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On the convergence of waveform relaxation methods for stiff nonlinear ordinary differential equations ☆

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Abstract

This paper concerns the numerical solution of stiff initial value problems for systems of ordinary differential equations. We focus on the class of waveform relaxation methods, which was introduced by Lelarasmee et al. (1982).

In waveform relaxation methods, a so-called *continuous time iteration* is set up, which is based on a decoupling of a given initial value problem into a number of subsystems. The continuous time iteration generates a sequence of functions that approximate the solution to the given initial value problem. After discretization of the initial value problems in the continuous time iteration, one obtains a so-called *discrete time iteration*.

In this paper we investigate the convergence of continuous time and discrete time iteration processes. We consider discrete time iteration processes that are obtained from Runge–Kutta methods, and derive convergence results that are relevant in applications to nonlinear, nonautonomous, stiff initial value problems.

Keywords: Ordinary differential equations; Stiff initial value problems; Waveform relaxation methods; Continuous time iteration; Runge–Kutta methods; Discrete time iteration; Convergence

1. Introduction

1.1. Waveform relaxation methods

In this paper we investigate waveform relaxation methods for the numerical solution of stiff initial value problems for systems of ordinary differential equations,

$$U'(t) = f(t, U(t)), \quad \text{for } t \geqslant t_0, \qquad U(t_0) = u_0. \tag{1.1}$$

Here, $t_0 \in \mathbb{R}$, $u_0 \in \mathbb{R}^d$ are given, f is a given continuous function mapping $[t_0, \infty) \times \mathbb{R}^d$ onto $\mathbb{R}^d$, and $U(t)$ is unknown (for $t > t_0$).

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Waveform relaxation methods were introduced by Lelarasmee, Ruehli and Sangiovanni-Vincentelli [14]. These authors successfully applied this type of methods in the numerical solution of initial value problems (1.1) that arise from the modelling of large-scale integrated circuits.

Let $T > t_0$, let $U^0 : [t_0, T] \to \mathbb{R}^d$ be a given approximation to U on $[t_0, T]$, and let F be a given *splitting* of f, i.e., $F : [t_0, T] \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ and $F(t, y, y) = f(t, y)$ (whenever $t_0 \leqslant t \leqslant T$, $y \in \mathbb{R}^d$), where we always assume that U^0 and F are continuous. The following iteration defines a sequence of functions $U^k : [t_0, T] \to \mathbb{R}^d$ $(k = 1, 2, 3, \ldots)$ that approximate U on $[t_0, T]$,

$$(U^k)'(t) = F(t, U^k(t), U^{k-1}(t)), \quad \text{for } t \in [t_0, T], \qquad U^k(t_0) = u_0. \tag{1.2}$$

The above iteration is called a *continuous time waveform relaxation process* whenever the splitting function F has the property that the system (1.2) is *decoupled* into a number of *subsystems*. After discretization of (1.2) (by a numerical step-by-step method) one arrives at a so-called *discrete time waveform relaxation process*. We note that Lelarasmee et al. [14] call the functions U^k *waveforms* and the iteration (1.2) the *relaxation process*.

A well-known example of a waveform relaxation method is *Gauss–Seidel* waveform relaxation. This method has the splitting function F given by

$$F_j(t, y, z) = f_j\left(t, (\eta_1, \ldots, \eta_j, \zeta_{j+1}, \ldots, \zeta_d)^{\mathrm{T}}\right), \quad \text{for } j = 1, 2, \ldots, d,$$

where f_j and F_j stand for the jth components of f and F, respectively, and we have written $y = (\eta_1, \eta_2, \ldots, \eta_d)^{\mathrm{T}} \in \mathbb{R}^d$, $z = (\zeta_1, \zeta_2, \ldots, \zeta_d)^{\mathrm{T}} \in \mathbb{R}^d$.

Two advantages of waveform relaxation methods can be observed a priori. Firstly, the different subsystems of (1.2) can be solved (numerically) with different sequences of stepsizes through the interval $[t_0, T]$. This, so-called, *multirate* property is very favourable in applications to stiff initial value problems (1.1) where the dimension d is large and many different rates of change exist among the different components of the exact solution U. Initial value problems of this type arise, for example, in the modelling of large-scale integrated circuits (cf. [14]).

A second advantage of waveform relaxation methods is the inherent *(large-scale) parallelism*. Consider e.g. *Jacobi* waveform relaxation, which has the splitting function F given by

$$F_j(t, y, z) = f_j\left(t, (\zeta_1, \ldots, \zeta_{j-1}, \eta_j, \zeta_{j+1}, \ldots, \zeta_d)^{\mathrm{T}}\right), \quad \text{for } j = 1, 2, \ldots, d.$$

In Jacobi waveform relaxation, the system (1.2) is decoupled into d subsystems (all of dimension 1). If, on a parallel computer, these subsystems are assigned to d different processors, they can be solved on $[t_0, T]$ in parallel. This obvious type of parallelism is present in all waveform relaxation methods. However, in many cases, such as Gauss–Seidel waveform relaxation, exploiting this parallelism is only possible when approximations are exchanged between the different processors as soon as they have been computed (cf. e.g. [10]). This leads to a large amount of communication during each waveform relaxation sweep, which forms a severe drawback. In Jacobi waveform relaxation, communication is only necessary once per sweep, and this method is attractive for parallel implementation. We mention that Burrage and Pohl [5] implemented, on a distributed memory computer, a variant of Jacobi waveform relaxation.

A problem in waveform relaxation methods can be storage. For example, in Jacobi waveform relaxation the approximation to the previous iterate U^{k-1} has to be stored on the whole interval $[t_0, T]$. Further, the use of a parallel computing environment gives rise to many additional considerations (cf. e.g. [3,5,10]). It is beyond the scope of this paper to discuss these in detail, but we note that it is particularly important that the communication time is small compared to the computation time (cf. above), and that there exists a good load balancing of the different processors.

1.2. Convergence of waveform relaxation methods

A main problem concerning waveform relaxation methods is the question of which splitting functions F yield fast convergence of the sequence $U^1, U^2, U^3, \ldots,$ generated by (1.2), to the solution U of (1.1). The choice of a suitable function F can be natural in cases where the initial value problem (1.1) forms a model to a certain real-life phenomenon (cf. e.g. [14]). However, for general stiff initial value problems (1.1) no useful criterion is known up to now.

A second important question is which numerical methods lead to discrete time waveform relaxation processes that preserve the convergence behaviour of the corresponding continuous time process, with no restrictions on the grid due to stiffness.

In view of the above, a detailed study of the convergence behaviour of waveform relaxation methods is necessary. In the literature, an extensive convergence analysis has been performed in the case of linear, autonomous initial value problems. This research was begun by Miekkala and Nevanlinna [17,18].

