qquad \text{for} \quad i = 1, \ldots, s.$$

This yields $\widehat{y}_1 - y_1 = K(z_1, \ldots, z_s)$, and shows that the right-hand expression of (2.4) is a lower bound of $\varphi_K(x)$. □

An analogous formula for the error growth function $\varphi_B(x)$ is based on the following result.

Lemma 2.1 *Let* a *and* b $(b \ne 0)$ *be two vectors in* $\mathbb{C}^n$ *satisfying* $\Re\langle a, b\rangle \le x\|b\|^2$. *Then, there exists a matrix* Z *such that*

$$a = Zb \qquad \text{and} \qquad \mu(Z) \le x.$$

Proof. We put $u_1 = b/\|b\|$, and complete it to an orthonormal basis $u_1, \ldots, u_n$ of $\mathbb{C}^n$. Then we define the matrix Z by

$$Zu_1 = a/\|b\|, \qquad Zu_i = xu_i - \langle u_i, a\rangle u_1/\|b\|, \qquad i = 2, \ldots, n.$$

We have $Zb = a$, and one readily verifies that $\Re\langle Zv, v\rangle \le x\|v\|^2$ for all $v = \sum_{i=1}^n \alpha_i u_i$. □

We now consider a system (1.1) of arbitrary dimension and assume (1.9). We take two different initial values $y_0, \widehat{y}_0$, and denote the corresponding internal stage values by g_i and $\widehat{g}_i$, respectively. The main observation is that we can find matrices Z_i satisfying $\mu(Z_i) \le h\nu = x$ such that

$$h\Big(f(t_0 + c_i h, g_i) - f(t_0 + c_i h, \widehat{g}_i)\Big) = Z_i(g_i - \widehat{g}_i). \tag{2.5}$$

If $g_i = \widehat{g}_i$ we can take any matrix Z_i satisfying $\mu(Z_i) \le x$; if $g_i \ne \widehat{g}_i$ this follows from Lemma 2.1 with $b = g_i - \widehat{g}_i$ and $a = h(f(t_0 + c_i h, g_i) - f(t_0 + c_i h, \widehat{g}_i))$. Equation (2.5) implies that the numerical solution can be written as $y_1 - \widehat{y}_1 = K(Z_1, \ldots, Z_s)(y_0 - \widehat{y}_0)$, where

$$K(Z_1, \ldots, Z_s) = I + (b^T \otimes I)Z\Big(I \otimes I - (A \otimes I)Z\Big)^{-1}(\mathbb{1} \otimes I) \tag{2.6}$$

and Z is the block diagonal matrix with $Z_1, \ldots, Z_s$ as entries in the diagonal.

Theorem 2.3 *It holds*

$$\varphi_B(x) = \sup_{\mu(Z_1)\le x, \ldots, \mu(Z_s)\le x} \|K(Z_1, \ldots, Z_s)\|, \tag{2.7}$$

where the matrix $K(Z_1, \ldots, Z_s)$ is given by (2.6).

Proof. The above considerations show that the supremum in (2.7) is an upper bound of $\varphi_B(x)$. It is also a lower bound of $\varphi_B(x)$, because all ingredients for the proof of Theorem 2.2 are still valid for systems of differential equations. □

Examples. For one-stage methods (the θ-method) it holds $K(Z_1) = R(Z_1)$, and Theorem 2.3 together with the Theorem of von Neumann yields $\varphi_A(x) = \varphi_K(x) = \varphi_B(x)$.

For two-stage methods the computation of $\varphi_A(x)$ and $\varphi_K(x)$ can be done with help of a formula manipulation program. For example, for the two-stage Radau IIA method we get

$$\varphi_A(x) = \begin{cases} \dfrac{|1 + x/3|}{1 - 2x/3 + x^2/6} & \text{if} \quad x \le -6 - 3\sqrt{10} \\ \dfrac{\sqrt{3\sqrt{12x^2 + 12x + 9} + 10x + 7}}{2(2 - x)} & \text{if} \quad -6 - 3\sqrt{10} \le x < 2, \end{cases}$$

$$\varphi_K(x) = \begin{cases} \dfrac{4}{5 - 2x} & \text{if} \quad x \le (9 - 3\sqrt{17})/8 \\ \dfrac{3 + 4x}{\sqrt{(3 - 2x)(3 + 4x - 2x^2)}} & \text{if} \quad (9 - 3\sqrt{17})/8 \le x < 3/2. \end{cases}$$

Since the function $\varphi_K(x)$ is identical to the upper bound for $\varphi_B(x)$, given in [2], it is equal to $\varphi_B(x)$.

