QR Methods and Error Analysis for Computing Lyapunov and Sacker-Sell Spectral Intervals for Linear Differential-Algebraic Equations *

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Abstract

In this paper, we propose and investigate numerical methods based on QR factorization for computing all or some Lyapunov or Sacker-Sell spectral intervals for linear differential-algebraic equations. Furthermore, a perturbation and error analysis for these methods is presented. We investigate how errors in the data and in the numerical integration affect the accuracy of the approximate spectral intervals. Although we need to integrate numerically some differential-algebraic systems on usually very long time-intervals, under certain assumptions, it is shown that the error of the computed spectral intervals can be controlled by the local error of numerical integration and the error in solving the algebraic constraint. Some numerical examples are presented to illustrate the theoretical results.

Keywords: differential-algebraic equation, strangeness index, Lyapunov exponent, Sacker-Sell spectrum, exponential dichotomy, spectral interval, smooth QR factorization, QR algorithm, kinematic equivalence, Steklov function

AMS(MOS) subject classification: 65L07, 65L80, 34D08, 34D09

1 Introduction

In this paper we discuss the construction and the analysis of numerical methods for computing spectral intervals of linear systems of differential-algebraic equations (DAEs)

$$E(t)\dot{x} = A(t)x + f(t), \tag{1}$$

on the half-line $\mathbb{I} = [0, \infty)$, together with an initial condition

$$x(0) = x_0. \tag{2}$$

The spectral intervals are associated with the homogenous equation

$$E(t)\dot{x} = A(t)x, \tag{3}$$

and they allow the analysis of the asymptotic behavior or the growth rate of solutions to initial value problems.

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Here we assume that $E, A \in C(\mathbb{I}, \mathbb{R}^{n \times n})$ and $f \in C(\mathbb{I}, \mathbb{R}^n)$ are sufficiently smooth functions. We use the notation $C(\mathbb{I}, \mathbb{R}^{n \times n})$ to denote the space of continuous functions from $\mathbb{I}$ to $\mathbb{R}^{n \times n}$.

Linear systems of the form (1) occur when one linearizes a general implicit nonlinear system of DAEs $F(t, x, \dot{x}) = 0,\ t \in \mathbb{I}$, along a particular solution [9]. In this paper we restrict ourselves to *regular* DAEs, i.e., we require that (1) has a unique solution for sufficiently smooth E, A, f and appropriately chosen (consistent) initial conditions, see [36] for a discussion of existence and uniqueness of solution of more general nonregular DAEs.

DAEs arise in constrained multibody dynamics [27], electrical circuit simulation [32, 33], chemical engineering [25, 26] and many other applications, i n particular when the dynamics of a system is constrained or when different physical models are coupled together in automatically generated models [42]. While DAEs provide a very convenient modelling concept, many numerical difficulties arise due to the fact that the dynamics is constrained to a manifold, which often is only given implicitly, see [36]. These difficulties are typically characterized by one of many index concepts see [7, 31, 34, 36].

The stability theory for ordinary differential equations (ODEs) and its important part, the spectral theory, whose basic concepts and fundamental results were already developed by Lyapunov in [41], was studied extensively in the last 100 years, see [1] and references therein. Numerical methods for computing spectral intervals were introduced and analyzed since 1980, see [4, 30, 28]. However, only recently, a sequence of works by Dieci and Van Vleck gave a mathematically rigorous verification for these methods [20, 21, 22, 23, 24].

The stability theory for DAEs has been developed much more recently. The fact that the dynamics of DAEs is constrained, also requires a modification of most classical concepts of the qualitative theory that was developed for ODEs. Only recently, the spectral theory has been extended from ODEs to DAEs, see [12, 13, 11] and [40]. In particular, in [40], the classical spectral concepts (Lyapunov, Bohl, Sacker-Sell spectral intervals) for ODEs were extended systematically to general linear DAEs with variable coefficients of the form (1). It was shown that substantial differences in the theory arise and that most statements in the classical ODE theory hold for DAEs only under further restrictions. Furthermore, in [40] also an initial attempt to develop QR methods for computing spectral intervals of DAEs was presented. These methods use the underlying implicit ODEs for the computation of the spectral intervals.

In this paper we develop new QR methods that apply directly to DAEs. Furthermore, following the ideas given in [21, 22, 24] for ODEs, we also present a perturbation and error analysis which proves the applicability of our algorithms. One of the most important results that we show here is that, although we need to numerically integrate some DAE systems on usually very long time-intervals, the error in the spectral intervals depends essentially only on the local error of the numerical integration, the error arising in the solution of the algebraic constraint equations, and on the degree to which the DAE is integrally separated. These errors, however, can be easily kept under control by using an appropriate integration method for strangeness-free DAEs accompanied with a local error estimator and stepsize control, while integral separation is a natural and prevalent structural condition that is also central to the robustness of Lyapunov exponents. Our emphasis in this work is on strangeness-free DAEs that enjoy the integral separation property. Results in the spirit of the present work in the non-integrally separated case for ODEs appear in [22] and [23].

The outline of the paper is as follows. In the next section, we recall some fundamental concepts and results from the spectral theory of differential-algebraic equations as developed in [40]. In Section 3, we construct new discrete and continuous QR methods for approximating the spectral intervals and discuss their implementation. These new QR methods are compared with those proposed in [40]. A detailed perturbation and error analysis for the new QR methods is given in Section 4. Finally, in Section 5 we present numerical examples to illustrate the theoretical results and the properties of the numerical methods. We finish the paper with some conclusions.

2 Spectral theory for DAEs

General linear DAEs with variable coefficients have been studied in detail in the last twenty years, see [36] and the references therein. In order to understand the solution behavior and to solve them numerically, it is essential to incorporate the necessary information about derivatives of equations into the system. This has led to the concept of the strangeness-index, which under very mild assumptions allows for the DAE and (some of) its derivatives to be reformulated as a system with the same solution, that is strangeness-free, i.e., no further differentiations are needed and the algebraic and differential part of the system are separated. Note that we have assumed that the system is regular, otherwise also consistency conditions would arise. With this in mind, we may assume that the homogeneous DAE in consideration is already strangeness-free and has the form

$$E(t)\dot{x} = A(t)x, \quad t \in \mathbb{I}, \tag{4}$$

where

$$E(t) = \begin{bmatrix} E_1(t) \\ 0 \end{bmatrix}, \; A(t) = \begin{bmatrix} A_1(t) \\ A_2(t) \end{bmatrix},$$

$E_1 \in C(\mathbb{I}, \mathbb{R}^{d\times n})$ and $A_2 \in C(\mathbb{I}, \mathbb{R}^{(n-d)\times n})$ are such that the matrix

$$\bar{E}(t) := \begin{bmatrix} E_1(t) \\ A_2(t) \end{bmatrix} \tag{5}$$

is invertible for all t. As a direct consequence, then E_1 and A_2 are of full row-rank. For the numerical analysis, the solutions of (4) (and the coefficients E, A) are supposed to be sufficiently smooth so that the convergence result for the numerical methods [36] applied to (4) hold. It should be already noted here that the conditioning of the matrix $\bar{E}$ with respect to inversion will be an essential factor in the error analysis.

2.1 Lyapunov exponents and Lyapunov spectral intervals

We first discuss the concepts of Lyapunov exponents and Lyapunov spectral intervals.

Definition 1 *A matrix function* $X \in C^1(\mathbb{I}, \mathbb{R}^{n\times k})$, $\quad d \le k \le n$, *is called* fundamental solution matrix of (4) *if each of its columns is a solution to (4) and* $\operatorname{rank} X(t) = d$ *for all* $t \in \mathbb{I}$.

A fundamental solution matrix is said to be maximal *if* $k = n$ *and* minimal *if* $k = d$*, respectively.*

A major difference between ODEs and DAEs is that fundamental solution matrices for DAEs are not necessarily square and of full-rank. Every fundamental solution matrix of a strangeness-free DAE (4) with d differential equations has exactly d linearly independent columns and a minimal fundamental matrix solution can be easily made maximal by adding $n-d$ zero columns.

Definition 2 *For a given fundamental solution matrix X of a strangeness-free DAE system of the form (4) and for $d \le k \le n$, we introduce*

$$\lambda_i^u = \limsup_{t\to\infty} \frac{1}{t} \ln \|X(t)e_i\| \;\; \textit{and} \;\; \lambda_i^\ell = \liminf_{t\to\infty} \frac{1}{t} \ln \|X(t)e_i\|, \quad i = 1, 2, ..., k,$$

where e_i denotes the i-th unit vector. The columns of a minimal fundamental solution matrix form a normal basis *if* $\Sigma_{i=1}^d \lambda_i^u$ *is minimal. The* $\lambda_i^u, i = 1, 2, ..., d$, *belonging to a normal basis are called* (upper) Lyapunov exponents *and the intervals* $[\lambda_i^\ell, \lambda_i^u], i = 1, 2, ..., d$, *are called* Lyapunov spectral intervals. *The set of the Lyapunov spectral intervals is called the* Lyapunov spectrum Σ_L *of (4). The DAE is called* Lyapunov regular *if all spectral intervals consist of single points.*

Definition 3 *Suppose that* $U \in C(\mathbb{I}, \mathbb{R}^{n\times n})$ *and* $V \in C^1(\mathbb{I}, \mathbb{R}^{n\times n})$ *are nonsingular matrix functions such that V and V^{-1} are bounded. Then the transformed DAE system*

$$\tilde{E}(t)\dot{\tilde{x}} = \tilde{A}(t)\tilde{x}, \tag{6}$$

with $\tilde{E} = UEV$, $\tilde{A} = UAV - UE\dot{V}$ *and* $x = V\tilde{x}$ *is called* globally kinematically equivalent *to (4) and the transformation is called a* global kinematic equivalence transformation. *If* $U \in C^1(\mathbb{I}, \mathbb{R}^{n\times n})$ *and, furthermore, also* U *and* U^{-1} *are bounded then we call this a* strong global kinematic equivalence transformation.

It is clear that the Lyapunov exponents of a DAE system as well as the normality of a basis formed by the columns of a fundamental solution matrix are preserved under global kinematic equivalence transformations. The following lemma is the key to constructing and understanding QR methods and it is in fact a simplified version of [40, Lemma 7].

Lemma 4 *Consider a strangeness-free DAE system of the form (4) with continuous coefficients and a minimal fundamental solution matrix* X*. Then there exist matrix functions* $V \in C(\mathbb{I}, \mathbb{R}^{n\times d})$ *and* $U \in C^1(\mathbb{I}, \mathbb{R}^{n\times d})$ *with orthonormal columns such that in the fundamental matrix equation* $E\dot{X} = AX$ *associated with (4), the change of variables* $X = UR$*, with* $R \in C^1(\mathbb{I}, \mathbb{R}^{d\times d})$ *upper triangular with positive diagonal elements, and the multiplication of both sides of the system from the left with* V^T *leads to the system*

$$\mathcal{E}\dot{R} = \mathcal{A}R, \tag{7}$$

where $\mathcal{E} := V^T EU$ *is nonsingular,* $\mathcal{A} := V^T AU - V^T E\dot{U}$*, and both of them are upper triangular.*

Proof. Since a smooth and full column rank matrix function has a smooth QR decomposition, see [15, Prop. 2.3], there exists a matrix function U with orthonormal columns such that $X = UR$, where R is nonsingular and upper triangular. This decomposition is unique if the diagonal elements of R are chosen positive. By substituting $X = UR$ into the fundamental matrix equation $E\dot{X} = AX$, we obtain

$$EU\dot{R} = (AU - E\dot{U})R. \tag{8}$$

Since we have assumed that the DAE is strangeness-free and since $A_2U = 0$, we have that the matrix EU must have full column-rank. Thus, there exists a smooth QR decomposition

$$EU = V\mathcal{E},$$

where the columns of V are orthornormal and $\mathcal{E}$ is upper triangular with positive diagonal elements. Multiplying both sides of (8) by V^T, we obtain

$$\mathcal{E}\dot{R} = [V^T AU - V^T E\dot{U}]R.$$

The matrix function $\mathcal{A} := V^T AU - V^T E\dot{U}$ is upper triangular as well. This completes the proof. □

Remark 5 Lemma 4 holds for arbitrary matrix functions $X \in C^1(\mathbb{I}, \mathbb{R}^{n\times p})$, with columns that are linearly independent solutions of (4). However, this lemma shows only the existence of a pair of orthogonal matrix functions U and V that brings the system into upper triangular implicit ODE form. In practice it is necessary to construct these transformation matrices numerically. The construction of U, V was introduced in [40] for implicit ODEs and also implemented in the continuous QR algorithm presented there. In Section 3, we will extend that construction to the general case of (4) and also to the case that only the QR decomposition of parts of the fundamental solution matrix is computed.