Miekkala and Nevanlinna [17] considered the convergence of continuous time waveform relaxation processes on the infinite interval $[0, \infty)$. Their analysis is based on a useful formula for $\rho[\mathscr{K}]$, where $\rho[\cdot]$ stands for spectral radius and $\mathscr{K}$ denotes the (linear) operator that maps $U - U^{k-1}$ onto $U - U^k$ (for $k = 1, 2, 3, \ldots$).

In [18] a closely related formula for $\rho[\mathscr{K}_h]$ was derived and investigated. Here, $\mathscr{K}_h$ denotes any discrete time analogue to $\mathscr{K}$ obtained from application of a linear multistep method with constant stepsize $h > 0$. In particular it was shown in [18] that if the linear multistep method is A-stable, then $\rho[\mathscr{K}_h] \leqslant \rho[\mathscr{K}]$ (whenever $h > 0$).

Results on discrete time analogues $\mathscr{K}_h$ to $\mathscr{K}$ obtained from Runge–Kutta methods were derived by Lubich and Ostermann [16]. These authors showed that if the Runge–Kutta method is algebraically stable (cf. Section 1.3), then $\rho[\mathscr{K}_h] \leqslant \rho[\mathscr{K}]$ and $\| \mathscr{K}_h \| \leqslant \| \mathscr{K} \|$ (whenever $h > 0$). Here, $\| \cdot \|$ stands for the operator norm induced by the L^2-norm in the continuous case, and for the operator norm induced by a (scaled) l^2-norm in the discrete case (cf. also Section 2.5).

Nevanlinna [19,20] considered convergence, in the case of linear, autonomous initial value problems, on finite intervals $[0, T]$. He investigated $\| \mathscr{K}^k \|$ and $\| \mathscr{K}_h^k \|$ (for $k = 1, 2, 3, \ldots$), where $\mathscr{K}$ denotes the continuous time operator relevant to $[0, T]$ and $\mathscr{K}_h$ is again any discrete time analogue to $\mathscr{K}$ obtained from application of a linear multistep method with constant stepsize $h > 0$. The norms under consideration are induced by a (scaled) L^∞-norm and a (scaled)l^∞-norm, respectively. In addition, Nevanlinna [20] investigated the convergence of discrete time waveform relaxation processes where the stepsize reduces with a constant factor in every sweep.

Bellen, Jackiewicz and Zennaro [1] obtained a convergence result relevant to a class of nonlinear, nonautonomous, stiff initial value problems (1.1). More precisely, Bellen et al. [1] considered the class of problems (1.1) that are dissipative in the maximum norm. They investigated discrete time waveform relaxation processes that are obtained from application of continuous Runge–Kutta methods to the Jacobi and Gauss–Seidel iterations (1.2). Under the assumption that the continuous Runge–Kutta method is semi-AN$_f$(0)-stable (see [1]), the authors derived a useful estimate for the error reduction in the corresponding discrete time waveform relaxation processes. Here, the error was measured in the l^∞-norm.

Finally, we mention the following, well-known, *superlinear* convergence estimate, which holds for the continuous time iteration (1.2) under mild assumptions on F (cf. e.g. [2,3,15,19])

$$|U(t)-U^k(t)| \leqslant \frac{\{C(t-t_0)\}^k}{k!} \max_{t_0 \leqslant s \leqslant t} |U(s)-U^0(s)|$$

(whenever $t\in[t_0, T]$, $k=1, 2, 3, \ldots$), where $|\cdot|$ is any given norm on $\mathbb{R}^d$ and C is a constant independent of t, k and U^0. Although the above estimate reveals a rapid convergence behaviour when $k\to\infty$, the estimate can be misleading when k is moderate and the initial value problem (1.1) is stiff. For example, in the case of the semi-discretized (one-dimensional) heat equation and the Jacobi splitting, it can be seen that the constant C should increase (at least) like $(\Delta x)^{-2}$ (for $\Delta x \downarrow 0$), where Δx denotes the spatial mesh width. On the other hand, it can also be shown (cf. e.g. [19]) that, if $|\cdot|$ is the Euclidean norm, then $|U(t)-U^k(t)| \leqslant \theta^k \max_{t_0\leqslant s\leqslant t}|U(s)-U^0(s)|$ (whenever $t\in[t_0, T]$, $k=1, 2, 3, \ldots$) with $\theta=\theta(\Delta x)\in(0, 1)$. Clearly, the latter estimate is far more accurate when k is moderate, Δx small and $t\neq t_0+\mathrm{O}((\Delta x)^2)$.

1.3. Scope of this paper

For the numerical solution of (1.2) we consider in this paper the class of Runge–Kutta methods. Let $h_n>0$ $(n=1, 2,\ldots, N)$ be given *stepsizes* with $h_1+h_2+\cdots+h_N=T-t_0$, and define the *gridpoints* t_n by $t_n=t_{n-1}+h_n$ (for $n=1, 2,\ldots, N$). In this paper, we assume that the stepsizes are independent of the subsystems of (1.2) and of the iteration index k. In general, an interpolation procedure would be required to adapt a given Runge–Kutta method to (1.2), but, in view of our assumption, we can immediately obtain a complete method for (1.2) by using known approximations to U^{k-1}. We arrive at the following discrete time waveform relaxation process, defining approximations u_n^k to $U^k(t_n)$ (for $n=1, 2,\ldots, N$ and $k=1, 2, 3,\ldots$).

$$u_n^k = u_{n-1}^k + h_n \sum_{j=1}^{s} b_j F\left(t_{n-1}+c_j h_n,\ y_{nj}^k,\ y_{nj}^{k-1}\right), \tag{1.3a}$$

where y_{ni}^k $(i=1, 2,\ldots, s)$ satisfy the equations

$$y_{ni}^k = u_{n-1}^k + h_n \sum_{j=1}^{s} a_{ij} F\left(t_{n-1}+c_j h_n,\ y_{nj}^k,\ y_{nj}^{k-1}\right). \tag{1.3b}$$

Here, a_{ij}, b_j, c_j $(i,j=1, 2,\ldots, s)$ denote given real coefficients that define the Runge–Kutta method. Further, $u_0^k=u_0$ (for $k=1, 2, 3,\ldots$) and $y_{ni}^0=U^0(t_{n-1}+c_i h_n)$ (whenever $1\leqslant i\leqslant s$,

$1 \leqslant n \leqslant N$). We let $A = (a_{ij})_{i,j=1}^{s}$, $b = (b_1, b_2, \ldots, b_s)^{\mathrm{T}}$, $c = (c_1, c_2, \ldots, c_s)^{\mathrm{T}}$, and denote the Runge–Kutta method by (A, b, c).

Process (1.3) was considered by Lubich and Ostermann [16] for the case where (1.2) is linear and autonomous. Further, when F is either the Jacobi or the Gauss–Seidel splitting function, (1.3) belongs to the class of discrete time waveform relaxation processes considered by Bellen et al. [1].