It is interesting to note that for all irreducible two-stage methods it holds

$$\varphi_B(x) = \varphi_K(x)$$

(see [7]). For the moment it is not clear, whether this is also true for methods with more than two stages. We do not know of a counterexample.

3 Elementary Upper Bounds

For Runge-Kutta methods with more than two stages the concrete computation of the supremum in (2.7) may be difficult or even impossible. In the case of (irreducible) *algebraically stable* Runge-Kutta methods, i.e.,

$$\begin{array}{ll} b_i > 0 \qquad \text{for} \quad i = 1, \dots, s & \\ M = (b_i a_{ij} + b_j a_{ji} - b_i b_j)_{i,j=1}^{s} & \text{positive semi-definite} \end{array} \tag{3.1}$$

(see e.g., [6], Sect. IV.12) the following theorem gives an upper bound of $\varphi_B(x)$ which is easily obtained from the coefficients of the method. Observe that the bound is sharp for $x = 0$ and for $x \to -\infty$, and assures that $\varphi_B(x) < 1$ for $x < 0$, if $|R(\infty)| < 1$.

Theorem 3.1 *Let the Runge-Kutta method (1.2) be irreducible and algebraically stable, i.e., (3.1) holds. Then the error growth function satisfies*

$$\varphi_B(x) \le \frac{\sqrt{1-2x\gamma(1-\rho^2)} - 2x\gamma\rho}{1-2x\gamma} \qquad \textit{for} \quad x \le 0, \tag{3.2}$$

where $\rho = |R(\infty)|$ *with* $R(z)$ *given by (1.3) and*

$$\gamma = \Big(\sum_{j=1}^{s} b_j^{-1} v_j^2\Big)^{-1} \tag{3.3}$$

with $(v_1, \ldots, v_s)^T = \lim_{\varepsilon\to 0} b^T(A+\varepsilon I)^{-1}$ *(see Lemma 3.1 for the existence of this limit).*

Proof. Let $y_0, \widehat{y}_0$ be two initial values and denote the differences of the numerical solution, the stage values and the function values (multiplied by h) by Δy_0, Δy_1, Δg_i, and Δf_i, respectively. The Runge-Kutta formula then becomes

$$\Delta y_1 = \Delta y_0 + \sum_{i=1}^{s} b_i \Delta f_i, \tag{3.4}$$

$$\Delta g_i = \Delta y_0 + \sum_{j=1}^{s} a_{ij} \Delta f_j, \tag{3.5}$$

and the one-sided Lipschitz condition (1.9) leads to $\Re\langle \Delta f_i, \Delta g_i\rangle \le x\|\Delta g_i\|^2$, where $x = h\nu$. If the method is algebraically stable, it holds (see for example [6], p. 144)

$$\|\Delta y_1\|^2 \le \|\Delta y_0\|^2 + 2x\sum_{i=1}^{s} b_i \|\Delta g_i\|^2. \tag{3.6}$$

We are looking for a lower bound of $\sum_i b_i\|\Delta g_i\|^2$.