System (7) is an implicit ODE, since $\mathcal{E}$ is nonsingular. It is called *essentially underlying implicit ODE system* (EUODE) of (4), and it can be turned into an ODE by multiplication with $\mathcal{E}^{-1}$ from the left. The idea of constructing EUODEs as in Lemma 4 was used in [3] for properly-formulated linear DAEs and their adjoints. Since orthonormal changes of basis keep the Euclidean norm invariant, the Lyapunov exponents of the columns of the matrices X and R, and therefore those of the two systems are the same. Thus, in theory, the spectral analysis of the DAE (4) can be carried via its EUODE, provided that the data of the EUODE can be computed accurately, which is not the case if $\mathcal{E}$ is ill-conditioned.

2.2 Stability of Lyapunov exponents

In order to study the behavior of Lyapunov exponents under small perturbations, we consider a perturbed system of DAEs

$$[E(t) + \Delta E(t)]\dot{x} = [A(t) + \Delta A(t)]x, \quad t \in \mathbb{I}, \tag{9}$$

where we restrict the perturbations to have the form

$$\Delta E(t) = \begin{bmatrix} \Delta E_1(t) \\ 0 \end{bmatrix}, \ \Delta A(t) = \begin{bmatrix} \Delta A_1(t) \\ \Delta A_2(t) \end{bmatrix}.$$

Here ΔE and ΔA are assumed to be as smooth as E and A, respectively. Perturbations of this structure are called *admissible*. The DAE (4) is said to be *robustly strangeness-free* if it is still strangeness-free under all sufficiently small admissible perturbations. Note that it is essential to restrict the perturbations to this structure, since otherwise arbitrary small perturbations can change the strangeness-index and therefore also the smoothness-requirements of the system, see [35].

It is also easy to see that the DAE (4) is robustly strangeness-free under admissible perturbations if and only if the matrix function $\bar{E}$ as in (5) is boundedly invertible.

In the following we restrict ourselves to robustly strangeness-free DAE systems under admissible perturbations.

Definition 6 *The upper Lyapunov exponents $\lambda_1^u \geq ... \geq \lambda_d^u$ of (4) are said to be* stable *if for any $\epsilon > 0$, there exists $\delta > 0$ such that the conditions $\sup_t \|\Delta E(t)\| < \delta$, $\sup_t \|\Delta A(t)\| < \delta$ on the admissible perturbations imply that the perturbed DAE system (9) is strangeness-free, with the same number of d differential equations and a algebraic equations, and*

$$|\lambda_i^u - \gamma_i^u| < \epsilon, \qquad \text{for all } i = 1, 2, ..., d,$$

where the γ_i^u are the ordered upper Lyapunov exponents of the perturbed system (9).

It is clear that the stability of upper Lyapunov exponents is invariant under strong global kinematic equivalence transformations.

Another concept that is needed in the following is that of integral separation.

Definition 7 *A minimal fundamental solution matrix X for (4) is called* integrally separated *if for $i = 1, 2, ..., d-1$ there exist constants $c_1 > 0$ and $c_2 > 0$ such that*

$$\frac{\|X(t)e_i\|}{\|X(s)e_i\|} \cdot \frac{\|X(s)e_{i+1}\|}{\|X(t)e_{i+1}\|} \geq c_2 e^{c_1(t-s)},$$

for all t, s with $t \geq s \geq 0$. If a DAE system has an integrally separated minimal fundamental solution matrix, then we say it has the integral separation property*.*

The integral separation property is invariant under strong global kinematic equivalence transformations. Furthermore, by using the EUODE (7) and the result on the stability of Lyapunov exponents for ODEs [1], it is not difficult to show that if the upper Lyapunov exponents of (4) are distinct, then they are stable under admissible perturbations if and only if there exists an integrally separated fundamental matrix and some extra boundedness conditions posed on E, A hold, see [40, Section 3.2].

The integral separation of a fundamental matrix solution can be equivalently expressed in terms of the integral separation of a sequence of functions. Two continuous and bounded functions g_1 and g_2 are said to be integrally separated if there exist constants $c_1, c_2 \geq 0$, such that

$$\int_s^t (g_1(r) - g_2(r))\, dr \geq c_1(t-s) - c_2, \quad \text{for all } t > s \geq 0.$$

In practice, the integral separation of two functions can be tested via their Steklov difference. Given $H > 0$, we introduce the *Steklov averages* defined by

$$g_i^H(t) := \frac{1}{H}\int_t^{t+H} g_i(r)dr, \quad (i = 1, 2).$$

It was shown in [1] that two functions g_1, g_2 are integrally separated if and only if there exists a scalar $H > 0$ such that their *Steklov difference* is positive, i.e., for H sufficiently large, there exists a constant $c > 0$ such that

$$g_1^H(t) - g_2^H(t) \geq c > 0, \qquad \text{for all } t \geq 0.$$

For further discussions on integral separation and its importance in the course of approximating Lyapunov exponents, see [20, 22, 23, 24].

2.3 Sacker-Sell spectrum and Bohl exponents

The second spectral concept that we discuss is that of exponential dichotomy. For this we introduce shifted DAE systems.

Definition 8 *Consider a strangeness-free DAE of the form (4). For $\lambda \in \mathbb{R}$, the DAE system*

$$E(t)\dot{x} = [A(t) - \lambda E(t)]x, \quad t \in \mathbb{I}, \tag{10}$$

is called a shifted DAE system.

By using the transformation as in Lemma 4, we obtain the corresponding shifted EUODE for (10)

$$\mathcal{E}\dot{z} = (\mathcal{A} - \lambda\mathcal{E})z. \tag{11}$$

The DAE (4) is said to have exponential dichotomy if its corresponding EUODE has exponential dichotomy.

Definition 9 *The* Sacker-Sell (or exponential dichotomy) spectrum *of the DAE system (4) is defined by*

$$\Sigma_S := \{\lambda \in \mathbb{R}, \text{ the shifted DAE (10) does not have an exponential dichotomy}\}. \tag{12}$$

This means that the Sacker-Sell spectrum of the DAE system (4) is exactly the Sacker-Sell spectrum of its EUODE (7).

For the numerical computation of the Sacker-Sell spectrum we actually make use of the Bohl exponents of the DAEs. These exponents were introduced in [6] for ODEs, see also [14], and extended to DAEs in [40].

Definition 10 *Let x be a nontrivial solution of (4). The* (upper) Bohl exponent $\kappa_B^u(x)$ *of this solution is the greatest lower bound of all those values ρ for which there exists a constant $N_\rho > 0$ such that*

$$\|x(t)\| \leq N_\rho e^{\rho(t-s)} \|x(s)\| \tag{13}$$

for all $t \geq s \geq 0$. If such numbers ρ do not exist, then one sets $\kappa_B^u(x) = +\infty$.

Similarly, the lower Bohl exponent $\kappa_B^\ell(x)$ is the least upper bound of all those values ρ' for which there exists a constant $N'_\rho > 0$ such that

$$\|x(t)\| \geq N'_\rho e^{\rho'(t-s)} \|x(s)\|, \quad 0 \leq s \leq t. \tag{14}$$

It follows directly from the definition that Lyapunov exponents and Bohl exponents are related via

$$\kappa_B^\ell(x) \le \lambda^\ell(x) \le \lambda^u(x) \le \kappa_B^u(x).$$

Bohl exponents characterize the uniform growth rate of solutions, while Lyapunov exponents simply characterize the growth rate of solutions departing from $t = 0$. The formulas of Bohl exponents for ODEs, see e.g. [14], directly generalize to solutions x of DAEs, i.e.

$$\kappa_B^u(x) = \limsup_{s,t-s\to\infty} \frac{\ln\|x(t)\| - \ln\|x(s)\|}{t-s}, \quad \kappa_B^\ell(x) = \liminf_{s,t-s\to\infty} \frac{\ln\|x(t)\| - \ln\|x(s)\|}{t-s}, \tag{15}$$

and therefore the endpoints of the Sacker-Sell spectral intervals can be computed by the Bohl exponents of certain fundamental solutions, see [40]. Moreover, unlike the Lyapunov exponents, under admissible perturbations, the Bohl exponents are stable without any extra assumption, see [11, 40]. We will use the Bohl exponents to compute the end-points of the Sacker-Sell spectral intervals.

2.4 Obtaining Rates and Directions

In this section we discuss why in the case of integrally separated EUODE (7) robust Lyapunov exponents and Sacker-Sell spectrum/Bohl exponents may be obtained from the diagonal of R. In particular, if for some nonsingular, upper triangular R_0 the fundamental matrix solution R of EUODE (7) with $R(0) = R_0$ is integrally separated, and for $\mathcal{E} = [e_{i,j}]$, $\mathcal{A} = [a_{i,j}]$ both upper triangular, then it follows from [23, Theorems 6.1 and 6.2] applied to $\mathcal{E}^{-1}\mathcal{A}$ that robust (upper) Lyapunov exponents are given by

$$\lambda_i = \limsup_{t\to\infty} \frac{1}{t}\int_0^t \frac{a_{i,i}(s)}{e_{i,i}(s)}ds$$

and the upper and lower Bohl exponents are given by

$$\alpha_i = \inf_{t_0}\liminf_{t\to\infty} \frac{1}{t}\int_{t_0}^{t_0+t} \frac{a_{i,i}(s)}{e_{i,i}(s)}ds, \;\; \beta_i = \sup_{t_0}\limsup_{t\to\infty} \frac{1}{t}\int_{t_0}^{t_0+t} \frac{a_{i,i}(s)}{e_{i,i}(s)}ds.$$

To obtain the directions associated with the rates of growth defined by the diagonal elements of $R(t)$, we consider the approach taken in [20] for the case of integrally separated fundamental solution matrices. In particular, consider $\mathrm{diag}(R(t))^{-1}R(t)$ with $R(t)$ integrally separated. Then it is shown in [20, Lemma 7.4] that $\lim_{t\to\infty}\mathrm{diag}(R(t))^{-1}R(t)$ exists and is a unit upper triangular matrix $\overline{Z}$. Thus, to determine initial conditions that asymptotically behave in accordance with the rate given by the i-th diagonal entry, one solves the linear system $\overline{Z}x_0 = e_i$ for the initial condition x_0.

3 QR Methods for DAEs

In this section we derive numerical methods to compute the Lyapunov and Bohl exponents. We extend the approaches using smooth QR factorizations that were derived for the computation of spectral intervals for ODEs in [19, 20, 23] to DAEs. We assume again that the DAE system is given in strangeness-free form (4), i.e., whenever the evaluation of the functions $E(t), A(t)$ is needed, this has to be computed from the derivative array as described in [36]. This can be done for example with the `FORTRAN` code `GELDA` [38] or the corresponding `MATLAB` version [39]. QR methods for computing Lyapunov and Sacker-Sell spectra of DAEs in strangeness-free form were first suggested in [40], on the basis of using the EUODE. In the following we will extend and improve these methods.

Let us briefly recall the main idea leading to the methods given in [40]. We determine a smooth orthogonal matrix function $\tilde{Q} \in C^1(\mathbb{I}, \mathbb{R}^{n\times n})$ such that

$$A_2\tilde{Q} = \begin{bmatrix} 0 & \tilde{A}_{22} \end{bmatrix}, \tag{16}$$

with $\tilde{A}_{22}$ pointwise nonsingular. It has been shown in [10, 15], that such a $\tilde{Q}$ always exists. Moreover, it can be assumed that $\tilde{A}_{22}$ is upper triangular. It is also clear that in general $\tilde{Q}$ is not unique. However, since this transformation is a kinematic equivalence transformation, the spectra of the original and the transformed system are the same. So, matrix functions $\tilde{Q}$ may be chosen to be different, but at the end the computed spectral intervals are the same.

The transformation $\tilde{x} = \tilde{Q}^T x$ leads to a transformed homogeneous DAE for $\tilde{x}$ with coefficients

$$\begin{bmatrix} \tilde{E}_{11} & \tilde{E}_{12} \\ 0 & 0 \end{bmatrix} := \begin{bmatrix} E_1 \\ 0 \end{bmatrix} \tilde{Q}, \quad \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix} := \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \tilde{Q} - \begin{bmatrix} E_1 \\ 0 \end{bmatrix} \dot{\tilde{Q}}. \tag{17}$$

Since in this form the solution component $\tilde{x}_2$ associated with the algebraic equations vanishes identically, i.e., $\tilde{x}_2 = 0$, the spectral intervals of the DAE are those of the underlying implicit ODE

$$\tilde{E}_{11}\dot{\tilde{x}}_1 = \tilde{A}_{11} x_1. \tag{18}$$

In this way, the discrete and continuous QR method for ODEs of [20] could be easily adopted to DAEs, see [40].

In this paper, however, we propose discrete and continuous QR methods which apply directly to (4). Furthermore, in contrast to [40] and all the methods for ODEs, we also consider the case that only parts of the spectral intervals are computed. For this, let $X \in C^1(\mathbb{I}, \mathbb{R}^{n\times p})$ be an arbitrary matrix function whose columns are linearly independent solutions of (4), with $X_0 := X(0)$ given, $1 \le p \le d$. For the computation of the spectral intervals, we want to determine a factorization $X(t) = Q(t)R(t)$, $t \in \mathbb{I}$, where the columns of $Q(t)$ are orthonormal, i.e., $Q^T(t)Q(t) = I_p$, and $R(t)$ is upper triangular. It is clear that if the diagonal elements of R are chosen positive, then such a pair of matrix functions Q and R exists and is unique.