Taking the (formal) limit $k \to \infty$ in (1.3), we obtain the following numerical process, which defines approximations u_n to $U(t_n)$ (for $n = 1, 2, \ldots, N$).

$$u_n = u_{n-1} + h_n \sum_{j=1}^{s} b_j f(t_{n-1} + c_j h_n, y_{nj}), \tag{1.4a}$$

where the y_{ni} ($i = 1, 2, \ldots, s$) satisfy

$$y_{ni} = u_{n-1} + h_n \sum_{j=1}^{s} a_{ij} f(t_{n-1} + c_j h_n, y_{nj}). \tag{1.4b}$$

Clearly, (1.4) is the numerical process of the Runge–Kutta method (A, b, c) when applied to (1.1) with (successive) stepsizes $h_1, h_2, \ldots, h_N$.

In this paper we investigate the convergence of the sequence of *discrete time waveforms* $(u_1^k, u_2^k, \ldots, u_N^k)$ ($k = 1, 2, 3, \ldots$), generated by (1.3), to the numerical solution $(u_1, u_2, \ldots, u_N)$ defined by (1.4). We derive a convergence result which is relevant to the case of nonlinear, nonautonomous, stiff initial value problems (1.1). In addition, we consider the convergence of the sequence of *continuous time waveforms* $U^1, U^2, U^3, \ldots$, generated by (1.2), to the solution U of (1.1), where we deal with a norm that forms a continuous analogue to the norm considered in the discrete case.

Let $\langle \cdot, \cdot \rangle$ be any given inner product on $\mathbb{R}^d$, and denote the associated norm on $\mathbb{R}^d$ by $|\cdot|$, i.e., $|x| = \sqrt{\langle x, x \rangle}$ (whenever $x \in \mathbb{R}^d$). Furthermore, let S be any real $d \times d$ matrix such that $\langle \cdot, \cdot \rangle_S$, given by $\langle x, y \rangle_S = \langle Sx, y \rangle$ (whenever $x \in \mathbb{R}^d$, $y \in \mathbb{R}^d$), defines a second inner product on $\mathbb{R}^d$. We deal with the following assumptions on F.

There exists a continuous function $m : [t_0, T] \to (-\infty, 0)$ such that

$$\langle S(F(t, \tilde{y}, z) - F(t, y, z)), \tilde{y} - y \rangle \leqslant m(t) |\tilde{y} - y|^2$$

$$\big(\text{whenever } t \in [t_0, T] \text{ and } y, \tilde{y}, z \text{ in } \mathbb{R}^d\big). \tag{1.5a}$$

There exists a continuous function $L : [t_0, T] \to [0, \infty)$ such that

$$|S(F(t, y, \tilde{z}) - F(t, y, z))| \leqslant L(t) |\tilde{z} - z|$$

$$\big(\text{whenever } t \in [t_0, T] \text{ and } y, z, \tilde{z} \text{ in } \mathbb{R}^d\big). \tag{1.5b}$$

Condition (1.5a) can be viewed as a *one-sided Lipschitz condition* on the function SF w.r.t. its second argument, and condition (1.5b) can be viewed as a *Lipschitz condition* on SF w.r.t. its third argument (cf. e.g. [6,9,11]).

Concerning the Runge–Kutta method (A, b, c), we will assume that it is *algebraically stable* (cf. e.g. [4,6,7,9,11]),

$$b_i > 0 \text{ (for } i = 1, 2, \ldots, s) \text{ and } BA + A^{\mathrm{T}}B - bb^{\mathrm{T}} \text{ is positive-semidefinite,} \tag{1.6a}$$

where B stands for the $s \times s$ diagonal matrix with diagonal entries $b_1, b_2, \dots, b_s$. We will further require that

$$A \text{ is invertible and } 0 \leqslant c_i \leqslant 1 \text{ (for } i = 1, 2, \dots, s). \tag{1.6b}$$

We note that the assumption on the c_i ($i = 1, 2, \dots, s$) is made for ease of presentation of our results.

Let $\Delta y_{ni}^k = y_{ni} - y_{ni}^k$ (whenever $1 \leqslant i \leqslant s$, $1 \leqslant n \leqslant N$, $k \geqslant 0$), $\Delta u_n^k = u_n - u_n^k$ (whenever $0 \leqslant n \leqslant N$, $k \geqslant 1$) and define

$$\Delta Y^k = \left((\Delta y_{11}^k)^{\mathrm{T}}, (\Delta y_{12}^k)^{\mathrm{T}}, \dots, (\Delta y_{Ns}^k)^{\mathrm{T}} \right)^{\mathrm{T}}, \quad \text{for } k = 0, 1, 2, \dots,$$

$$\Delta Z^k = \left((\Delta u_1^k)^{\mathrm{T}}, (\Delta u_2^k)^{\mathrm{T}}, \dots, (\Delta u_N^k)^{\mathrm{T}} \right)^{\mathrm{T}}, \quad \text{for } k = 1, 2, 3, \dots.$$

A short outline of our paper is as follows.

In Section 2.1 we derive an estimate for $|||\, \Delta Y^k \,|||_m$. Here, $|||\cdot|||_m$ denotes a scaled l^2-norm on $((\mathbb{R}^d)^s)^N$, which depends on the function m given by (1.5a). Using the result of Section 2.1, we obtain in Section 2.2 an estimate for $|||\, \Delta Z^k \,|||$. Here, $|||\cdot|||$ is a scaled l^2-norm on $(\mathbb{R}^d)^N$, which is independent of m. Section 2.3 deals with the existence and uniqueness of solutions to the schemes (1.3), (1.4). In Section 2.4 we turn to the continuous time iteration (1.2), and derive an estimate for $|||\, U - U^k \,|||_m$, where, in this case, $|||\cdot|||_m$ denotes a scaled L^2-norm that depends on m, and corresponds to $|||\cdot|||_m$ from the discrete case. If (1.2) is linear and autonomous and the stepsizes h_n ($1 \leqslant n \leqslant N$) are equal, then our norms reduce to the norms considered by Lubich and Ostermann [16]. In Section 2.5 we compare our estimates, specialized to this case, to the optimal estimates that were obtained by Lubich and Ostermann [16] for this situation.

We conclude this introduction with some remarks on assumptions (1.5), (1.6). Firstly, we note that if G is the symmetric, positive-definite matrix such that $\langle x, y \rangle = y^{\mathrm{T}} G x$ (whenever $x \in \mathbb{R}^d$, $y \in \mathbb{R}^d$), then $\langle \cdot, \cdot \rangle_S$ defines an inner product on $\mathbb{R}^d$ if and only if GS is symmetric and positive-definite. Clearly, a suitable matrix S is the $d \times d$ identity matrix. However, this choice for S does not always lead to optimal estimates in our case. By adapting the choice of S to the splitting function F, our estimates often (strongly) improve, cf. Section 2.5.