Suppose for the moment that the inverse of the Runge-Kutta matrix A exists and denote its elements by ω_{ij}. From (3.5) we get

$$\Delta f_i = \sum_{j=1}^{s} \omega_{ij}\Delta g_j - \Big(\sum_{j=1}^{s} \omega_{ij}\Big)\Delta y_0,$$

and, inserted into (3.4), this yields

$$\Delta y_1 = R(\infty)\Delta y_0 + \sum_{j=1}^{s}\Big(\sum_{i=1}^{s} b_i\omega_{ij}\Big)\Delta g_j,$$

where $R(\infty)$ is the value at infinity of the stability function (1.3). Using the Cauchy-Schwarz inequality for the estimation of the right-hand expression, we arrive at

$$\Big|\|\Delta y_1\| - \rho\,\|\Delta y_0\|\Big| \le \|\Delta y_1 - R(\infty)\,\Delta y_0\| \le \sqrt{\sum_{j=1}^{s} b_j^{-1}\Big(\sum_{i=1}^{s} b_i\omega_{ij}\Big)^2}\cdot\sqrt{\sum_{i=1}^{s} b_i\|\Delta g_i\|^2}$$

and consequently we get the lower bound

$$\sum_{i=1}^{s} b_i\|\Delta g_i\|^2 \ge \gamma(\|\Delta y_1\| - \rho\,\|\Delta y_0\|)^2 \tag{3.7}$$

where γ is given by (3.3). Therefore, by substituting (3.7) in (3.6), we get the second degree inequality

$$(1-2x\gamma)\|\Delta y_1\|^2 + 4x\gamma\rho\|\Delta y_1\|\cdot\|\Delta y_0\| - (1+2x\gamma\rho)^2\|\Delta y_0\|^2 \le 0,$$

which, in turn, implies the desired result.

If the Runge-Kutta matrix A is singular, we replace it everywhere by the regular matrix $(A+\varepsilon I)$ and consider the limit $\varepsilon \to 0$. The existence of the limits in the considered formulas are assured by Lemma 3.1 below. □

Lemma 3.1 *For irreducible algebraically stable Runge-Kutta methods the following limit exists*

$$\lim_{\varepsilon\to 0} b^T(A+\epsilon I)^{-1} = v^T.$$

Proof. If the coefficient matrix A is regular, the result is obvious. Therefore assume that A is singular. We first show that the Jordan blocks of A corresponding to zero eigenvalues have a size at most 1. Let $u \ne 0$ be an eigenvector (i.e., $Au = 0$) and assume that there exists a vector w satisfying $Aw = u$. From algebraic stability it follows that $u^TMu = -(b^Tu)^2 \ge 0$ and thus $b^Tu = 0$, $u^TMu = 0$. Since M is positive semi-definite we get $0 = u^TMw = u^TBAw = u^TBu$, which is impossible because of (3.1).

The inverse of $A+\epsilon I$ can then be expanded in a series as $(A+\epsilon I)^{-1} = \epsilon^{-1}A_{-1} + A_0 + \epsilon A_1 + \epsilon^2 A_2 + \ldots$. Comparing the coefficient of ϵ^{-1} in the identity $I = (A+\epsilon I)(A+\epsilon I)^{-1}$, we get $AA_{-1} = 0$. Hence, using algebraic stability (3.1), we conclude $A_{-1}^TMA_{-1} = -A_{-1}^Tbb^TA_{-1} \ge 0$. This yields $b^TA_{-1} = 0$ and thus multiplying the above expansion of $(A+\epsilon I)^{-1}$ by b^T on the left yields the desired result with $v^T = b^TA_0$. □

If the stability function of an algebraically stable Runge-Kutta method satisfies $|R(\infty)| = 1$, then we have $\varphi_B(x) = 1$ and $\varphi_A(x) = 1$ for all $x \leq 0$. In order to get sharper estimates also in this case, one has to restrict the class of problems. Let us consider nonlinear problems $y' = f(t, y)$ that satisfy

$$\|f(t, y) - f(t, z)\| \leq L\|y - z\| \tag{3.8}$$

in addition to (1.9). It is clear that, under this condition, the problem has limited stiffness and that $L \geq |\nu|$.