3.1 Discrete QR algorithm

In the discrete QR algorithm, the fundamental solution matrix X and its triangular factor R are indirectly evaluated by a reorthogonalized integration of the DAE system (4) via an appropriate QR factorization. We first choose a mesh $0 = t_0 < t_1 < ... < t_{N-1} < t_N = T$. At t_0, we perform the QR factorization

$$X_0 = Q(t_0)R(t_0),$$

where $R(t_0)$ has positive diagonal elements.

For $j = 1, 2, \ldots, N$, let $X(t, t_{j-1})$ be the numerical solution (via numerical integration) to the matrix initial value problem

$$\begin{aligned} E(t)\dot{X}(t, t_{j-1}) &= A(t)X(t, t_{j-1}), \quad t_{j-1} \le t \le t_j, \\ X(t_{j-1}, t_{j-1}) &= Q(t_{j-1}). \end{aligned} \tag{19}$$

We stress that $Q(t_{j-1})$ defined in this way is a consistent initial value assigned at t_{j-1} for the DAE system (4).

Then we carry out the QR factorization

$$X(t_j, t_{j-1}) = Q(t_j)R(t_j, t_{j-1}), \tag{20}$$

where $R(t_j, t_{j-1}) =: [r_{k,\ell}(t_j, t_{j-1})]$ has positive diagonal elements. The value of the matrix function X at time t_j is then determined by

$$X(t_j) = Q(t_j)R(t_j, t_{j-1})R(t_{j-1}, t_{j-2}) \ldots R(t_2, t_1)R(t_1, t_0)R(t_0), \tag{21}$$

which is again a QR factorization with positive diagonal elements. Since this is unique, for the QR factorization $X(t_j) = Q(t_j)R(t_j)$ with positive diagonal elements in $R(t_j) =: [r_{k,\ell}(t_j)]$, we have

$$R(t_j) = R(t_j, t_{j-1})R(t_{j-1}, t_{j-2}) \ldots R(t_2, t_1)R(t_1, t_0)R(t_0). \tag{22}$$

Thus, in particular, we have

$$\frac{1}{t_j}\ln[r_{i,i}(t_j)] = \frac{1}{t_j}\ln\prod_{\ell=1}^{j}[r_{i,i}(t_j,t_{j-1})] = \frac{1}{t_j}\sum_{\ell=1}^{j}\ln[r_{i,i}(t_j,t_{j-1})], \quad i=1,2,\ldots,p, \tag{23}$$

and we define functions $\lambda_i(t)$ via

$$\lambda_i(t) := \frac{1}{t}\ln[r_{i,i}(t)], \quad i=1,2,\ldots,p. \tag{24}$$

Then, under the assumption that the columns of X (or equivalently those of R) are integrally separated, we can approximate the Lyapunov spectral intervals by solving the associated optimization problems $\inf_{\tau\le t\le T}\lambda_i(t)$ and $\sup_{\tau\le t\le T}\lambda_i(t)$, $i=1,2,\ldots,p$, respectively, with a given $\tau\in(0,T)$.

The approximation of the Bohl exponents and hence of the Sacker-Sell spectrum is carried out analogously, see [40], by solving appropriate optimization problems associated with (15). Namely, with $H>0$, we define

$$\psi_{H,i}(t) := \frac{1}{H}(\ln[r_{i,i}(t+H)] - \ln[r_{i,i}(t)]). \tag{25}$$

It has been shown in [20, 40] that the Sacker-Sell spectral intervals for (4) can be approximated by $\inf_{0\le t\le T-H}\psi_{H,i}(t)$ and $\sup_{0\le t\le T-H}\psi_{H,i}(t)$, where $H>0$ is chosen sufficiently large.

We summarize the discrete QR algorithm in the following procedure.

Algorithm 1 (Discrete QR algorithm for computing Lyapunov spectra)

- **Input:** `A pair of sufficiently smooth matrix functions` (E,A) `in the form of the strangeness-free DAE (4) (if they are not available directly they must be computed pointwise as output of a routine such as GELDA), a time interval` $[0,T]$, $\tau, H \in (0,T)$, `a mesh` $0=t_0<t_1<\ldots<t_{N-1}<t_N=T$ `and an initial matrix` $X_0\in\mathbb{R}^{n\times p}$.
- **Output:** `Approximate bounds for the spectral intervals` $\{\lambda_i^l,\lambda_i^u\}_{i=1}^p$, `associated with the first` p `columns of the fundamental solution matrix` $X(t)$.
- **Initialization:**
  1. Set $t_0:=0$, and determine the QR factorization

     $$X(t_0)=Q_0R_0,$$

     where R_0 has positive diagonal elements.
  2. Set $\lambda_i(t_0):=0$ and $s_i(t_0):=0$ for $i=1,\ldots,p$ (for computing the sum in (23)).

  While $j<N$

  1. $j:=j+1$.
  2. Solve the initial value problem (19) for $X(t,t_{j-1})$ on $[t_{j-1},t_j]$. Denote the computed numerical solution at $t=t_j$ by $\bar{X}(t_j,t_{j-1})$.
  3. Compute the QR factorization $\bar{X}(t_j,t_{j-1}) = Q_jR_j$ with positive diagonal elements $(r^j)_{i,i}$, $i=1,\ldots,p$.
  4. Update $s_i(t_j):=s_i(t_{j-1})+\ln[r^j_{i,i}]$ and $\lambda_i(t_j)=\frac{1}{t_j}s_i(t_j)$, $\quad i=1,2,\ldots,p$.
  5. If desired, check the integral separation property by using $\{s_i\}_{i=1}^p$.
  6. Update $\min_{\tau\le t\le t_j}\lambda_i(t)$ and $\max_{\tau\le t\le t_j}\lambda_i(t)$, $i=1,2,\ldots,p$.

The corresponding algorithm for computing the Bohl exponents and hence the Sacker-Sell spectra is almost the same. The only difference is that in Step 6 of the algorithm, we update

$$\min_{0\le t\le t_j-H} s_i^H(t), \quad \max_{0\le t\le t_j-H} s_i^H(t),$$

for $t_j > H$, where

$$s_i^H(t) := \frac{1}{H}(s_i(t+H) - s(t)).$$

Remark 11 Algorithm 1 is almost the same as the corresponding discrete QR algorithm for ODEs. The only differences are that an appropriate implicit DAE solver, e.g., a BDF or IRK method, see [36], must be used for integrating the initial value problem (19) and that a consistent initial value has to be computed to start the integration in each step.

It is not difficult to see that Algorithm 1 and the discrete QR method suggested in [40] are mathematically equivalent, i.e., in exact arithmetic they produce the same factors R_j, and consequently, also the same Lyapunov exponents $\lambda_i(t_j)$. Indeed, if at $t = t_j$ we compute $\tilde{Q}(t_j)$ defined by (16), then,

$$X(t_j) = \tilde{Q}(t_j)^T \begin{bmatrix} \tilde{X}(t_j) \\ 0 \end{bmatrix}$$

and

$$X(t_j, t_{j-1}) = \tilde{Q}(t_j)^T \begin{bmatrix} \tilde{X}(t_j, t_{j-1}) \\ 0 \end{bmatrix} = \tilde{Q}(t_j)^T \begin{bmatrix} \hat{Q}(t_j) \\ 0 \end{bmatrix} \hat{R}(t_j, t_{j-1}),$$

where $\tilde{X}(t_j, t_{j-1})$ is the corresponding solution to the underlying ODE (18) that satisfies $\tilde{X}(t_{j-1}, t_{j-1}) = \hat{Q}(t_{j-1})$ and the factorization $\tilde{X}(t_j, t_{j-1}) = \hat{Q}(t_j)\hat{X}(t_j, t_{j-1})$ is determined for the first p columns of the matrices computed in [40]. Due to the uniqueness of the QR factorization, we obtain

$$R(t_j, t_{j-1}) = \hat{R}(t_j, t_{j-1}) \text{ and } Q(t_j) = \tilde{Q}(t_j)^T \begin{bmatrix} \hat{Q}(t_j) \\ 0 \end{bmatrix}.$$

This variant is less advantageous from a computational point of view, because the extra task of evaluating $\tilde{Q}(t_j)$ is needed. However, this computationally redundant transformation gives us an insight in what happens in the background of the algorithm. In fact, we actually compute QR factorizations of the solutions to the implicit underlying ODE (18). This observation will be useful in the perturbation and error analysis of the QR methods in Section 4.

3.2 Continuous QR algorithm

For the continuous QR algorithm we assume that the unique factorization $X(t) = Q(t)R(t)$ with positive diagonal elements in R is to be determined for $t \in \mathbb{I}$. For this we determine differential equations for the Q factor and the scalar equations for the logarithms of the diagonal elements of R elementwise. We will see that once the factor Q is obtained by numerical integration, then we also obtain the logarithms of the diagonal elements of R.

Differentiating $X = QR$ and inserting this into the DAE yields $E\dot{Q}R + EQ\dot{R} = AQR$, or equivalently

$$E\dot{Q} + EQ\dot{R}R^{-1} = AQ. \tag{26}$$

Note that the linear independence of the columns of X implies the invertibility of R. The DAE (26) is a nonlinear strangeness-free (differentiation-index one) DAE system for Q with the same algebraic part as that of the DAE system (4) for X. The differential part is linear in $\dot{Q}$, but nonlinear in Q, since R depends on Q. Now, following the idea of the continuous QR method for ODEs, e.g., see [20], we will derive a formula for $Q^T\dot{Q}$ and then use the fact that this matrix function is skew-symmetric to determine its elements.

To achieve this, we use the algebraic equation $A_2Q = 0$ and replace it by its derivative $\dot{A}_2Q + A_2\dot{Q} = 0$ to obtain the system

$$\bar{E}(\dot{Q} + Q\dot{R}R^{-1}) = \bar{A}Q, \tag{27}$$

where $\bar{E}$ is defined as in (5) and

$$\bar{A} = \begin{bmatrix} A_1 \\ \dot{A}_2 \end{bmatrix}. \tag{28}$$

Note that here we have to assume differentiability of A_2, but comparing with [40], this is not an extra assumption, since the same is assumed to have (16), too.

Since the original system is assumed to be strangeness-free, we have that $\bar{E}$ is nonsingular and hence (27) is an implicit ODE. The following lemma is the key for obtaining $Q^T\dot{Q}$.

Lemma 12 *Consider a strangeness-free DAE of the form (4) and assume that A_2 is differentiable, so that the implicit ODE (27) can be formed. Then there exist a bounded, full-column rank matrix function $P \in C(\mathbb{I}, \mathbb{R}^{n\times p})$, and an upper triangular nonsingular matrix function $\mathcal{E} \in C(\mathbb{I}, \mathbb{R}^{p\times p})$ such that*

$$P^T\bar{E} = \mathcal{E}Q^T \tag{29}$$

holds. Furthermore, if we require $P^TP = I_p$ and the diagonal elements of $\mathcal{E}$ to be positive, then P and $\mathcal{E}$ are unique. In this case, we also have the following estimates

$$\|\mathcal{E}\| \leq \left\|\bar{E}\right\|, \quad \left\|\mathcal{E}^{-1}\right\| \leq \left\|\bar{E}^{-1}\right\|.$$

Proof. It is obvious that (29) is equivalent to $\bar{E}^{-T}Q = P\mathcal{E}^{-T}$. The right hand side is nothing but the QR factorization of the left-hand side matrix. In order to obtain $\mathcal{E}$ in upper triangular form, we apply a Gram-Schmidt orthogonalization to the columns of $\bar{E}^{-T}Q$ from right to left. Thus, the proof follows immediately from the existence result for smooth QR factorizations, see [15]. The estimates for $\|\mathcal{E}\|$ and $\left\|\mathcal{E}^{-1}\right\|$ follow directly from the identities $P^T\bar{E}Q = \mathcal{E}$ and $P^T\bar{E}^{-T}Q = \mathcal{E}^{-T}$, respectively. □

In our numerical methods, we want to avoid the computation of P and $\mathcal{E}$ as in the proof of Lemma 12. Following the concept of pencil arithmetic introduced in [5], we first perform a QR factorization

$$\begin{bmatrix} \bar{E} \\ Q^T \end{bmatrix} = \begin{bmatrix} \tilde{T}_{1,1} & \tilde{T}_{1,2} \\ \tilde{T}_{2,1} & \tilde{T}_{2,2} \end{bmatrix} \begin{bmatrix} \tilde{M}_{1,1} \\ 0 \end{bmatrix},$$

from which we obtain that $\tilde{T}_{1,2}^T\bar{E} = -\tilde{T}_{2,2}^TQ^T$. In general, this factorization does not guarantee that $\tilde{T}_{2,2}$ is invertible. To obtain this, we compute the QR factorization of the augmented matrix

$$\begin{bmatrix} \bar{E} & 0 \\ Q^T & I_p \end{bmatrix} = \begin{bmatrix} T_{1,1} & T_{1,2} \\ T_{2,1} & T_{2,2} \end{bmatrix} \begin{bmatrix} M_{1,1} & M_{1,2} \\ 0 & M_{2,2} \end{bmatrix}, \tag{30}$$

where the block matrix $[T_{i,j}]$ is orthogonal and the block matrix $[M_{i,j}]$ is upper triangular. Then we have that $T_{2,2}^T = M_{2,2}$ is nonsingular and upper triangular. In order to get the desired matrices P and $\mathcal{E}$, we use an additional QR factorization $T_{1,2} = PG$, where P fulfills $P^TP = I_p$ and G is lower triangular (the fact that $T_{1,2}$ is full column-rank is implied directly by the nonsingularity of $T_{2,2}$). Finally, we set $\mathcal{E} = -G^{-T}T_{2,2}$.