Next, we remark that conditions (1.5a) and (1.5b) imply

$$\langle f(t, \tilde{y}) - f(t, y), \tilde{y} - y \rangle_S \leqslant \{m(t) + L(t)\} | \tilde{y} - y |^2 \tag{1.7}$$

(whenever $t \in [t_0, T]$, $y \in \mathbb{R}^d$, $\tilde{y} \in \mathbb{R}^d$). This follows directly from (1.5) by using the Cauchy–Schwarz inequality.

Finally, we mention that condition (1.6) is satisfied by many Runge–Kutta methods that are of practical interest, see e.g. [6,9,11]. Our assumption on a Runge–Kutta method is of a different nature than the assumption that was made by Bellen et al. [1] on a (continuous) Runge–Kutta method. It was shown (In 't Hout [13]) that the latter assumption implies a barrier $p \leqslant 4$ on the classical order p of the underlying Runge–Kutta method. On the other hand, it is well known (see e.g. [6,9,11]) that there exist Runge–Kutta methods of arbitrary order which satisfy (1.6).

2. Convergence results

Throughout this paper, I denotes the $d \times d$ identity matrix, O denotes the $s \times s$ zero matrix, $e = (1, 1, \dots, 1)^{\mathrm{T}} \in \mathbb{R}^s$, and $\otimes$ stands for the Kronecker product (see e.g. [9]).

2.1. Estimate for ΔY^k

Processes (1.3) and (1.4) define a mapping of ΔY^{k-1} onto ΔY^k. In this section, we bound ΔY^k in terms of ΔY^{k-1}. We consider the following inner product on $((\mathbb{R}^d)^s)^N$,

$$[X, \tilde{X}]_m = \sum_{n=1}^{N} \sum_{i=1}^{s} h_n\{-m(t_{n-1} + c_i h_n)\} b_i \langle x_{ni}, \tilde{x}_{ni} \rangle,$$

whenever $X = (x_{11}^{\mathrm{T}}, x_{12}^{\mathrm{T}}, \dots, x_{Ns}^{\mathrm{T}})^{\mathrm{T}}$, $\tilde{X} = (\tilde{x}_{11}^{\mathrm{T}}, \tilde{x}_{12}^{\mathrm{T}}, \dots, \tilde{x}_{Ns}^{\mathrm{T}})^{\mathrm{T}}$ with x_{ni}, $\tilde{x}_{ni}$ in $\mathbb{R}^d$ (for $1 \leqslant i \leqslant s$, $1 \leqslant n \leqslant N$). Further, we denote the norm associated with $[\cdot, \cdot]_m$ by $||| \cdot |||_m$. We have:

Theorem 2.1. *Assume the splitting function F satisfies* (1.5) *and the Runge–Kutta method* (A, b, c) *satisfies* (1.6). *Then*

$$||| \Delta Y^k |||_m \leqslant \left(\max_{t \in [t_0, T]} \frac{L(t)}{-m(t)} \right) ||| \Delta Y^{k-1} |||_m, \quad \textit{for } k = 1, 2, 3, \dots.$$

As an immediate corollary of Theorem 2.1 we obtain that, if (1.5) and (1.6) are fulfilled and $m(t) + L(t) < 0$ (for $t \in [t_0, T]$), then $\Delta Y^k \to 0$ (for $k \to \infty$).

Proof. (1) Write

$$\Delta f_{ni}^k = f(t_{n-1} + c_i h_n, y_{ni}) - F\big(t_{n-1} + c_i h_n, y_{ni}^k, y_{ni}^{k-1}\big)$$

(whenever $1 \leqslant i \leqslant s$, $1 \leqslant n \leqslant N$). Then (1.3) and (1.4) imply

$$\Delta u_n^k = \Delta u_{n-1}^k + h_n \sum_{j=1}^{s} b_j \Delta f_{nj}^k, \qquad \Delta y_{ni}^k = \Delta u_{n-1}^k + h_n \sum_{j=1}^{s} a_{ij} \Delta f_{nj}^k.$$

Using that $\Delta u_0^k = 0$, we see

$$\Delta u_n^k = \sum_{m=1}^{n} \sum_{j=1}^{s} h_m b_j \Delta f_{mj}^k,$$

and this yields

$$\Delta y_{ni}^k = \sum_{m=1}^{n-1} \sum_{j=1}^{s} h_m b_j \Delta f_{mj}^k + \sum_{j=1}^{s} h_n a_{ij} \Delta f_{nj}^k$$

(whenever $1 \leqslant i \leqslant s$, $1 \leqslant n \leqslant N$). Defining $\Delta F^k = ((\Delta f_{11}^k)^{\mathrm{T}}, (\Delta f_{12}^k)^{\mathrm{T}}, \dots, (\Delta f_{Ns}^k)^{\mathrm{T}})^{\mathrm{T}}$, we obtain

$$\Delta Y^k = (\hat{A} \otimes I) \Delta F^k,$$

where $\hat{A} = (\hat{A}_{nm})_{n,m=1}^{N}$ with $\hat{A}_{nm} = h_m e b^{\mathrm{T}}$ (whenever $m < n$), $\hat{A}_{nm} = h_n A$ (whenever $m = n$)

and $\hat{A}_{nm} = O$ (for $m > n$). From the assumption that A is invertible it follows that $\hat{A}$ and $(\hat{A} \otimes I)$ are invertible and $(\hat{A} \otimes I)^{-1} = \hat{A}^{-1} \otimes I$ (cf. e.g. [9]). Hence,

$$(\hat{A}^{-1} \otimes I)\Delta Y^k = \Delta F^k.$$

Consider on $((\mathbb{R}^d)^s)^N$ the (second) inner product

$$[X, \tilde{X}]_S = \sum_{n=1}^{N} \sum_{i=1}^{s} h_n b_i \langle x_{ni}, \tilde{x}_{ni} \rangle_S,$$

whenever $X = (x_{11}^{\mathrm{T}}, x_{12}^{\mathrm{T}}, \dots, x_{Ns}^{\mathrm{T}})^{\mathrm{T}}$, $\tilde{X} = (\tilde{x}_{11}^{\mathrm{T}}, \tilde{x}_{12}^{\mathrm{T}}, \dots, \tilde{x}_{Ns}^{\mathrm{T}})^{\mathrm{T}}$ with $x_{ni} \in \mathbb{R}^d$, $\tilde{x}_{ni} \in \mathbb{R}^d$. Then we have

$$[(\hat{A}^{-1} \otimes I)\Delta Y^k, \Delta Y^k]_S = [\Delta F^k, \Delta Y^k]_S.$$

(2) Let (cf. e.g. [9, Definition 5.1.1] and [11, Definition 14.1])

$$\psi[\hat{A}^{-1} \otimes I] = \min \frac{[(\hat{A}^{-1} \otimes I)X, X]_S}{[X, X]_S},$$

where the minimum is taken over all $X \in ((\mathbb{R}^d)^s)^N$ with $X \neq 0$. We will prove that $\psi[\hat{A}^{-1} \otimes I] \geqslant 0$.