Theorem 3.2 *Let the Runge-Kutta method be irreducible and algebraically stable and assume that the differential equation satisfies (1.9) and (3.8). For any pair of numerical solutions we then have for* $\nu \leq 0$

$$\|\Delta y_1\| \leq \varphi(h\nu, hL)\|\Delta y_0\| \tag{3.9}$$

where

$$\varphi(x, \ell) = \sqrt{1 + \frac{2x}{(1 + \beta\ell)^2}} \tag{3.10}$$

and $\quad \beta = \sqrt{\sum_{j=1}^{s} b_j^{-1}\Big(\sum_{i=1}^{s} b_i a_{ij}\Big)^2}\ .$

Proof. Multiplying (3.5) by b_i and summing up yields (because of $\sum_i b_i = 1$)

$$\Delta y_0 = \sum_{i=1}^{s} b_i \Delta g_i - \sum_{j=1}^{s}\Big(\sum_{i=1}^{s} b_i a_{ij}\Big)\Delta f_j .$$

The Lipschitz condition of f together with $b_i > 0$ then imply

$$\|\Delta y_0\| \leq \sum_{i=1}^{s} b_i\|\Delta g_i\| + \ell \sum_{j=1}^{s}\left|\sum_{i=1}^{s} b_i a_{ij}\right| \cdot \|\Delta g_j\|,$$

where we have used the abbreviation $\ell = hL$. With the Cauchy-Schwarz inequality we can conclude that

$$\|\Delta y_0\| \leq \left(1 + \ell\sqrt{\sum_{j=1}^{s} b_j^{-1}\Big(\sum_{i=1}^{s} b_i a_{ij}\Big)^2}\ \right)\sqrt{\sum_{i=1}^{s} b_i\|\Delta g_i\|^2}.$$

This yields a lower bound for $\sum_i b_i\|\Delta g_i\|^2$ which, inserted into (3.6), gives the desired estimate. □

4 Superexponential Growth Functions

For a problem (1.1) satisfying the one-sided Lipschitz condition (1.9), the difference of two solutions grows at most like $\exp(\nu(t-t_0))\|\Delta y_0\|$. The characteristic property of the exponential function is $\exp(x_1)\exp(x_2) = \exp(x_1+x_2)$. The aim of this section is to show a similar relation for the error growth functions $\varphi_A(x)$, $\varphi_K(x)$ and $\varphi_B(x)$. This will be useful for the study of asymptotic stability.

Definition 4.1 *Let I be an interval containing* 0*. A continuous function $\varphi : I \to \mathbb{R}$ is called* superexponential *if it satisfies $\varphi(0) = 1$ and*

$$\varphi(x_1)\varphi(x_2) \le \varphi(x_1 + x_2) \tag{4.1}$$

for all $x_1, x_2 \in I$ having the same sign and satisfying $x_1 + x_2 \in I$.

Proposition 4.1 *For a superexponential function it holds*

$$\varphi(x) \ge e^{\alpha_r x} \quad \textit{for} \;\; x \ge 0, \qquad \varphi(x) \ge e^{\alpha_l x} \quad \textit{for} \;\; x \le 0,$$

where $$\alpha_r = \limsup_{h\to 0, h>0} \frac{\varphi(h)-\varphi(0)}{h}, \qquad \alpha_l = \liminf_{h\to 0, h<0} \frac{\varphi(h)-\varphi(0)}{h}.$$

Proof. Because of $\varphi(x) \ge \varphi(x/2)\varphi(x/2) \ge 0$, a superexponential function cannot assume negative values. By Definition 4.1 it holds $\varphi(x)\varphi(h) \le \varphi(x+h)$ and hence

$$\frac{\varphi(x+h)-\varphi(x)}{h} \ge \varphi(x)\frac{\varphi(h)-1}{h}$$

whenever x and h are positive. Consequently, we get $D^+\varphi(x) \ge \varphi(x)\cdot\alpha_r$ for $x \ge 0$ (here $D^+\varphi(x) = \limsup_{h\to 0,h>0}(\varphi(x+h)-\varphi(x)))/h$ denotes the Dini derivate; see [5], Section I.10). Solving this differential inequality yields the statement for $x \ge 0$.