Remark 13 The last QR factorization in the above process of computing P and $\mathcal{E}$ could be omitted, if we require P not be orthogonal but only continuous and bounded. In this case, we can simply set $P = T_{1,2}$ and $\mathcal{E} = -T_{2,2}^T$ and we have that P and $\mathcal{E}$ are in this way uniquely defined via (30). For an alternative way to determine P, see Remark 17. Finally, the computation of P and $\mathcal{E}$ becomes rather simple if P, Q are square matrices of the same size as $\bar{E}$, i.e., when $p = d = n$. Then, only one QR factorization of the form $\bar{E}Q = P\mathcal{E}$ is needed. Moreover, in the ODE case, when $E = I$, then we have immediately $P = Q$ and $\mathcal{E} = I$, and no extra calculation is needed.

Multiplying (27) from the left by P^T defined as in (29), one obtains

$$\mathcal{E}Q^T\dot{Q} + \mathcal{E}\dot{R}R^{-1} = P^T\bar{A}Q.$$

Setting $B := \dot{R}R^{-1}$, $S(Q) := [s_{i,j}(Q)] = Q^T\dot{Q}$, and $K := P^T\bar{A}Q$, it follows that $S(Q) = \mathcal{E}^{-1}K - B$. Since $S(Q)$ is skew-symmetric and B is upper triangular, the strictly lower part of $S(Q)$ is defined by the lower part $\mathrm{low}(W)$ of $W := [w_{i,j}] = \mathcal{E}^{-1}K$ and its upper triangular part is determined by the skew-symmetry. We have $S(Q) = \mathrm{low}(W) - [\mathrm{low}(W)]^T$, i.e.,

$$s_{i,j} = \begin{cases} w_{i,j}, & i > j, \\ 0, & i = j, \\ -w_{j,i}, & i < j, \end{cases} \quad 1 \le i, j \le p. \tag{31}$$

Thus, Q is obtained by solving the initial value problem for the strangeness-free DAE

$$E\dot{Q} = AQ - EQB,$$

or equivalently

$$E\dot{Q} = -EQ[W - S(Q)] + AQ. \tag{32}$$

Note that the system (32) is again strangeness-free, since the nonlinear part only effects the first block row.

For the numerical integration, an appropriate solver which preserves the algebraic constraint as well as the orthogonality condition $Q^TQ = I_p$ should be used, see [34], combined with reorthogonalization. Note that $B = W - S(Q) = \mathrm{upp}(W) + [\mathrm{low}(W)]^T$, where $\mathrm{upp}(W)$ denotes the upper triangular part of W.

Remark 14 In order to determine $B = \dot{R}R^{-1}$, we first compute W by solving the upper triangular algebraic system $\mathcal{E}W = K$. Note that due to Lemma 12, the condition number of this problem is not worse than that of the original DAE problem (4). The computational cost for this is $p^3/2 + O(p^2)$ per time step. In the special case that $p = n$, i.e., that E is a nonsingular matrix and Q is an orthogonal matrix, then the differential equation for Q is simply $\dot{Q} = QS(Q)$. In this case we need to calculate only the lower triangular part and the diagonal of W and the computational cost is $n^3/6 + O(n^2)$. However, in general we expect to use this procedure for the case that $p << n$, i.e. $p^3/2 << n^3/6$.

If we set $\mathcal{A} := K - \mathcal{E}S(Q) = P^T\bar{A}Q - \mathcal{E}Q^T\dot{Q}$, then the differential equation for the factor R is given by the upper triangular matrix equation of size $p \times p$

$$\mathcal{E}\dot{R} = \mathcal{A}R, \tag{33}$$

or equivalently

$$\dot{R} = BR.$$

However, we are in fact interested only in the diagonal elements $r_{i,i}$ of R (or more exactly, in their logarithm). The fact that the system is upper-triangular leads to the differential equations

$$\dot{r}_{i,i} = w_{i,i}r_{i,i}, \tag{34}$$

where $w_{i,i},\ i = 1, \ldots, p$ is the i-th diagonal element of the matrix $W = \mathcal{E}^{-1}K$ (Note that the diagonal of the latter matrix and that of $B = \mathcal{E}^{-1}\mathcal{A}$ coincide). To determine these quantities, we introduce the auxiliary functions $\phi_i(t)$ defined by the solution of the initial value problems

$$\dot{\phi}_i(t) = w_{i,i}(t), \quad \phi_i(0) = 0. \quad (i = 1, \ldots, p) \tag{35}$$

Finally, the functions $\lambda_i(t)$, defined as in the discrete QR method are obtained via

$$\lambda_i(t) = \frac{1}{t}\phi_i(t), \quad i = 1, 2, \ldots, p. \tag{36}$$

To check the integral separation of the functions $\{w_{i,i}\}_{i=1}^p$ in practice, we use their Steklov differences. Choosing a sufficiently large H, then the Steklov difference of $w_{i,i}$ and $w_{i+1,i+1}$ is given by

$$\psi_i(t, H) := \frac{1}{H}\left\{[\phi_i(t+H) - \phi_i(t)] - [\phi_{i+1}(t+H) - \phi_{i+1}(t)]\right\}, t \in \mathbb{I}, \ \ i = 1, ..., p-1. \tag{37}$$

We summarize the continuous QR procedure for computing approximations to Lyapunov spectral intervals in the following algorithm.

Algorithm 2 (Continuous QR algorithm for computing Lyapunov spectra)

- **Input:** A pair of sufficiently smooth matrix functions (E, A) in the form of the strangeness-free DAE (4) (if they are not available directly they must be obtained pointwise as output of a routine such as GELDA); the first derivative of A_2 (if it is not available directly, we use a finite difference approximation); values T, H, τ such that $H \in (0, T)$ and $\tau \in (0, T)$, and $Q_0 = Q(t_0)$ as initial value for (32).
- **Output:** Approximate bounds for spectral the intervals $\{\lambda_i^l, \lambda_i^u\}_{i=1}^p$.
- **Initialization:**
  1. Set $j = 0, t_0 := 0$. Compute $P(t_0)$, $\mathcal{E}(t_0)$, and $K(t_0)$ as in (29) and (30).
  2. Compute $W(t_0)$ as in Remark 14.
  3. Set $\lambda_i(t_0) = 0,\ \phi_i(t_0) = 0,\ i = 1, ..., p$.

  While $t_j < T$
  1. $j := j + 1$.
  2. Choose a stepsize h_j and set $t_j = t_{j-1} + h_j$.
  3. Evaluate $Q(t_j)$ by solving (32).
  4. Compute $P(t_j), \mathcal{E}(t_j), K(t_j)$ as in (30) and by their definitions, respectively.
  5. Solve for $W(t_j)$ as in Remark 14.
  6. Compute $\phi_i(t_j)$, $\lambda_i(t_j)$, $i = 1, ..., p$ as in (35), (36).
  7. If desired, compute the Steklov differences $\psi_i(t, H)$, $i = 1, 2, ..., p - 1$, by (37) to check integral separation.
  8. Update $\min_{\tau \le t \le t_j} \lambda_i(t)$ and $\max_{\tau \le t \le t_j} \lambda_i(t)$.

The corresponding algorithm for computing Sacker-Sell spectra is similar, except that instead of computing $\lambda_i(t)$ at each meshpoint (see Step 6.), we evaluate the Steklov averages $\psi_{H,i}(t)$ by the formula

$$\psi_{H,i}(t) = \frac{1}{H}(\phi_i(t + H) - \phi_i(t)), \quad i = 1, 2, ..., p.$$

Finally, in the last step we compute $\inf_{0 \le t \le T-H} \psi_{H,i}(t)$ and $\sup_{0 \le t \le T-H} \psi_{H,i}(t)$.

Remark 15 If the same mesh is used in Algorithms 1 and 2 and all calculations are done in exact arithmetic and without discretization errors, then the quantities s_i at the end of the j-th step of Algorithm 1 are exactly the values $\phi_i(t_j)$ defined in Algorithm 2.

An advantage of the discrete algorithm is a simpler implementation and that existing efficient DAE solvers for strangeness-free problems like BDF or implicit Runge-Kutta methods, see [2, 7, 34, 36] can be used. On first look the discrete method also seems to be cheaper than its continuous counterpart. However, this is not true at all. A disadvantage of the discrete method is that it creates numerical integration errors on each of the local intervals and these may grow very fast, in particular if the DAE system is very unstable and the subintervals are very long. Consequently, in order to keep a prescribed accuracy, in the discrete algorithm much smaller stepsizes need to be used than in the continuous algorithm. The key difference is that in the discrete version, we evaluate indirectly the whole matrix X and thus its factor R, while in the continuous version, we integrate the numerically stable factor Q and only the logarithm of the diagonal elements $r_{i,i}$. In the next section, we will show that the numerical integration of the factor Q is globally stable. This property shows that the continuous QR method is clearly superior.

Let us for a moment recall the variant of the continuous QR method suggested in [40], which uses a pre-transformation $\tilde{Q}$ as at the beginning of this section. Let $Q = \tilde{Q}U$, where U is the Q factor in the QR factorization of $\tilde{X} = \tilde{Q}^T X$. Then we have $\dot{Q} = \dot{\tilde{Q}}U + \tilde{Q}\dot{U}$. Inserting this formula for $\dot{Q}$ into (26), we have

$$E\tilde{Q}\dot{U} + E\tilde{Q}U\dot{R}R^{-1} = (A\tilde{Q} - E\dot{\tilde{Q}})U. \tag{38}$$

Let us use again the notation as in (17) and partition U conformably as $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$. Then from the algebraic equation, we obtain $U_2 = 0$ and thus we get the implicit underlying ODE for U_1 as

$$\tilde{E}_{11}\dot{U}_1 + \tilde{E}_{11}U_1\dot{R}R^{-1} = \tilde{A}_{11}U_1. \tag{39}$$

We stress that R is the same upper triangular factor as that of X. Since $\tilde{E}_{11}$ is nonsingular, by Lemma 12, there exist matrices V_1 and $\mathcal{E}_1$, where $V_1^T V_1 = I_p$ and $\mathcal{E}_1$ is upper triangular and nonsingular, such that $V_1^T \tilde{E}_{1,1} = \mathcal{E}_1 U_1^T$. Similarly as above, multiplying equation (39) by V_1^T from the left, we obtain

$$\mathcal{E}_1 U_1^T \dot{U}_1 + \mathcal{E}_1 \dot{R}R^{-1} = V_1^T \tilde{A}_{11}U_1.$$

By defining $K_1 = V_1^T \tilde{A}_{11} U_1$ and $W_1 = \mathcal{E}_1^{-1}K_1$ and the same argument as that for determining $S(Q)$, we have that $S(U_1) = U_1^T\dot{U}_1 = \mathrm{low}(W_1) - [\mathrm{low}(W_1)]^T$. Furthermore, U_1 can be obtained numerically by solving the initial value problem for the implicit ODE

$$\tilde{E}_{11}\dot{U}_1 + \tilde{E}_{11}U_1[W_1 - S(U_1)] = \tilde{A}_{11}U_1. \tag{40}$$

The calculation of the $\{\lambda_i(t)\}_{i=1}^p$ can then be carried out in the same manner as (35) and (36).

Remark 16 Theoretically, one may multiply (40) by $\tilde{E}_{11}^{-1}$ and obtain the ODE

$$\dot{U}_1 + U_1[W_1 - S(U_1)] = \tilde{E}_{11}^{-1}\tilde{A}_{11}U_1.$$

It is also easily verified by elementary calculations that $W_1 = U_1^T \tilde{E}_{11}^{-1}\tilde{A}_{11}U_1$. Thus, the appearance as well as the role of V_1 may be eliminated. Furthermore, if U_1 is a square matrix (i.e., in the case $p = d$), then $U_1^T U_1 = U_1 U_1^T = I_d$, and the differential equation for U_1 simplifies to

$$\dot{U}_1 = U_1 S(U_1).$$

This alternative formulation is exactly that of the continuous QR method for ODEs [20, 21, 22, 24] and will be useful for the perturbation and error analysis in Section 4. However, in practice, we avoid the direct computation of $\tilde{E}_{11}^{-1}$ because it may be costly and very ill-conditioned.