Denote by $\hat{B}$ the block-diagonal matrix with diagonal blocks $h_1 B, h_2 B, \dots, h_N B$. Consider on $(\mathbb{R}^s)^N$ the inner product $(V, W) = W^{\mathrm{T}}\hat{B}V$, and define

$$\psi[\hat{A}^{-1}] = \min \frac{(\hat{A}^{-1}V, V)}{(V, V)},$$

where the minimum is over all $V \in (\mathbb{R}^s)^N$ with $V \neq 0$. Then it can be shown (cf. e.g. [9]) that

$$\psi[\hat{A}^{-1} \otimes I] = \psi[\hat{A}^{-1}].$$

In the following, we prove that a Runge–Kutta method with matrix $\hat{A}$ and vector of weights $\hat{b} = (h_1 b^{\mathrm{T}}, h_2 b^{\mathrm{T}}, \dots, h_N b^{\mathrm{T}})^{\mathrm{T}}$ is algebraically stable, and next we obtain that $\psi[\hat{A}^{-1}] \geqslant 0$.

Let $V = (v_1^{\mathrm{T}}, v_2^{\mathrm{T}}, \dots, v_N^{\mathrm{T}})^T \in (\mathbb{R}^s)^N$. Then we have

$$\begin{aligned}
& V^{\mathrm{T}}\left(\hat{B}\hat{A} + \hat{A}^{\mathrm{T}}\hat{B} - \hat{b}\hat{b}^{\mathrm{T}}\right)V \\
&= 2V^{\mathrm{T}}\hat{B}\hat{A}V - (\hat{b}^{\mathrm{T}}V)^2 \\
&= 2\sum_{n=1}^{N} h_n v_n^{\mathrm{T}} B\Big(\sum_{m<n} h_m e b^{\mathrm{T}} v_m + h_n A v_n\Big) - \left(\sum_{n=1}^{N} h_n b^{\mathrm{T}} v_n\right)^2 \\
&= 2\sum_{n=1}^{N} \sum_{m<n} h_n h_m v_n^{\mathrm{T}} b b^{\mathrm{T}} v_m + 2\sum_{n=1}^{N} h_n^2 v_n^{\mathrm{T}} B A v_n - \left(\sum_{n=1}^{N} h_n b^{\mathrm{T}} v_n\right)^2 \\
&\geqslant 2\sum_{n=1}^{N} \sum_{m<n} h_n h_m b^{\mathrm{T}} v_n b^{\mathrm{T}} v_m + \sum_{n=1}^{N} (h_n b^{\mathrm{T}} v_n)^2 - \left(\sum_{n=1}^{N} h_n b^{\mathrm{T}} v_n\right)^2 = 0,
\end{aligned}$$

where the inequality "$\geqslant$" holds by the algebraic stability of (A, b, c).

Next, we have

$$(\hat{A}V, V) = V^{\mathrm{T}}\hat{B}\hat{A}V \geqslant \tfrac{1}{2}(\hat{b}^{\mathrm{T}}V)^2 \geqslant 0 \quad \big(\text{whenever } V \in (\mathbb{R}^s)^N\big),$$

and consequently, $\psi[\hat{A}^{-1}] \geqslant 0$.

(3) Combining parts (1) and (2) we obtain

$$0 \leqslant [\Delta F^k, \Delta Y^k]_S = \sum_{n=1}^{N} \sum_{i=1}^{s} h_n b_i \langle \Delta f_{ni}^k, \Delta y_{ni}^k \rangle_S.$$

Define

$$\Delta g_{ni}^k = F(t_{n-1} + c_i h_n, y_{ni}^k, y_{ni}) - F(t_{n-1} + c_i h_n, y_{ni}^k, y_{ni}^{k-1})$$

(whenever $1 \leqslant i \leqslant s$, $1 \leqslant n \leqslant N$). Using (1.5a), it follows that

$$\begin{aligned}
\langle \Delta f_{ni}^k, \Delta y_{ni}^k \rangle_S &= \langle f(t_{n-1} + c_i h_n, y_{ni}) - F(t_{n-1} + c_i h_n, y_{ni}^k, y_{ni}), \Delta y_{ni}^k \rangle_S \\
&\quad + \langle \Delta g_{ni}^k, \Delta y_{ni}^k \rangle_S \\
&\leqslant m(t_{n-1} + c_i h_n) |\Delta y_{ni}^k|^2 + \langle \Delta g_{ni}^k, \Delta y_{ni}^k \rangle_S \\
&= -m(t_{n-1} + c_i h_n)\left\{ -|\Delta y_{ni}^k|^2 + \langle \Delta \tilde{g}_{ni}^k, \Delta y_{ni}^k \rangle \right\},
\end{aligned}$$

where $\Delta \tilde{g}_{ni}^k = \{-m(t_{n-1} + c_i h_n)\}^{-1} S \Delta g_{ni}^k$ (for $1 \leqslant i \leqslant s$, $1 \leqslant n \leqslant N$). Hence,

$$[\Delta F^k, \Delta Y^k]_S \leqslant -|||\, \Delta Y^k \,|||_m^2 + [\Delta \tilde{G}^k, \Delta Y^k]_m,$$

where $\Delta \tilde{G}^k = ((\Delta \tilde{g}_{11}^k)^{\mathrm{T}}, (\Delta \tilde{g}_{12}^k)^{\mathrm{T}}, \ldots, (\Delta \tilde{g}_{Ns}^k)^{\mathrm{T}})^{\mathrm{T}}$. Thus we obtain

$$|||\, \Delta Y^k \,|||_m^2 \leqslant [\Delta \tilde{G}^k, \Delta Y^k]_m,$$

and from the Cauchy–Schwarz inequality it follows that

$$|||\, \Delta Y^k \,|||_m \leqslant |||\, \Delta \tilde{G}^k \,|||_m.$$

Finally,

$$|||\, \Delta \tilde{G}^k \,|||_m = \sqrt{\sum_{n=1}^{N} \sum_{i=1}^{s} h_n \{-m(t_{n-1} + c_i h_n)\} b_i |\Delta \tilde{g}_{ni}^k|^2},$$

and by (1.5b) we have

$$|\Delta \tilde{g}_{ni}^k| = \{-m(t_{n-1} + c_i h_n)\}^{-1} |S \Delta g_{ni}^k| \leqslant \frac{L(t_{n-1} + c_i h_n)}{-m(t_{n-1} + c_i h_n)} |\Delta y_{ni}^{k-1}|.$$

This yields

$$|||\, \Delta \tilde{G}^k \,|||_m \leqslant \left(\max_{t \in [t_0, T]} \frac{L(t)}{-m(t)} \right) |||\, \Delta Y^{k-1} \,|||_m. \qquad \square$$