The lower bound for $x < 0$ is obtained by applying the just proved estimate to the superexponential function $\psi(x) := \varphi(-x)$. □

Theorem 4.1 *If the Runge-Kutta method is A-stable, the error growth function $\varphi_A(x)$ is superexponential. If it is B-stable, the error growth functions $\varphi_K(x)$ and $\varphi_B(x)$ are superexponential.*

Proof. a) A-stability is equivalent to $\varphi_A(0) = 1$. It therefore remains to verify (4.1). Let x_1 and x_2 be fixed (both ≤ 0 or both ≥ 0) and assume $\varphi_A(x_1 + x_2) < \infty$. The idea is to consider the rational function

$$S(z) = R(a - z)R(z)$$

where $a \in \mathbb{C}$ is a parameter satisfying $\Re a \leq x_1 + x_2$. Due to A-stability and $\varphi_A(x_1 + x_2) < \infty$, $S(z)$ is analytic on the strip $0 \leq \Re z \leq x_1 + x_2$ (or $x_1 + x_2 \leq \Re z \leq 0$). At the border of this strip the modulus of $S(z)$ is bounded by $\varphi_A(x_1 + x_2)$, because $|R(z)| \leq 1$ on the imaginary axis (see Theorem 2.1). By the maximum principle we therefore have for all z in the considered strip

$$|R(a - z)R(z)| \leq \varphi_A(x_1 + x_2).$$

We now choose z on the line $\Re z = x_2$ in such a way that $|R(z)|$ becomes maximal; then, we choose a on the line $\Re a = x_1 + x_2$ (i.e., $\Re(a - z) = x_1$) such that $|R(a-z)|$ becomes maximal (eventually one has to consider limits). This shows that $\varphi_A(x_1)\varphi_A(x_2) \leq \varphi_A(x_1 + x_2)$.

b) For the function $\varphi_K(x)$ of (2.4) the argumentation is similar. This time we consider the rational function

$$S(z) = K(a_1 - z, \ldots, a_s - z)K(b_1 + z, \ldots, b_s + z),$$

where $\Re a_j \leq x_1 + x_2$ and $\Re b_j \leq 0$. The maximum principle applied to $S(z)$ on the same strip as before yields

$$|K(a_1 - z, \ldots, a_s - z)K(b_1 + z, \ldots, b_s + z)| \leq \varphi_K(x_1 + x_2).$$

We now fix $b_1, \ldots, b_s$ on the line $\Re b_j = 0$ such that $|K(b_1 + x_2, \ldots, b_s + x_2)|$ is maximal; then, we fix $a_1, \ldots, a_s$ on the line $\Re a_j = x_1 + x_2$ such that $|K(a_1 - x_2, \ldots, a_s - x_2)|$ is maximal. This proves that $\varphi_K(x)$ is superexponential.

c) For the proof of the last statement we consider the rational function

$$S(z) = u_A^* K(A_1 - zI, \ldots, A_s - zI)v_A u_B^* K(B_1 + zI, \ldots, B_s + zI)v_B,$$

where the matrices A_j, B_j satisfy $\mu(A_j) \leq x_1 + x_2$ and $\mu(B_j) \leq 0$, and u_A, v_A, u_B, v_B are vectors of $\mathbb{C}^m$. Using the property $\mu(A_j - zI) = \mu(A_j) - \Re z$ and the fact that $\|C\| = \sup_{\|u\|=1,\|v\|=1} |u^* Cv|$, one obtains as above that also $\varphi_B(x)$ is superexponential (see Theorem 2.3). □

The upper bound of Theorem 3.1 can also be shown to be superexponential. The computations, however, are very long and tedious, and need the use of a formula manipulation program.

Theorem 4.2 *For given $\nu < 0$ and $L \geq -\nu$ the function $\Phi(h) = \varphi(h\nu, hL)$ with $\varphi(x, \ell)$ given by (3.10) is superexponential, provided that $\beta \geq 8/15$. The function $\Phi(h)$ is strictly decreasing for $h < 1/(\beta L)$ and strictly increasing for $h > 1/(\beta L)$.*

Proof. The property $\Phi(0) = 1$ is easy to check. On the contrary, about two pages of tedious standard calculations are necessary to conclude that $\Phi(h_1)\Phi(h_2) \leq \Phi(h_1 + h_2)$ is equivalent to the inequality

$$-\frac{2\nu}{L\beta} \leq \frac{4 + 7L\beta(h_1 + h_2) + 4L^2\beta^2(h_1 + h_2)^2 + L^3\beta^3(h_1 + h_2)(h_1^2 + h_1h_2 + h_2^2)}{(1 + L\beta(h_1 + h_2))^2}.$$

It can be checked that the right hand side is $> 15/4$ for all $h_1, h_2 \geq 0$ and thus, by $L \geq -\nu$, the condition $\beta \geq 8/15$ is sufficient to guarantee (4.1).