Remark 17 If we apply the continuous QR technique presented in this section to (38), then we have to determine $P^T = \begin{bmatrix} P_1^T & P_2^T \end{bmatrix}$ such that

$$\begin{bmatrix} P_1^T & P_2^T \end{bmatrix} \begin{bmatrix} \tilde{E}_{11} & \tilde{E}_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix} = \mathcal{E} \begin{bmatrix} U_1^T & U_2^T \end{bmatrix}.$$

Using that $U_2 = 0$, we obtain that

$$P_1^T\tilde{E}_{11} = \mathcal{E}U_1^T, \text{ and } P_1^T\tilde{E}_{12} + P_2^T\tilde{A}_{22} = 0.$$

Once P_1 is available, then $P_2 = -\tilde{A}_{22}^{-T}\tilde{E}_{12}^T P_1$. If we want to have $P^T P = I_p$, then an additional orthogonalization process must be applied to P. Furthermore, we get

$$P^T \begin{bmatrix} \tilde{E}_{11} & \tilde{E}_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix} U = P_1^T\tilde{E}_{11}U_1, \quad P^T \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ 0 & \dot{\tilde{A}}_{22} \end{bmatrix} U = P_1^T\tilde{A}_{11}U_1.$$

This shows that the difference between the previous version suggested in [40] and the current version of the continuous QR algorithm lies only in the normalization of P and V_1. Here P_1 plays a similar role as V_1 in the reduced version, but $P_1^T P_1 \neq I_p$, in general. Nevertheless, the explicit ODE for R is the same, but the implicit forms obtained by different versions are different, in general. In our opinion, the new version presented in this paper better reflects the nature of the problem, because in the previous version, the terms associated with $\tilde{E}_{12}, \tilde{A}_{12}$ and $\tilde{A}_{22}$ are simply omitted, but instabilities that arise from these terms may effect the solution, in particular in the non-homogeneous case. Since these are omitted in the analysis and not checked, this may lead to false conclusions.

4 Perturbation and Error Analysis

A systematic perturbation and error analysis for the QR methods in the ODE case has been given in [21, 22, 24]. The framework and the results presented there can be used, modified and extended to the QR methods for DAEs constructed in Section 3. In the light of Lemma 4, we in fact compute the spectral intervals for the implicit EUODE of triangular form (33). Furthermore, in both the discrete and continuous variants, we have to numerically integrate strangeness-free DAE systems such as (19) or (32) instead of ODE systems as in the ODE case. Hence, some extra assumptions and some more effort are needed in the error analysis for DAEs.

In the following, for simplicity of notation, we perform the error analysis for the case that all spectral intervals are calculated, i.e., we discuss the case $p = d$. The case of $p < d$ can be treated in a completely analogous way.

There are several sources for the error in computing spectral intervals;

a) the error arising in the computation of the strangeness-free form, i.e., in obtaining E_1, A_1, A_2 (and also $\dot{A}_2$ in the continuous QR algorithm),

b) the integration (discretization) error in the course of solving DAE systems occurring in the discrete and continuous methods,

c) the error in solving the linear systems in the context of the implicit integration method and in the evaluation of W in the continuous method (see Remark 14),

d) the error in performing the occurring QR factorizations in finite precision arithmetic, and

e) the error in the early termination or truncation of the optimization process.

We discuss here only the errors a)–c). The errors d) arising from the QR factorization will be ignored, since there are excellent backward stable numerical methods available for this task, [29], and the resulting errors are typically much smaller than the errors resulting from the numerical integration. The errors e) in the early termination/truncation of the optimization process arise by considering the system on $[0, T]$ with a large T instead of $[0, \infty)$. Similarly to the ODE case, see [21, Section 3.3], these errors depend strongly on the difference between the asymptotic behavior of the system in consideration and its very long, but finite-time, dynamics. One may easily construct simple examples, where the approximate spectral exponents computed even for a very large T are completely different from their exact values. However, it is clear that by taking larger intervals of optimization these errors can be reduced.

In contrast to the case of ordinary differential equations, where only the discretization error, the error in the QR factorizations and the error in an early termination/truncation of the optimization process have to be considered, in the DAE case the computation of the strangeness-free form may be an essential factor in the analysis that cannot be influenced significantly by reducing the stepsize. The computation of the strangeness-free form may be ill-conditioned or even ill-posed if the assumptions for its existence do not hold, see [36]. So as before, we assume that the data E_1, A_1, A_2 are well-determined and available to a high accuracy, which is at least as good as the one that we can expect from the discretization method. But this clearly has to be checked and supervised during the computation of the spectral intervals and it has to be incorporated into the error analysis.

While in the ODE case explicit integration methods can be used for the numerical integration, the second critical point in the DAE case is the solution of the linear systems in the necessary implicit integration methods. The most important term in the solution of these linear systems (regardless whether one-step or multi-step methods are used) (see [36]) is the matrix (or submatrix)

$$\begin{bmatrix} E_1 - h_j c A_1 \\ A_2 \end{bmatrix},$$

or

$$\begin{bmatrix} E_1 - h_j c A_1 \\ A_2 - h_j c \dot{A}_2 \end{bmatrix}$$

where c is a constant arising from the method. These linear systems may be ill-conditioned even for strangeness-free systems, this happens for example when the second block row in these systems is near rank-deficient, or if E_1 is near rank-deficient.

In general, for sufficiently small stepsize it is the condition number of the matrix function $\bar{E}$ in (5) which determines the error in the solution of these linear systems, provided that a numerically stable method is used for the solution. The ill- or well-conditioning of these linear systems is again a property of the DAE under consideration and it should be noted that reducing the step-size typically does not cure this problem.

In the following, we assume that for all values t the matrix $\bar{E}$ is sufficiently well-conditioned, in the sense that the numerical solution to the associated linear system can be obtained within the accuracy dominated by the desired tolerance for the discretization error. But this needs to be checked during the computational process at every time instance t, and it has to be incorporated into the error analysis.

Under the assumption that the reduction process to strangeness-free form and the matrix $\bar{E}$ are sufficiently well-conditioned, i.e., that the errors resulting from these problems can be bounded, we will show that for systems that are integrally separated, the error in the spectral intervals, e.g., that of $\{\lambda_i^u\}_{i=1}^d$, can be estimated by a bound for the local integration errors multiplied by a factor that depends on the norm of the strict upper triangular part of R (i.e., the deviation from normality).

To analyze the global error, two kinds of error analysis are necessary. While a forward error analysis is sufficient for the investigation of the error in computing the DAE solution, a combination of backward and forward error analysis is used for investigating how the integration error accumulates and effects the accuracy of the computed spectral intervals.

4.1 Backward error analysis for the discrete QR method

Let us first study the backward error analysis for the discrete QR method. Let $\Phi \in C(\mathbb{I}_j, \mathbb{R}^{n\times n})$ and $\bar{\Phi} \in C(\mathbb{I}_j, \mathbb{R}^{n\times n})$ be defined as the exact and the approximate (via the numerical integrator) solutions, respectively, to the initial value problems

$$E(t)\dot{\Phi}(t,t_{j-1}) = A(t)\Phi(t,t_{j-1}), \quad E(t_{j-1})[\Phi(t_{j-1},t_{j-1}) - I_n] = 0, \tag{41}$$

in the interval $\mathbb{I}_j = [t_{j-1}, t_j]$ of width $h_j = t_j - t_{j-1}$, $j = 1, 2, \ldots$. Here we assume that the data matrices $E(t), A(t)$ are exact data given in strangeness-free form (4). Note that $X(t_j, t_{j-1}) = \Phi(t_j, t_{j-1})Q(t_{j-1}) = Q(t_j)R(t_j, t_{j-1})$ is the exact QR decomposition with positive diagonal elements in $R(t_j, t_{j-1})$.

As already mentioned before, we have to use implicit methods for the numerical integration, and in each step we have to solve a linear system, for which we assume that the error in the solution is small enough compared to the discretization error. On the other hand, for the next interval we need consistent initial conditions and for this we have to make sure that the approximate solution exactly satisfies the algebraic constraint

$$A_2(t)\bar{\Phi}(t,t_{j-1}) = 0. \tag{42}$$

In order to guarantee that this is the case, it may be necessary to project the numerically computed solution to satisfy the constraint exactly. This is typically easy if the changes of the constraint equation (in t) are not too large compared with the dynamics of the differential part. If this is not the case, then this may lead to fundamental stability problems in the DAE integrator, which require special techniques, [37]. Here we will assume that this problems is handled by the DAE integrator. As in the ODE case, we furthermore assume that the local integration errors in the solution can be estimated, i.e., altogether, we make the following assumption.

Assumption 18 *Assume that the approximate solution $\bar{\Phi}(t_j, t_{j-1})$ satisfies the exact algebraic constraint (42), that the local errors $\mathcal{N}_j := \bar{\Phi}(t_j, t_{j-1}) - \Phi(t_j, t_{j-1})$ $(j = 1, 2, \ldots)$ are available (or can be estimated) in terms of the maximal local stepsize ℓ_j in $\mathbb{I}_j$, and that the roundoff and solution error in the solution of the linear systems that have to be solved at each integration step is negligible compared with the discretization error.*

We assume further that the initial condition $X_0 = X(t_0)$ is consistent and exact and has the exact QR decomposition $X_0 = Q_0 R_0$, where R_0 has positive diagonal elements.

Denoting by X_j the numerical (via the numerical integration) solution that approximates the rectangular fundamental solution $X(t_j)$, and assuming that we have determined the exact and unique QR decomposition $X_j = Q_j R_j$, $j = 0, 1, \ldots$, where R_j has positive diagonal elements, we then have that

$$X_k = \bar{\Phi}(t_k, t_{k-1}) \ldots \bar{\Phi}(t_2, t_1)\bar{\Phi}(t_1, t_0)X_0.$$

Recalling that $\bar{X}(t, t_{j-1})$ is the approximate solution to (19)), at $t = t_j$ we also get

$$\bar{X}(t_j, t_{j-1}) = \bar{\Phi}(t_j, t_{j-1})Q_{j-1} = Q_j R_j, \quad j = 1, \ldots, k,$$

and thus we have

$$X_j = Q_j R_j R_{j-1} \ldots R_1 R_0. \tag{43}$$

Similarly to [21, Theorem 3.1], we obtain the following Lemma for the backward error in the numerical integration process.

Lemma 19 *Consider a DAE in strangeness-free form (4) and let X_j be the approximate fundamental solution that approximates $X(t_j)$. Then, under Assumption 18, we have that*

$$X_j = Q(t_j)[R(t_j, t_{j-1}) + \mathcal{E}_j] \ldots [R(t_2, t_1) + \mathcal{E}_2][R(t_1, t_0) + \mathcal{E}_1]R_0, \tag{44}$$

where the backward error $\mathcal{E}_i$ in time-step i satisfies $\mathcal{E}_i = Q^T(t_i)\mathcal{N}_i Q(t_{i-1})$, $i = 1, 2, \ldots, j$, i.e., the numerical realization of the discrete QR method by (43) computes the exact QR factorization of the right-hand side of (44).

Proof. By comparing with the proof in the ODE case [21], the only difference occurring here is that the matrices $Q(t_j)$ are rectangular matrices and thus $Q(t_j)Q^T(t_j)$ in general is singular. However, we still have that $Q(t_j)Q^T(t_j)$ is the orthogonal projector onto $\operatorname{Im} Q(t_j)$. Hence, under Assumption 18, we have that

$$\begin{aligned} Q(t_j)Q^T(t_j)\mathcal{N}_j &= Q(t_j)Q^T(t_j)[\bar{\Phi}(t_j, t_{j-1}) - \Phi(t_j, t_{j-1})] \\ &= Q(t_j)Q^T(t_j)\bar{\Phi}(t_j, t_{j-1}) - Q(t_j)Q^T(t_j)\Phi(t_j, t_{j-1}) \\ &= \bar{\Phi}(t_j, t_{j-1}) - \Phi(t_j, t_{j-1}) = \mathcal{N}_j. \end{aligned} \tag{45}$$

Using this observation, the proof of [21, Theorem 3.1] can be repeated here. Indeed, considering the first integration step, we have

$$Q_1 R_1 = \bar{\Phi}(t_1, t_0)Q_0 = [\Phi(t_1, t_0) + \mathcal{N}_1]Q_0 = Q(t_1)R(t_1, t_0) + \mathcal{N}_1 Q_0 = Q(t_1)[R(t_1, t_0) + Q^T(t_1)\mathcal{N}_1 Q_0].$$

For the next step we have $X_2 = \bar{\Phi}(t_2, t_1)\bar{\Phi}(t_1, t_0)Q_0 R_0$. Similarly as above, we then have

$$\bar{\Phi}(t_2, t_1)Q(t_1) = Q(t_2)[R(t_2, t_1) + Q^T(t_2)\mathcal{N}_2 Q(t_1)].$$

Using this and that $Q(t_1)Q^T(t_1)\bar{\Phi}(t_1,t_0) = \bar{\Phi}(t_1,t_0)$, we obtain that

$$X_2 = Q(t_2)[R(t_2,t_1) + \mathcal{E}_2][R(t_1,t_0) + \mathcal{E}_1]R_0.$$

Continuing this way, the assertion follows. □

Remark 20 We note that the matrix solutions Φ and $\bar{\Phi}$ play only the roles of auxiliary variables in the error analysis. In the numerical method, we do not determine $\Phi(t_j,t_{j-1})$, but directly compute $X(t_j,t_{j-1}) = \Phi(t_j,t_{j-1})Q(t_{j-1})$ by solving (19).