2.2. Estimate for ΔZ^k

Using the result for $|||\ \Delta Y^k\ |||_m$ obtained in the previous section, we arrive below at an estimate for $|||\ \Delta Z^k\ |||$. We deal with the following norm on $(\mathbb{R}^d)^N$,

$$|||\ X\ ||| = \sqrt{\sum_{n=1}^{N} h_n |x_n|^2},$$

whenever $X = (x_1^{\mathrm{T}}, x_2^{\mathrm{T}}, \ldots, x_N^{\mathrm{T}})^{\mathrm{T}}$ with $x_n \in \mathbb{R}^d$ $(1 \leqslant n \leqslant N)$,

and define

$$\alpha = 1 - b^{\mathrm{T}}A^{-1}e, \qquad \beta = \max\left\{\frac{|b^{\mathrm{T}}A^{-1}v|}{\sqrt{v^{\mathrm{T}}Bv}} : v \in \mathbb{R}^s,\ v \neq 0\right\}.$$

Theorem 2.2. *Assume F satisfies* (1.5) *and the Runge–Kutta method (A, b, c) satisfies* (1.6). *Let q and r be real numbers with $r|\alpha| < 1$ such that*

$$\sqrt{h_n} \leqslant q r^{n-m} \sqrt{h_m} \quad (\textit{whenever } 1 \leqslant m \leqslant n \leqslant N).$$

Then

$$|||\ \Delta Z^k\ ||| \leqslant \frac{q\beta}{1 - r|\alpha|} \max_{t \in [t_0, T]} \frac{1}{\sqrt{-m(t)}} \left(\max_{t \in [t_0, T]} \frac{L(t)}{-m(t)} \right)^k |||\ \Delta Y^0\ |||_m,$$

for $k = 1, 2, 3, \ldots$.

Proof. Write $\Delta y_{n\cdot}^k = ((\Delta y_{n1}^k)^{\mathrm{T}}, (\Delta y_{n2}^k)^{\mathrm{T}}, \ldots, (\Delta y_{ns}^k)^{\mathrm{T}})^{\mathrm{T}}$ (whenever $1 \leqslant n \leqslant N$). It is easily seen from (1.3), (1.4) that

$$\Delta u_n^k = \alpha \Delta u_{n-1}^k + (b^{\mathrm{T}}A^{-1} \otimes I)\Delta y_{n\cdot}^k,$$

and this implies

$$\text{(i)} \qquad \sqrt{h_n}\,\Delta u_n^k = \sum_{m=1}^{N} c_{nm}\sqrt{h_m}(b^{\mathrm{T}}A^{-1} \otimes I)\Delta y_{m\cdot}^k, \quad \text{for } n = 1, 2, \ldots, N,$$

with $c_{nm} = \sqrt{(h_n/h_m)}\,\alpha^{n-m}$ (for $m \leqslant n$) and $c_{nm} = 0$ (for $m > n$). Let $C = (c_{nm})_{n,m=1}^N$. Define

$$|||\ X\ |||' = \sqrt{\sum_{n=1}^{N} |x_n|^2},$$

whenever $X = (x_1^{\mathrm{T}}, x_2^{\mathrm{T}}, \ldots, x_N^{\mathrm{T}})^{\mathrm{T}}$ with $x_n \in \mathbb{R}^d$ $(1 \leqslant n \leqslant N)$,

and let the matrix norm subordinate to $|||\cdot|||'$ again be denoted by $|||\cdot|||'$. From (i) we obtain

$$\text{(ii)} \qquad |||\ \Delta Z^k\ ||| \leqslant |||\ C \otimes I\ |||' \sqrt{\sum_{n=1}^{N} h_n |(b^{\mathrm{T}}A^{-1} \otimes I)\Delta y_{n\cdot}^k|^2}.$$

Let $\|C\|_1$, $\|C\|_2$ and $\|C\|_\infty$ denote the matrix norms of C subordinate to the sum norm, the Euclidean norm and the maximum norm on $\mathbb{R}^N$, respectively. It can be shown (cf. e.g. [9, Theorem 3.7.8]) that $|||\, C \otimes I\, |||' = \|C\|_2$. Further, it is well known that $\|C\|_2 \leqslant \sqrt{\|C\|_1 \|C\|_\infty}$. We have

$$\|C\|_1 = \max_m \sum_{n=m}^{N} \sqrt{\frac{h_n}{h_m}}\, |\alpha|^{n-m}, \qquad \|C\|_\infty = \max_n \sum_{m=1}^{n} \sqrt{\frac{h_n}{h_m}}\, |\alpha|^{n-m}.$$

One easily sees that $\|C\|_1$ and $\|C\|_\infty$ are both bounded by $q(1-r|\alpha|)^{-1}$, and consequently

$$\text{(iii)} \qquad |||\, C \otimes I\, |||' \leqslant \frac{q}{1-r|\alpha|}.$$

Next, it can be verified (cf. e.g. [9,Theorem 3.7.8]) that

$$|(b^{\mathrm{T}}A^{-1} \otimes I)\Delta y_{n\cdot}^k| \leqslant \beta \sqrt{\sum_{i=1}^{s} b_i |\Delta y_{ni}^k|^2}.$$

Therefore,

$$\begin{aligned}\sqrt{\sum_{n=1}^{N} h_n |(b^{\mathrm{T}}A^{-1} \otimes I)\Delta y_{n\cdot}^k|^2} &\leqslant \beta \sqrt{\sum_{n=1}^{N} \sum_{i=1}^{s} h_n b_i |\Delta y_{ni}^k|^2} \\ &\leqslant \beta \max_{t \in [t_0, T]} \frac{1}{\sqrt{-m(t)}}\, |||\, \Delta Y^k\, |||_m.\end{aligned}$$

By application of Theorem 2.1 we obtain

$$\begin{aligned}\text{(iv)} \qquad &\sqrt{\sum_{n=1}^{N} h_n \left|(b^{\mathrm{T}}A^{-1} \otimes I)\Delta y_{n\cdot}^k\right|^2} \\ &\leqslant \beta \max_{t \in [t_0, T]} \frac{1}{\sqrt{-m(t)}} \left(\max_{t \in [t_0, T]} \frac{L(t)}{-m(t)} \right)^k |||\, \Delta Y^0\, |||_m.\end{aligned}$$

Combining (ii) with inequalities (iii) and (iv), the theorem follows. □

2.3. Existence and uniqueness of solutions to (1.3), (1.4)

Consider the system of equations

$$x_i = \sum_{j=1}^{s} a_{ij} g_j(x_j), \quad \text{for } i = 1, 2, \dots, s, \tag{2.1}$$

where $g_i : \mathbb{R}^d \to \mathbb{R}^d$ ($i = 1, 2, \dots, s$) are given continuous functions. Let $|\cdot|_S$ denote the (vector) norm associated with $\langle \cdot, \cdot \rangle_S$. The following result is well known (cf. e.g. [8,9,11,12]).