The rest of the proof is easily obtained by computing and analyzing the derivative $\Phi'(h) = \nu(1 - \beta hL)/(\Phi(h)(1 + \beta hL)^3)$. □

5 Asymptotic Stability

The results of this section illustrate the role of superexponential functions in the asymptotic stability analysis of Runge-Kutta methods. Recall that a problem $y' = f(t, y)$ satisfying the one-sided Lipschitz condition (1.9) with $\nu < 0$ is asymptotically stable (see (1.10)). Other results about asymptotic stability have been recently obtained by Stuart & Humphries [9].

Definition 5.1 *A B-stable numerical method is called* asymptotically B-stable *if for the difference Δy_n of any two numerical solutions, when applied to $y' = f(t, y)$ satisfying (1.9) with $\nu < 0$, it holds $\lim_{n\to\infty} \|\Delta y_n\| = 0$ for any mesh $t_0, t_1, \ldots$ with $t_n \to \infty$.*

Observe that, even if a Runge-Kutta method is B-stable, it is not guaranteed that the numerical solution $\{y_n\}_{n\geq 0}$ of the test equation $y' = \lambda y$,

$\Re\lambda < 0$, tends to zero if the step sizes are not uniformly bounded. This may happen when $|R(\infty)| = 1$. In fact, in such a case, it is possible to choose a diverging sequence of step sizes h_n such that, even being $|R(h_n\lambda)| < 1$ for all n, the product $\prod_{k=0}^{n-1} |R(h_k\lambda)|$ tends to some limit $r \neq 0$ as $n \to \infty$. The same situation arises for constant step sizes, if we consider a problem $y' = \lambda(t)y$, where $\lambda(t)$ tends sufficiently fast to $-\infty$ as $t \to \infty$. In order to get asymptotic stability results, we either have to restrict the class of methods ($|R(\infty)| < 1$) or to consider only problems with limited stiffness.

Theorem 5.1 *Consider a B-stable Runge-Kutta method satisfying* $|R(\infty)| < 1$ *and suppose that the differential equation satisfies (1.9) with* $\nu < 0$. *For the difference* Δy_n *of any two numerical solutions (corresponding to a mesh* $t_0, t_1, \ldots$ *with* $t_n \to \infty$, $h_n = t_{n+1} - t_n$*) we have:*
a) the method is asymptotically B-stable, i.e., without any restriction on the step sizes it holds

$$\|\Delta y_n\| \to 0 \qquad \text{for} \quad n \to \infty;$$

b) under the restriction $h_{n+1} \leq ch_n$ $(c > 1)$ *there exist* $C > 0$ *and* $\alpha > 0$ *such that*

$$\|\Delta y_n\| \leq C(t_n - t_0)^{-\alpha}\|\Delta y_0\| \qquad \text{for} \quad n = 1, 2, \ldots;$$

c) if the step sizes are uniformly bounded, there exist $C > 0$ *and* $\beta > 0$ *such that*

$$\|\Delta y_n\| \leq Ce^{-\beta(t_n - t_0)}\|\Delta y_0\| \qquad \text{for} \quad n = 0, 1, 2, \ldots.$$

Remark 5.1 *The same statements hold if we replace "B-stable" by "A-stable" and if we consider only linear systems with constant coefficients.*

Proof. a) We assume that the considered method is irreducible (otherwise we replace it by an equivalent, irreducible one without changing the numerical solution), so that the Runge-Kutta coefficients satisfy (3.1) (see e.g., Theorem IV.12.18 of Hairer & Wanner [6]). By definition of the error growth function $\varphi_B(x)$ we have that

$$\|\Delta y_n\| \leq \Big(\prod_{k=0}^{n-1} \varphi_B(h_k\nu) \Big) \|\Delta y_0\|. \tag{5.1}$$