Then with the usual error estimates for strangeness-free systems, see [36], along with the numerical solution, we obtain estimates for the local error

$$\mathcal{M}_j := \bar{\Phi}(t_j,t_{j-1})Q(t_{j-1}) - \Phi(t_j,t_{j-1})Q(t_{j-1}) = \mathcal{N}_j Q(t_{j-1}). \tag{46}$$

Using this, for the backward errors $\mathcal{E}_j$ we obtain the estimate

$$\|\mathcal{E}_j\| = \left\|Q^T(t_j)\mathcal{N}_j Q(t_{j-1})\right\| \le \|\mathcal{N}_j Q(t_{j-1})\| = \|\mathcal{M}_j\| \le \|\mathcal{N}_j\|.$$

If a q-th order integrator is used for the numerical solution of (19), then it follows from [36] that the local errors $\mathcal{N}_j, \mathcal{M}_j$ and thus also the backward error $\mathcal{E}_j$ are $\mathcal{O}(\ell_j^{q+1})$. For small intervals $\mathbb{I}_j$ of width h_j we then have $h_j = c_j\ell_j$ with a small constant c_j and thus the local errors are $\mathcal{O}(h_j^{q+1})$.

We remark that Lemma 19 may be formulated for ODEs when one is computing some but not all Lyapunov exponents or on the Stiefel manifold [8, 18] in the special case in which the error $\mathcal{N}_j$ is in $\operatorname{Im} Q(t_j)$ (or alternatively in $\operatorname{Im} Q_j$).

It follows that we have the same error estimate as in the ODE case and hence, the backward error analysis given in [21] can be applied directly. For this, let us rephrase some results from [21] in our notation.

Lemma 21 *For $j = 1,2,\ldots$, the matrices $R(t_j,t_{j-1})$ in (21) are the solution matrices evaluated at t_j of the upper-triangular matrix differential equations*

$$\dot{R}(t,t_{j-1}) = B(t)R(t,t_{j-1}), \quad R(t_{j-1},t_{j-1}) = I_d,$$

where $B(t)$ is given in (33).

At any $\hat{t} = t_k$, the solution $R(t_k)$ of (33) is the same matrix as the exact solution of the piecewise constant triangular system

$$\dot{\tilde{R}} = B_j\tilde{R},\ t_{j-1} \le t < t_j,\ \tilde{R}(0) = R(t_0),\ j = 1,2,\ldots,k, \tag{47}$$

evaluated at t_j, where the matrices $B_j \in \mathbb{R}^{d\times d}$ are upper triangular and satisfy

$$R(t_j,t_{j-1}) = e^{h_jB_j},\ j = 0,1,\ldots,k-1. \tag{48}$$

Proof. See [21, Lemma 2.3, Lemma 2.4]. □

Introducing the auxiliary notation

$$\hat{R}(t_j,t_{j-1}) := R(t_j,t_{j-1}) + \mathcal{E}_j,\ \text{and}\ \hat{R}(t_k) = \left[\prod_{j=k}^{1}\hat{R}(t_j,t_{j-1})\right]R_0,$$

we can rewrite the representation (44) as

$$X_j = Q(t_j)\hat{R}(t_j,t_{j-1})\ldots\hat{R}(t_2,t_1)\hat{R}(t_1,t_0)R_0, \tag{49}$$

Then, similarly as in Lemma 21, $\hat{R}(t_k)$ is the exact solution at t_k of the piecewise constant problem

$$\dot{\hat{R}} = \hat{B}_j \hat{R},\ t \in \mathbb{I}_j,\ \hat{R}(0) = R_0,\ j = 1, 2, \ldots, k, \tag{50}$$

where the matrices $\hat{B}_j \in \mathbb{R}^{d \times d}$ satisfy

$$\hat{R}(t_j, t_{j-1}) = e^{h_j \hat{B}_j},\ j = 0, 1, \ldots, k-1. \tag{51}$$

Note that the matrices $\hat{B}_j$ are not necessarily upper triangular.

To bound the norm of the differences $\hat{B}_j - B_j$, we introduce the following assumption.

Assumption 22 *Let*

$$\delta_i := \min_{1 \le \ell \le d} \frac{1}{\min\left(1, \exp(\int_{t_{i-1}}^{t_i} w_{\ell,\ell}(t)dt\right)}, \tag{52}$$

where $w_{\ell,\ell}$ is as defined in (34) and let $\xi_i := \|\Xi_i\|$, where Ξ_i denotes the strict upper triangular part of $R(t_i, t_{i-1})$. We assume that there exist constants $\xi, \delta < 1$ such that

$$\|\mathcal{E}_i\|\, \delta_i \le \delta < 1,\ \textit{and}\ \xi_i \delta_i \le \xi < 1 \quad \text{for all } i = 0, 1, \ldots, j.$$

It is easy to see that $\xi_i = \mathcal{O}(h_i)$, and since we have that $\|\mathcal{E}_i\| = \mathcal{O}(h_i^{q+1})$ for small h_i if a q-th order integrator is used, it follows that the conditions in Assumption 22 can be easily fulfilled by reducing the stepsize h_i.

In the following we will make use of the following theorem of [21] on the comparison of the piecewise constant problem (47) and its perturbation (50) rephrased in terms of strangeness-free DAEs.

Theorem 23 *Consider a well-conditioned strangeness-free DAE system of the form (4). Let $\{t_i\}_{i=0}^{\infty}$ be a sequence of points (converging to ∞) generated by the numerical realization of the discrete QR method. Suppose that for a given tolerance* `TOL` *the backward error satisfies $\|\mathcal{E}_i\| \le$* `TOL` *for all $i = 0, 1, \ldots$, and that Assumptions 18 and 22 hold.*

Then, at $t = t_j$, the numerically computed QR factorization computed by the discrete QR method determines the (exact) QR factorization (49), where the upper-triangular factor $\hat{R}(t_j)$ is the exact solution of problem (50), with perturbed coefficient matrix

$$h_j \hat{B}_j = h_j B_j + \mathcal{Z}_j + \mathcal{O}(\|\mathcal{E}_j^2\|),$$

and where the perturbation matrix $\mathcal{Z}_j$ satisfies the componentwise estimate

$$|\mathcal{Z}_j| \le \left[\frac{1 - (\delta_j \xi_j)^d}{1 - \delta_j \xi_j}\right]^2 |\Pi_j|,$$

and the (ℓ, k) element of the matrix Π_j satisfies

$$(|\Pi_j|)_{\ell,k} \le \mathtt{TOL} \,/ \min_{i=\ell,k} \left(\exp(\int_{t_{j-1}}^{t_j} w_{i,i}(t)dt)\right).$$

Proof. The proof is identical to the proof of Theorem 3.12 in [21]. ◻

It follows that, if all the assumptions in Theorem 23 hold and the numerical integration method for (19) has order q, then the perturbation $\hat{B}_j - B_j$ has magnitude $O(h_j^q)$.

4.2 Backward error analysis for the continuous QR method

For the continuous QR method, the backward error analysis of [21] can be extended in a straightforward way. We again need Assumption 18 and make use of (45) shown in the proof of Lemma 19. The key difference between the discrete and the continuous QR methods is that in the continuous variant, we neither approximate the matrix solution $X(t)$ nor its upper triangular factor $R(t)$, but only $Q(t)$ and (the logarithm of) the diagonal elements of $R(t)$.

For $j = 0, 1, \ldots$, let $\hat{Q}(t, t_j)$ be the Q-factor in the QR factorization of $\Phi(t, t_{j-1})Q_j$. Then, by direct differentiation, it is easy to see that $\hat{Q}(t, t_j)$ satisfies the differential equation (32), but with $\hat{Q}(t, t_j)$ replacing $Q(t)$ there. Let us introduce

$$H(E, A, Q) := -EQ[W - S(Q)] + AQ,$$

where $W := [w_{k,\ell}] = W(E, A, Q)$ and $S(Q)$ are defined as in Section 3. Note that these expressions depend on the matrix function P as well, but P can be considered as a function of Q by Lemma 12. Then, on the intervals $\mathbb{I}_j$, $j = 1, 2, \ldots$, we compute approximations to the solutions of the initial value problems

$$\begin{array}{rcl} E(t)\frac{d}{dt}\hat{Q}(t, t_{j-1}) & = & H(E(t), A(t), \hat{Q}(t, t_{j-1})), \quad \hat{Q}(t_{j-1}, t_{j-1}) = Q_{j-1}, \\ \frac{d}{dt}\hat{\phi}_i(t, t_{j-1}) & = & w_{i,i}(t), \quad \hat{\phi}(t_{j-1}, t_{j-1}) = 0. \end{array} \tag{53}$$

Suppose that we have obtained approximations $\hat{Q}^c(t_j, t_{j-1})$ and $\phi_i^c(t_j)$ instead of the exact solutions $\hat{Q}(t_j, t_{j-1})$ and $\phi_i(t_j, t_{j-1})$ and then use $Q_j := \hat{Q}^c(t_j, t_{j-1})$ as the initial value for the next interval.

Similar to Assumption 18, to guarantee consistent initial conditions for the DAEs in (53), we also need the following assumption.

Assumption 24 *In addition to the normalization condition $(\hat{Q}^c(t_j, t_{j-1}))^T\hat{Q}^c(t_j, t_{j-1}) = I_d$, we require that $\hat{Q}^c(t_j, t_{j-1})$ exactly satisfies the algebraic equation at t_j, i.e., $A_2(t_j)\hat{Q}^c(t_j, t_{j-1}) = 0$.*

Then, at $t = t_k$, we evaluate

$$\frac{1}{t_k}\sum_{j=1}^{k}\phi_i^c(t_j, t_{j-1}),$$

which gives an approximation to $\lambda_i(t_k)$. We stress that here we can control the local error for the initial value problem (53), i.e., the bounds for the differences $\hat{Q}(t_j, t_{j-1})^c - \hat{Q}(t_j, t_{j-1})$ and $\phi_i^c(t_j, t_{j-1}) - \phi_i(t_j, t_{j-1})$.

Since the off-diagonal elements of R_j are not evaluated in the numerical process, we can achieve that the difference

$$Q_jR_j - \hat{Q}(t_j, t_{j-1})\hat{R}(t_j, t_{j-1})$$

has the same order of magnitude as the differences $Q_j - \hat{Q}(t_j, t_{j-1})$ and the difference in the diagonal of $R_j - \hat{R}(t_j, t_{j-1})$, e.g., by setting the off-diagonal elements of R_j to be exactly those of $\hat{R}(t_j, t_{j-1})$. We could also have another option to minimize the Frobenius norm $\left\|Q_jR_j - \hat{Q}(t_j, t_{j-1})\hat{R}(t_j, t_{j-1})\right\|_F$, see [21, Lemma 3.15].

The following theorem then is an analogue of [21, Theorem 3.16].

Theorem 25 *Let $\{Q_j\}_{j=1}^{\infty}$ with $Q_j = \hat{Q}^c(t_j, t_{j-1})$, be the numerical approximations computed by the continuous QR method to the exact Q-factors of $X(t_j)$ for which Assumption 24 holds, let $\{\phi_i^c(t_j, t_{j-1})\}_{j=1}^{\infty}$ be the approximations to $\{\phi_i(t_j, t_{j-1})\}_{j=1}^{\infty}$, and let $\hat{Q}(t_j, t_{j-1})\hat{R}(t_j, t_{j-1})$ be the exact QR factorization of $\Phi(t_j, t_{j-1})Q_{j-1}$. Finally, let the matrices R_j be upper triangular matrices with diagonal given by $\{\exp(\phi_i^c(t_j, t_{j-1}))\}_{i=1}^{d}$ and the off-diagonal elements be chosen so that the difference in the off diagonal elements of $R_j - \hat{R}(t_j, t_{j-1})$ has the same order of magnitude as the differences on the diagonal.*

Let $\hat{\mathcal{N}}_j := Q_j - \hat{Q}(t_j, t_{j-1})$ *and* $\Delta_j := R_j - \hat{R}(t_j, t_{j-1})$*, then the local error in the computation of* $\Phi(t_j, t_{j-1})Q_{j-1}$ *satisfies*

$$\begin{aligned} \bar{\Phi}(t_j, t_{j-1})Q_{j-1} - \Phi(t_j, t_{j-1})Q_{j-1} &= Q_j R_j - \hat{Q}(t_j, t_{j-1})\hat{R}(t_j, t_{j-1}) \\ &= \hat{\mathcal{N}}_j \hat{R}(t_j, t_{j-1}) + \hat{Q}(t_j, t_{j-1})\Delta_j + \hat{\mathcal{N}}_j \Delta_j. \end{aligned} \tag{54}$$

Remark 26 Since the approximations to the orthogonal factors Q_{j-1} are rectangular, one cannot obtain an explicit expression for $\mathcal{N}_j = \bar{\Phi}(t_j, t_{j-1}) - \Phi(t_j, t_{j-1})$ as in [21, Theorem 3.16]. Furthermore, the local error on the left-hand side of (54), denoted by $\hat{\mathcal{M}}_j$, is not the same as $\mathcal{M}_j$ in (46). The matrices $\mathcal{M}_j$ are local errors of the numerical solution of (19) starting with the exact initial value $Q(t_j)$, while the matrices $\hat{\mathcal{M}}_j$ are local errors obtained with the approximate initial value $Q_j = \hat{Q}^c(t_j, t_{j-1})$. However, we know from the numerical analysis of differential equations, see [2], that they are asymptotically equivalent, i.e., when the stepsize h_j is small enough, $\mathcal{M}_j$ has the same order of magnitude as $\hat{\mathcal{M}}_j$ for which practical estimates are available.