Lemma 2.3. *If the Runge–Kutta method* (A, b, c) *satisfies* (1.6a) *and there exists a real number* $\lambda < 0$ *such that*

$$\langle g_i(\tilde{x}) - g_i(x), \tilde{x} - x\rangle_S \leqslant \lambda\,|\tilde{x} - x|_S^2 \quad (\textit{whenever } x \in \mathbb{R}^d,\ \tilde{x} \in \mathbb{R}^d,\ 1 \leqslant i \leqslant s), \tag{2.2}$$

then system (2.1) *has a unique solution* $x_1, x_2, \ldots, x_s$.

From the above lemma, we immediately obtain:

Theorem 2.4. *Assume* F *satisfies* (1.5a) *and* (A, b, c) *satisfies* (1.6). *Then system* (1.3b) *has a unique solution* $y_{n1}^k, y_{n2}^k, \ldots, y_{ns}^k$. *If, in addition,* (1.5b) *holds and* $m(t) + L(t) < 0$ (*for* $t \in [t_0, T]$), *then system* (1.4b) *has a unique solution* $y_{n1}, y_{n2}, \ldots, y_{ns}$.

Note that in Theorem 2.4 there is no restriction on the stepsize h_n.

Proof. System (1.3b) can be written in the form (2.1) with $x_i = y_{ni}^k - u_{n-1}^k$ and $g_i(x) = h_n F(t_{n-1} + c_i h_n, x + u_{n-1}^k, y_{ni}^{k-1})$ (for $i = 1, 2, \ldots, s$). Condition (1.5a) implies that

$$\langle g_i(\tilde{x}) - g_i(x), \tilde{x} - x\rangle_S \leqslant h_n m(t_{n-1} + c_i h_n)\,|\tilde{x} - x|^2$$

(whenever $x \in \mathbb{R}^d$, $\tilde{x} \in \mathbb{R}^d$, $1 \leqslant i \leqslant s$). By equivalence of norms, there exists a real number $\gamma > 0$ such that $|x| \geqslant \gamma\,|x|_S$ (whenever $x \in \mathbb{R}^d$). Therefore, (2.2) is fulfilled with $\lambda = \gamma^2 h_n \max_i m(t_{n-1} + c_i h_n) < 0$, and Lemma 2.3 implies that (1.3b) has a unique solution.

System (1.4b) can be written in the form (2.1) with $x_i = y_{ni} - u_{n-1}$ and $g_i(x) = h_n f(t_{n-1} + c_i h_n, x + u_{n-1})$ (for $i = 1, 2, \ldots, s$). Similarly as above, and using (1.7), it follows that (1.4b) has a unique solution. □

2.4. Estimate for ΔU^k

In this section we obtain a convergence result for the continuous time iteration (1.2). Consider the inner product

$$[\varphi, \tilde{\varphi}]_m = \int_{t_0}^{T} \{-m(t)\}\langle \varphi(t), \tilde{\varphi}(t)\rangle\, \mathrm{d}t,$$

for continuous $\varphi : [t_0, T] \to \mathbb{R}^d$, $\tilde{\varphi} : [t_0, T] \to \mathbb{R}^d$,

denote the norm associated with $[\cdot, \cdot]_m$ by $|||\cdot|||_m$, and let $\Delta U^k = U - U^k$ (for $k = 0, 1, 2, \ldots$). Then we have the following, continuous analogue to Theorem 2.1.

Theorem 2.5. *Assume* F *satisfies* (1.5). *Then*

$$|||\Delta U^k|||_m \leqslant \left(\max_{t \in [t_0, T]} \frac{L(t)}{-m(t)} \right) |||\Delta U^{k-1}|||_m, \quad \textit{for } k = 1, 2, 3, \ldots.$$

Proof. (Cf. part (3) in the proof of Theorem 2.1.) Since

$$\begin{aligned} \tfrac{1}{2}|\Delta U^k(T)|_S^2 &= \tfrac{1}{2}\{|\Delta U^k(T)|_S^2 - |\Delta U^k(t_0)|_S^2\} \\ &= \int_{t_0}^{T} \langle (\Delta U^k)'(t), \Delta U^k(t)\rangle_S\, \mathrm{d}t, \end{aligned}$$

it holds that

$$0 \leqslant \int_{t_0}^{T} \langle (\Delta U^k)'(t),\ \Delta U^k(t) \rangle_S \, \mathrm{d}t.$$

Define

$$\Delta g(t) = F(t,\ U^k(t),\ U(t)) - F(t,\ U^k(t),\ U^{k-1}(t)), \quad \text{for } t \in [t_0,\ T].$$

Then, by (1.5a),

$$\begin{aligned} &\langle (\Delta U^k)'(t),\ \Delta U^k(t) \rangle_S \\ &\quad = \langle F(t,\ U(t),\ U(t)) - F(t,\ U^k(t),\ U(t)),\ \Delta U^k(t) \rangle_S + \langle \Delta g(t),\ \Delta U^k(t) \rangle_S \\ &\quad \leqslant m(t) \,|\, \Delta U^k(t) \,|^2 + \langle \Delta g(t),\ \Delta U^k(t) \rangle_S \\ &\quad = -m(t) \left\{ -|\, \Delta U^k(t) \,|^2 + \langle \Delta \tilde{g}(t),\ \Delta U^k(t) \rangle \right\}, \end{aligned}$$

where $\Delta \tilde{g}(t) = \{-m(t)\}^{-1} S \Delta g(t)$ (for $t \in [t_0,\ T]$). Thus,

$$\int_{t_0}^{T} \langle (\Delta U^k)'(t),\ \Delta U^k(t) \rangle_S \, \mathrm{d}t \leqslant -\ |||\ \Delta U^k\ |||_m^2 + [\Delta \tilde{g},\ \Delta U^k]_m,$$

and we obtain

$$|||\ \Delta U^k\ |||_m^2 \leqslant [\Delta \tilde{g},\ \Delta U^k]_m.$$

Application of the Cauchy–Schwarz inequality yields

$$|||\ \Delta U^k\ |||_m \leqslant\ |||\ \Delta \tilde{g}\ |||_m.$$

Finally, by using (1.5b), it easily follows that

$$|||\ \Delta \tilde{g}\ |||_m \leqslant \left(\max_{t \in [t_0,\ T]} \frac{L(t)}{-m(t)} \right) |||\ \Delta U^{k-1}\ |||_m. \qquad \square$$

2.5. *A comparison for linear autonomous initial value problems*

In this section we specialize our results of Sections 2.1 and 2.4 to the case where (1.2) is linear and autonomous and the stepsizes h_n ($n = 1, 2, \ldots, N$) are equal. We compare the resulting estimates to the optimal estimates that were derived by Lubich and Ostermann [16] in this case, and assess a nontrivial situation in which our estimates are equal.