Since $\nu < 0$ and $|R(\infty)| < 1$, it follows from Theorem 3.1 that the factors $\varphi_B(h_k\nu)$ are all smaller than one and that they are close to one only for small values of h_k. However, due to the fact that $\varphi_B(x)$ is superexponential we have

$$\varphi_B(h_k\nu)\varphi_B(h_{k+1}\nu) \le \varphi_B((h_k + h_{k+1})\nu).$$

Hence, replacing two consecutive steps by one large step of size $h_k + h_{k+1}$, increases the upper bound in (5.1). After combining several consecutive steps (if necessary) we can assume that $h_k \ge h > 0$ for all k. From the monotonicity of $\varphi_B(x)$ it thus follows that $\|\Delta y_n\| \le (\varphi_B(h\nu))^n\|\Delta y_0\| \to 0$ for $n \to \infty$, because $\varphi_B(h\nu) < 1$ (again by Theorem 3.1).

b) We remove points of the mesh until $h_k \ge h > 0$ and $h_{k+1} \le c_1 h_k$ for all k, where $c_1 > 1$ is a suitable constant depending on c. This implies that $t - t_0 \le c_0 c_1^n$ for $t \in [t_n, t_{n+1}]$, where $c_0 > 0$ is another suitable constant. Computing n from this inequality and inserting it into $\|\Delta y_n\| \le (\varphi_B(h\nu))^n\|\Delta y_0\|$, we get the desired estimate.

c) We remove mesh-points until $0 < h \le h_k \le H$ for all k. This yields $t - t_0 \le c_2 n$ for $t \in [t_n, t_{n+1}]$, where $c_2 > 0$ is a suitable constant, and the exponential decay can be obtained as above. □

Theorem 5.2 *Consider a B-stable Runge-Kutta method ($|R(\infty)| = 1$ is admitted) and suppose that the differential equation satisfies (1.9) with $\nu < 0$ and (3.8) with some $L \ge -\nu$. Then the conclusion (c) of the preceding theorem can be drawn.*

Proof. We consider the function $\varphi(h\nu, hL)$ of Theorem 3.2 instead of $\varphi_B(x)$. Since $\varphi(h\nu, hL)$ is an increasing function of β, we can assume without restrictions that $\beta \ge 8/15$, so that this function is superexponential by Theorem 4.2. As $\varphi(h_k\nu, h_kL) \le q < 1$ for $h \le h_k \le H$, the proof of the preceding theorem can be applied. □

Acknowledgment. We would like to thank Gerhard Wanner for his useful comments during the preparation of this paper.

References

[1] K. Burrage & J.C. Butcher: *Stability critera for implicit Runge-Kutta methods*, SIAM J. Numer. Anal. 16 (1979), 46-57.

[2] K. Burrage & J.C. Butcher: *Non-linear stability of a general class of differential equation methods*, BIT 20 (1980), 185-203.

[3] J.C. Butcher: *The numerical analysis of ordinary differential equations*, Wiley, London, 1987.

[4] K. Dekker & J.G. Verwer: *Stability of Runge-Kutta methods for stiff nonlinear differential equations*, North Holland, Amsterdam, 1984.

[5] E. Hairer, S.P. Nørsett & G. Wanner: *Solving ordinary differential equations I, Nonstiff problems*, Springer-Verlag, New York, 1987 (second edition 1993).

[6] E. Hairer & G. Wanner: *Solving ordinary differential equations II, Stiff and differential algebraic problems*, Springer-Verlag, New York, 1991 (second edition 1996).

[7] E. Hairer & G. Wanner: *On a generalization of a theorem of von Neumann*, to appear in ZAMM, 1996.

[8] W.H. Hundsdorfer & M.N. Spijker: *A note on B-stability of Runge-Kutta methods*, Numer. Math. 36 (1981), 319-331.

[9] A.M. Stuart & A.R. Humphries: *Model problems in numerical stability theory for initial value problems*, SIAM Review 36 (1994), 226-257.