The remainder of the error analysis is as in the discrete QR method. By the same arguments, Lemma 21 and Theorem 23 hold, i.e., the numerical realization of the continuous QR method computes the exact QR factorization (44), where the triangular factor is the exact solution of a perturbed piecewise constant problem. The perturbation in the coefficient matrix of the piecewise constant problem can be estimated elementwise (and also in norm) by the local integration error amplified by a factor, see Theorem 23.

In this section we have seen that under some certain assumptions on the DAE, the backward error analysis for the discrete and continuous QR method applied to DAEs is similar to that for ODEs in [21]. The reason is that both the discrete and the continuous QR realizations (indirectly but) essentially lead to upper triangular ODE systems for the triangular factors, independently of the fact whether the original system is an ODE or a DAE. As the main result, we have shown that the exact realization of the QR methods can be interpreted as the solution of a piecewise-constant and upper triangular differential system, while the numerical realization can be interpreted as the solution of a perturbed system. The perturbation arising in the coefficient matrix has the same magnitude as the local discretization error.

There are only two differences. First, the orthogonal factors in the DAE case in general are not square matrices. Thus, the formulations and the analysis for the DAEs had to be modified. Second, we have to solve linear DAEs (19) or nonlinear DAEs (32) instead of ODE systems as in the ODE case. We have shown that if the original systems is strangeness-free then this also holds for the DAEs (19) and (32) which then allows to control the local error and to have a rigorous analysis, see [36], in using efficient numerical integration methods for DAEs and established software packages see [7, 34, 36].

After deriving the backward analysis for strangeness-free DAEs, in the next section we will study the forward error analysis.

4.3 Forward error analysis

In this section we study the forward error analysis for the discrete and continuous QR methods, which is applied to more general problems than that in [22, 24]. Consider an implicitly given linear time-varying system

$$\hat{E}(t)\dot{U}(t) = \hat{A}(t)U(t), \quad t \in \mathbb{I}, \tag{55}$$

where $\hat{E}, \hat{A}$ are numerically computed, piecewise continuous, upper triangular matrix functions taking values in $\mathbb{R}^{d\times d}$, and where $U(t) \in \mathbb{R}^{d\times d}$. We assume that $\hat{E}(t)$ is nonsingular for all $t \in \mathbb{I}$, and that both $\hat{E}^{-1}$ and $\hat{E}^{-1}\hat{A}$ are uniformly bounded. This class of upper triangular differential systems includes both (33) and (47).

We then consider the case that the coefficients of (55) are subjected to small perturbations, i.e., we solve the perturbed system

$$[\hat{E}(t) + \Delta\hat{E}(t)]\dot{V}(t) = [\hat{A}(t) + \Delta\hat{A}(t)]V(t), \quad t \geq 0, \tag{56}$$

where $\Delta\hat{E}, \Delta\hat{A}$ are small perturbations that are also piecewise continuous with the same discontinuity points as $\hat{E}, \hat{A}$, but they are not necessarily upper triangular.

We will show that there exists a pair of orthogonal matrix functions $\hat{P}, \hat{Q}$ that bring the coefficients in (56) to upper triangular form (in fact we apply the continuous QR method described in Section 3 to (56)) such that $\hat{P}$ and $\hat{Q}$ are close to identity matrices. Furthermore, we will estimate the differences $\hat{Q}(t) - I_d$ and $\hat{P}(t) - I_d$ for all $t \in \mathbb{I}$. As a consequence, then combining the error estimation with the backward error analysis, the analysis of the conditioning of the strangeness-free DAE and the errors in solving the linear systems and QR factorizations in the integration method, we will obtain explicit error bounds for the computed Lyapunov and Sacker-Sell exponents of (4) as well as global error bounds for the orthogonal matrices P, Q in the continuous QR method. For this purpose we will extend the concepts of [22, 24] to strangeness-free DAEs.

To do this, first we carry out an auxiliary calculation.

Lemma 27 *Consider the implicit ODEs (55) and (56). Suppose that* $\sup_{t\geq 0} \left\| \Delta\hat{E} \right\| \leq \omega_1$, $\sup_{t\geq 0} \left\| \Delta\hat{A} \right\| \leq \omega_2$, *and furthermore that* $\sup_{t\geq 0} \left\| \hat{E}^{-1} \right\| \leq \kappa$, *where* ω_1, ω_2, κ *are given positive numbers. If* $\kappa\omega_1 < 1$, *then the perturbed system (56) is equivalent to the explicit ODE system*

$$\dot{V}(t) = [\hat{B}(t) + \Delta\hat{B}(t)]V(t), \quad t \geq 0, \tag{57}$$

where $\hat{B}(t) = \hat{E}^{-1}(t)\hat{A}(t)$ *and the estimate*

$$\left\| \Delta\hat{B} \right\| \leq \frac{1}{1-\varepsilon_1}(\mathcal{M}\varepsilon_1 + \varepsilon_2)$$

holds with $\mathcal{M} = \sup_{t\geq 0} \left\| \hat{B}(t) \right\|$, $\varepsilon_1 = \sup_{t\geq 0} \left\| \hat{E}^{-1}(t)\Delta\hat{E}(t) \right\| \leq \kappa\omega_1$, *and* $\varepsilon_2 = \sup_{t\geq 0} \left\| \hat{E}^{-1}(t)\Delta\hat{A}(t) \right\| \leq \kappa\omega_2$.

Proof. The proof is straightforward using elementary calculations. □

Using Lemma 27 we can extend the forward error analysis for explicit ODEs of [24] to our implicit ODEs.

Lemma 28 *Consider the implicit ODEs (55) and (56) and suppose that the system (55) is integrally separated, i.e., the diagonal elements* $\hat{b}_{i,i}$, $i = 1\ldots, d$ *are integrally separated. Suppose further, that all the assumptions of Lemma 27 hold and let* $\omega := (\mathcal{M}\varepsilon_1 + \varepsilon_2)/(1-\varepsilon_1)$. *Then there exist a global kinematic equivalence transformation with orthogonal matrices* $\hat{P}$ *and* $\hat{Q}$ *(that are close to identity matrices) that bring* $\hat{E}, \hat{A}$ *to upper triangular form*

$$\hat{\mathcal{E}} = \hat{P}^T\hat{E}\hat{Q}, \quad \hat{\mathcal{A}} = \hat{P}^T\hat{A}\hat{Q} - \hat{Q}^T\dot{\hat{Q}}.$$

Moreover, let $\left|\hat{b}_{k,\ell}(t)\right| \leq \kappa_{k,\ell}$ *for* $k < \ell$ *and for all* $t \in \mathbb{I}$. *Then there exist computable positive numbers* $\{\alpha_{k,\ell}\}_{k\neq\ell}$, *and* $\{\omega_{k,\ell}\}_{k\neq\ell}$ *such that if* $\omega < \min_{k\neq\ell}\{\omega_{k,\ell}\} = \omega_m$, *then for* $\hat{Q} = [\hat{q}_{k,\ell}]$ *one has* $|\hat{q}_{k,\ell}(t)| \leq \rho_{k,\ell}$ *for* $k \neq \ell$ *and for all* $t \in \mathbb{I}$, *where* $\rho_{k,\ell} = \alpha_{k,\ell}\kappa_{k,\ell}\omega$.

Proof. We apply the classical QR factorization to the solution of perturbed ODE system (57). By the same argument as that in Remark 16 and the uniqueness of QR factorization, the Q-factor obtained from (57) and that of (56) are the same. By this observation, we apply [24, Lemma 4.1] to (57) and immediately conclude that Q is near the identity matrix and also obtain the error bounds for $\hat{Q}(t) - I_d$ as in the assertion. Note that the parameters $\{\kappa_{k,\ell}\}_{k\neq\ell}$, $\{\alpha_{k,\ell}\}_{k\neq\ell}$ and the bounds $\{\omega_{k,\ell}\}_{k\neq\ell}$ can be constructed explicitly as in [24, Lemma 4.1]. By the definition of $\hat{P}$, we have that $\tilde{E}\hat{Q} = \hat{P}\hat{\mathcal{E}}$. Since the left-hand side is a nearly upper triangular matrix, by invoking the classical perturbation result for the QR factorization, see e.g. [43], we see that $\hat{P}$ is close to the identity matrix as well and a bound of $\left\| \hat{P}(t) - I_d \right\|$ is available. □

As a corollary we get a simplified bound for $\hat{Q}$.

Corollary 29 *In the notation of Lemma 28, let* $\tilde{\rho} = \max_{k\neq\ell} \rho_{k,\ell}$ *and assume that* $\rho := (n-1)(\tilde{\rho}+\tilde{\rho}^2) \leq 1$ *and* $\omega < \omega_m$. *Then,* $\left\|\hat{Q}(t) - I_d\right\| \leq \rho$ *and* $\left\|\hat{Q}(t) - I_d\right\|_F \leq \sqrt{2(n^2-n)}\tilde{\rho}$ *for all* $t \in \mathbb{I}$.

Now combining the forward error analysis with the backward error analysis and applying Corollary 29 to (47) and (50) as a particular case of (55) and (56), we obtain a global error bound for the components P, Q of the continuous QR method. The bound for the component Q of the discrete QR method is the same as that for the continuous variant.

Theorem 30 *Consider a well-conditioned DAE of the form (4). Let the assumptions of Lemma 28 and Corollary 29 hold. Then we have the following global error bound for the Q factor in the QR methods presented in Section 3*

$$\|Q_j - Q(t_j)\| \leq \rho, \quad j = 0, 1, 2, \ldots,$$

where $Q(t_j)$ *and* Q_j *are the exact and approximate values of the matrix function* Q *at* t_j, *respectively. Furthermore, if the condition number* $\operatorname{cond}(\bar{E})$ *of* $\bar{E}$ *defined in (5) satisfies* $\operatorname{cond}(\bar{E})\rho < 1/2$, *then*

$$\|P_j - P(t_j)\| \leq \frac{3\operatorname{cond}(\bar{E})\rho}{1 - 2\operatorname{cond}(\bar{E})\rho}, \quad j = 0, 1, 2, \ldots,$$

where $P(t_j)$ *and* P_j *are the exact and the approximate values of the orthogonal scaling factor* P *evaluated at* t_j, *respectively, which is defined by (29).*

Proof. By carrying out the backward error analysis first, then next the forward error analysis, from (44), we have the relation $Q_j = Q(t_j)\hat{Q}(t_j)$. By Corollary 29, we get

$$\|Q_j - Q(t_j)\| = \left\|Q(t_j)[\hat{Q}(t_j) - I_d]\right\| = \left\|\hat{Q}(t_j) - I_d\right\| \leq \rho.$$

To show the error bound for P, we refer to formula (29) and its equivalent formulation $\bar{E}^{-T}Q = P\mathcal{E}^{-T}$ for determining P. This is in fact a QR factorization and the perturbation in the left-hand side is $\left\|\bar{E}^{-T}Q_j - \bar{E}^{-T}Q(t_j)\right\| \leq \left\|\bar{E}^{-T}\right\|\rho$. Invoking [43, Theorem 3.1], we have

$$\|P_j - P(t_j)\| \leq \frac{3\left\|(\bar{E}^{-T}Q)^+\right\|\left\|\bar{E}^{-T}\right\|\rho}{1 - 2\left\|(\bar{E}^{-T}Q)^+\right\|\left\|\bar{E}^{-T}\right\|\rho},$$

where for a matrix M, M^+ denotes the Moore-Penrose inverse of M.

Using that $\left\|\bar{E}^{-T}\right\| = \left\|\bar{E}^{-1}\right\|$ and $\left\|(\bar{E}^{-T}Q)^+\right\| \leq \left\|\bar{E}^T\right\| = \left\|\bar{E}\right\|$, we obtain the estimate for $\|P_j - P(t_j)\|$. □

Finally, we obtain a perturbation result for the comparison of the spectral exponents in (55) and (56).