Let $F(t,\ y,\ z) = Py + Qz$ (whenever $t \in [t_0,\ T]$, $y \in \mathbb{R}^d$, $z \in \mathbb{R}^d$), where P and Q are given real $d \times d$ matrices. Assume $h_n = h > 0$ (for $n = 1, 2, \ldots, N$), and assume the Runge–Kutta method $(A,\ b,\ c)$ satisfies (1.6). For an arbitrary real $d \times d$ matrix M, define its norm and *logarithmic norm* by

$$|\, M \,| = \max\left\{ \frac{|\, Mx \,|}{|\, x \,|} : x \in \mathbb{R}^d,\ x \neq 0 \right\},$$

$$\mu[M] = \max\left\{ \frac{\langle Mx,\ x \rangle}{\langle x,\ x \rangle} : x \in \mathbb{R}^d,\ x \neq 0 \right\},$$

respectively (cf. e.g. [6,9,11]). Further, define

$$||| X ||| = \sqrt{h \sum_{n=1}^{N} \sum_{i=1}^{s} b_i \,| x_{ni} |^2}, \quad \text{whenever } X = \left(x_{11}^{\mathrm{T}}, x_{12}^{\mathrm{T}}, \ldots, x_{Ns}^{\mathrm{T}}\right)^{\mathrm{T}} \in \left((\mathbb{R}^d)^s\right)^N,$$

and

$$||| \varphi ||| = \sqrt{\int_{t_0}^{T} | \varphi(t) |^2 \, \mathrm{d}t}, \quad \text{whenever } \varphi : [t_0, T] \to \mathbb{R}^d \text{ is continuous.}$$

Let $\mathscr{S}$ denote the set of all real $d \times d$ matrices S such that $\langle \cdot, \cdot \rangle_S$ is an inner product on $\mathbb{R}^d$, i.e., $\mathscr{S} = \{S\colon GS$ is symmetric and positive-definite$\}$, where the matrix G is given by $\langle x, y \rangle = y^{\mathrm{T}} G x$ (whenever $x \in \mathbb{R}^d$, $y \in \mathbb{R}^d$). Theorems 2.1 and 2.5 yield

$$||| \Delta Y^k ||| \leqslant \theta \, ||| \Delta Y^{k-1} |||, \qquad ||| \Delta U^k ||| \leqslant \theta \, ||| \Delta U^{k-1} |||, \tag{2.3}$$

with

$$\theta = \theta_1 = \inf\left\{ \frac{| SQ |}{-\mu[SP]} : S \in \mathscr{S},\ \mu[SP] < 0 \right\},$$

provided there exists an $S \in \mathscr{S}$ such that $\mu[SP] < 0$.

Next, let $\langle \cdot, \cdot \rangle^{(\mathrm{c})}$ denote the inner product which forms the extension of $\langle \cdot, \cdot \rangle$ to the complex vectorspace $\mathbb{C}^d$. Let $| x |^{(\mathrm{c})} = \sqrt{\langle x, x \rangle^{(\mathrm{c})}}$ (whenever $x \in \mathbb{C}^d$), and define for any given complex $d \times d$ matrix M, its norm

$$| M |^{(\mathrm{c})} = \max\left\{ \frac{| Mx |^{(\mathrm{c})}}{| x |^{(\mathrm{c})}} : x \in \mathbb{C}^d,\ x \neq 0 \right\}.$$

Lubich and Ostermann [16] showed that, if all eigenvalues of P have negative real parts, then (2.3) is fulfilled with

$$\theta = \theta_2 = \max\left\{ | (\zeta I - P)^{-1} Q |^{(\mathrm{c})} : \zeta \in \mathbb{C},\ \mathrm{Re}(\zeta) \geqslant 0 \right\}.$$

Moreover, the value $\theta = \theta_2$ is the smallest possible bound on $||| \Delta U^k ||| \,/\, ||| \Delta U^{k-1} |||$ which is independent of T and of (continuous) $\Delta U^{k-1} : [t_0, T] \to \mathbb{R}^d$ (cf. [16]). Hence, we have:

Theorem 2.6. *Assume there exists an $S \in \mathscr{S}$ such that $\mu[SP] < 0$. Then $\theta_1 \geqslant \theta_2$.*

Below we give an alternative proof of Theorem 2.6, which does not require the knowledge that θ_2 is optimal.

Proof. Let $S \in \mathscr{S}$ be such that $\mu[SP] < 0$ and let ζ be given with $\mathrm{Re}(\zeta) \geq 0$. It is easily seen that $(\zeta I - P)$ and $(\zeta S - SP)$ are invertible, and

(i) $\quad | (\zeta I - P)^{-1} Q |^{(\mathrm{c})} \leqslant | (\zeta S - SP)^{-1} |^{(\mathrm{c})} \, | SQ |^{(\mathrm{c})}.$

For complex $d \times d$ matrices M, we consider the logarithmic norm

$$\mu^{(c)}[M] = \max\left\{ \operatorname{Re} \frac{\langle Mx, x\rangle^{(c)}}{\langle x, x\rangle^{(c)}} : x \in \mathbb{C}^d,\ x \neq 0 \right\}.$$

By two well-known properties of the logarithmic norm (see e.g. [9]), it holds that

$$|(\zeta S - SP)^{-1}|^{(c)} \leqslant \frac{1}{-\mu^{(c)}[SP - \zeta S]} \quad (\text{whenever } \mu^{(c)}[SP - \zeta S] < 0),$$

and

$$\mu^{(c)}[SP - \zeta S] \leqslant \mu^{(c)}[SP] + \mu^{(c)}[-\zeta S].$$

For $x = v + \mathrm{i}w$ with $v \in \mathbb{R}^d$, $w \in \mathbb{R}^d$, we have

$$\operatorname{Re}\langle -\zeta Sx, x\rangle^{(c)} = \operatorname{Re}(-\zeta)\{\langle v, v\rangle_S + \langle w, w\rangle_S\}.$$

Thus $\mu^{(c)}[-\zeta S] \leqslant 0$, and we obtain

$$\text{(ii)} \qquad |(\zeta S - SP)^{-1}|^{(c)} \leqslant \frac{1}{-\mu^{(c)}[SP]} \quad (\text{whenever } \mu^{(c)}[SP] < 0).$$

From (i) and (ii), and the fact that for real $d \times d$ matrices M one has $|M|^{(c)} = |M|$ and $\mu^{(c)}[M] = \mu[M]$, it follows that

$$|(\zeta I - P)^{-1}Q|^{(c)} \leqslant \frac{|SQ|}{-\mu[SP]}. \qquad \square$$

As a first result on the sharpness of our estimates, we have:

Theorem 2.7. *Suppose* $|\cdot|$ *is the Euclidean norm and* P *is symmetric and negative-definite. Then* $\theta_1 = \theta_2 = |P^{-1}Q|$.

Proof. This follows by considering $S = -P^{-1}$, $\zeta = 0$, and by using Theorem 2.6. □

In particular, the above theorem applies to the case of Jacobi waveform relaxation.

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