Theorem 31 *Consider the problems (55) and (56) with upper Lyapunov exponents* λ_i *and* μ_i, *respectively, and suppose that the unperturbed system (55) is integrally separated. If all the assumptions of Theorem 30 hold, then for sufficiently small* ω, *the perturbed system is (56) is integrally separated as well. Furthermore, the following perturbation bound holds:*

$$|\lambda_i - \mu_i| \leq \sum_{k\neq i} \rho_{k,i}^2 \gamma_{i,k} + \hat{\beta} \sum_{j=1}^{d} \rho_{j,i} \left(\sum_{k<j} \rho_{k,i}\right) + \beta \sum_{j\neq i} \rho_{i,j} + \omega, \tag{58}$$

for $i = 1, 2, \ldots, d$, *where* $\hat{\beta} = \max_{i\neq k} \sup_{t\in\mathbb{I}} \left|\hat{b}_{i,k}(t)\right|$, *and* $\gamma_{i,k} = \sup_{t\in\mathbb{I}} \left|\hat{b}_{i,i}(t) - \hat{b}_{k,k}(t)\right|$ *for* $1 \leq i, k \leq d$.

The same estimate holds for the differences between the lower Lyapunov exponents.

Proof. We have
$$(\hat{E}+\Delta\hat{E})^{-1}(\hat{A}+\Delta\hat{A}) = \hat{B}+\Delta\hat{B} = \hat{D}+\hat{U}+\Delta\hat{B},$$
where $\hat{D}=[\hat{d}_{i,j}]$ is the diagonal matrix with $d_{i,i}=\hat{b}_{i,i}$ and $\hat{U}=[\hat{u}_{i,k}]$ is the strict upper triangular matrix with $\hat{u}_{i,k}=\hat{b}_{i,k}$ for $i<k$.

The transformation with $\hat{P}$ and $\hat{Q}=[\hat{q}_{i,k}]$ transforms the perturbed system (56) to a system in upper triangular form
$$\hat{\mathcal{E}}\dot{Z} = \hat{\mathcal{A}}Z \tag{59}$$
which is equivalent to
$$\dot{Z} = \hat{\mathcal{B}}Z,$$
where $\hat{\mathcal{E}},\hat{\mathcal{A}}$ are defined as in Lemma 28 and $\hat{\mathcal{B}}=[\hat{\beta}_{i,j}]=\hat{\mathcal{E}}^{-1}\hat{\mathcal{A}}$.

It is easy to check that the diagonal elements of $\hat{\mathcal{B}}$ are equal to the corresponding diagonal elements of $\hat{Q}^T(\hat{B}+\Delta\hat{B})Q$, i.e.,
$$\hat{\beta}_{i,i} = \left[\hat{Q}^T(\hat{B}+\Delta\hat{B})Q\right]_{i,i}.$$
In order to estimate the difference between $\hat{\beta}_{i,i}$ and $\hat{b}_{i,i}$, recall that for the diagonal elements we have
$$\left[\hat{Q}^T(\hat{B}+\Delta\hat{B})\hat{Q}\right]_{i,i} = \left[\hat{Q}^T(\hat{D}+\hat{U}+\Delta\hat{B})\hat{Q}\right]_{i,i}.$$
Similar as in the proof of [22, Theorem 3.2], we have
$$\left[\hat{Q}^T\hat{D}\hat{Q}\right]_{i,i} - \hat{d}_{i,i} = (\hat{q}_{i,i}^2-1)\hat{d}_{i,i} + \sum_{k\neq i}\hat{q}_{k,i}^2\hat{d}_{k,k} = \sum_{k\neq i}\hat{q}_{k,i}^2(\hat{d}_{k,k}-\hat{d}_{i,i}).$$
Furthermore, we have
$$\begin{aligned}\left[\hat{Q}^T\hat{U}\hat{Q}\right]_{i,i} &= \sum_{j=1}^{d}\left(\sum_{k<j}\hat{q}_{k,i}\hat{b}_{k,j}\right)\hat{q}_{j,i}\\ &= \hat{q}_{i,i}\left(\sum_{k<i}\hat{q}_{k,i}\hat{b}_{k,i}+\sum_{j>i}\hat{b}_{i,j}\hat{q}_{j,i}\right)+\sum_{j=1,j\neq i}^{d}\left(\sum_{k<j,k\neq i}\hat{q}_{k,i}\hat{b}_{k,j}\right)\hat{q}_{j,i}.\end{aligned}$$
Then, using the estimates $|\hat{q}_{i,k}|\leq\rho_{i,k}$ for $i\neq k$ from Lemma 28, $|\hat{q}_{i,i}|\leq 1$ from the orthonormality, and $\left|\hat{b}_{i,k}\right|\leq\hat{\beta}$ for all $i\neq k$ from the definition of $\hat{\beta}$, we have that
$$\begin{aligned}\left|\hat{\beta}_{i,i}-\hat{b}_{i,i}\right| &\leq \left|\left[\hat{Q}^T\hat{D}Q\right]_{i,i}-\hat{d}_{i,i}\right|+\left|\left[\hat{Q}^T\hat{U}Q\right]_{i,i}\right|+\left|\left[\hat{Q}^T\Delta\hat{B}Q\right]_{i,i}\right|\\ &\leq \sum_{k\neq i}\rho_{k,i}^2\gamma_{i,k}+\hat{\beta}\sum_{j=1,j\neq i}^{d}\rho_{j,i}\left(\sum_{k<j,k\neq i}\rho_{k,i}\right)+\beta\sum_{j\neq i}\rho_{i,j}+\omega.\end{aligned}$$
Taking into account that $\rho_{i,k}=\alpha_{i,k}\kappa_{i,k}\omega$ for all i,k, there exists $\zeta_i\geq 0$ such that $\left|\hat{\beta}_{i,i}-\hat{b}_{i,i}\right|\leq\zeta_i\omega$ for $i=1,2,\ldots,d$.

With these preparations, we are able to check the integral separation of the upper triangular system (59). Since (55) is an upper triangular system, it is integrally separated if and only if its diagonal elements are integrally separated [23, Theorem3.4], i.e., there exist constants $c_1>0$ and $c_2\geq 0$ such that
$$\int_s^t\left(\hat{b}_{i,i}(r)-\hat{b}_{i+1,i+1}(r)\right)dr \geq c_1(t-s)-c_2, \quad \text{for all } t\geq s\geq 0,\ i=1,2,\ldots,d-1.$$

Then, it follows that

$$\begin{aligned}
\int_s^t \left(\hat{\beta}_{i,i}(r) - \hat{\beta}_{i+1,i+1}(r)\right) dr &= \int_s^t \left(\hat{b}_{i,i}(r) - \hat{b}_{i+1,i+1}(r)\right) dr + \int_s^t \left(\hat{\beta}_{i,i}(r) - \hat{b}_{i,i}(r)\right) dr \\
&+ \int_s^t \left(\hat{\beta}_{i+1,i+1}(r) - \hat{b}_{i+1,i+1}(r)\right) dr \\
&\geq c_1(t-s) - c_2 - \zeta_i \omega(t-s) - \zeta_{i+1}\omega(t-s) \\
&= (c_1 - \omega(\zeta_i + \zeta_{i+1}))(t-s) - c_2, \quad \text{for all } t \geq s \geq 0.
\end{aligned}$$

If ω is small enough such that $c_1 - \omega(\zeta_i + \zeta_{i+1})$ is strictly positive for $i = 1, 2, \dots d-1$, then the system (59) is integrally separated. Then, it is possible to approximate the Lyapunov exponents via the diagonal elements of $\hat{\mathcal{B}}$ [20]. Finally, we have

$$\begin{aligned}
|\lambda_i - \mu_i| &= \left| \limsup_{t\to\infty} \frac{1}{t}\int_0^t \hat{\beta}_{i,i}(r)dr - \limsup_{t\to\infty} \frac{1}{t}\int_0^t \hat{b}_{i,i}(r)dr \right| \\
&\leq \left| \limsup_{t\to\infty} \frac{1}{t}\int_0^t \left[\hat{\beta}_{i,i}(r) - \hat{b}_{i,i}(r)\right] dr \right| \\
&\leq \limsup_{t\to\infty} \frac{1}{t}\int_0^t \left|\hat{\beta}_{i,i}(r) - \hat{b}_{i,i}(r)\right| dr \\
&\leq \sum_{k\neq i} \rho_{k,i}^2 \gamma_{i,k} + \hat{\beta} \sum_{j=1, j\neq i}^{d} \rho_{j,i} \left(\sum_{k<j, k\neq i} \rho_{k,i} \right) + \hat{\beta} \sum_{j\neq i} \rho_{i,j} + \omega.
\end{aligned}$$

The proof for the lower exponents is analogous by using the identity

$$\liminf_{t\to\infty} f(t) = -\limsup_{t\to\infty}(-f(t)),$$

which holds for arbitrary $f(t) \in C(\mathbb{I}, \mathbb{R})$. □

As a Corollary we get the following upper bounds

Corollary 32 *Let the assumptions of Theorem 31 hold. Then, using the same notation as in Corollary 29, we have*

$$|\lambda_i - \mu_i| \leq \rho^2 \sum_{k\neq i} \gamma_{i,k} + (d-1)\hat{\beta}\rho + (\frac{d}{2} - 1)(d-1)\hat{\beta}\rho^2 + \omega = \mathcal{O}(\omega), \quad i = 1, 2, \dots d. \tag{60}$$

Remark 33 It can be shown in a similar way that analogous estimates as (58) and (60) hold for the upper and the lower Bohl exponents (the upper and lower endpoints of Sacker-Sell intervals). Note again that if we consider only the discretization error arising from numerical integration, i.e., the case of (47) and (50), then the perturbation bound ω has magnitude $\mathcal{O}(h^q)$, where $h = \max_{j\geq 1} h_j$ is the maximal stepsize and q is the order of the integrator.

4.4 Discussion of the error analysis

The analysis of the previous sections shows that in the case of the discrete QR method, for well-conditioned strangeness-free DAEs, the main error source is the error arising from numerical integration. However, the local error on each interval $\mathbb{I}_j = [t_{j-1}, t_j]$, $j = 1, 2, \dots$, can be controlled and kept below a given tolerance via an appropriate stepsize control. Then, by the backward error analysis, the problem is transferred to the perturbation analysis of a piecewise constant, upper triangular system, which has been analyzed in the forward error analysis. The perturbation occurring in the coefficient matrix of this piecewise constant system has the same magnitude as the local integration error if the errors in the QR factorizations and the errors in generating the strangeness-free formulation and those in solving the linear systems can be controlled. Thus, under the assumptions stated in the backward and the forward error analysis, we can conclude that the error of the spectral exponents has the same order of magnitude as the local error tolerance, too.

In the case of the continuous QR method, similarly, we apply again the backward and the forward error analysis results to estimate the errors arising from the numerical integration of the Q-factor and the logarithm of the diagonal elements of R. Besides the errors arising from the use of a numerical integrator, we have to face also round-off errors arising in QR factorizations (both, in the discrete and the continuous variants), the errors arising in approximating $\dot{A}_2$ (in the continuous QR, if the derivative of A_2 is not available), and the errors in solving linear algebraic system of upper triangular form, see (Remark 14). Again we have to be able to control these errors by incorporating them within the integration error in the backward error analysis and (or) within the data perturbation in the forward error analysis.

However, it is clear that the discrete QR method will in general produce less accurate results if the stepsize is small, but not small enough, because the fundamental solution matrix X may grow very fast which makes the columns of X become nearly linearly-dependent and then the QR factorization may produce bad results.

Furthermore, the exponential growth of the different columns of X may be quite different, e.g., there may exist simultaneously large positive and large negative exponents. This means that controlling the absolute error in the computation of X is not enough. In this case, one should use the relative error for the stepsize control (popular software packages for solving initial value problems for ODEs and DAEs use mixed error control, i.e., a combination involving both the absolute and the relative error). In the continuous QR method, not only the integration error of the Q-component, also the accumulation of round-off errors depends strongly on the condition number of $\bar{E}$, that is, on the DAE nature of the problem. We refer to [36] for more details on numerical methods for strangeness-free DAEs.

An alternative approach to the error analysis in the orthogonal factor, the upper triangular factors, and the Lyapunov and Bohl exponents is presented in [44]. The main idea is that once one has a backward error result such as Lemma 19, then one would like to show the existence of an orthogonal change of variables that brings the sequence of perturbed triangular factors, $R(t_j, t_{j-1}) + \mathcal{E}_j$, to upper triangular form again. In this work and in [22, 24] for ODEs this was done by determining a perturbed triangular differential equation and then showing via the continuous QR method the existence of and bounds on a near identity orthogonal change of variables (assuming that the integral separation is strong enough as compared to the size of the perturbation) via the equations for Q in the continuous QR method. Alternatively, in [44] one works directly with the perturbed triangular factor and by defining an appropriate zero finding problem in terms of the discrete QR method one shows the existence of and bounds on the near identity change orthogonal change of variables. In particular, this avoids forming the perturbed triangular differential equation and finding bounds on its perturbation.

5 Numerical examples

We have implemented both the continuous and the discrete variants of the QR methods described in Section 3 in MATLAB. The following preliminary results are obtained with Version Matlab Version 7.4(R2007a) on an Intel CPU T9300 processor with 2.5 GHz.

To illustrate the properties of the procedures, we consider two examples, one of a Lyapunov regular DAE system and another DAE system which is not Lyapunov regular. In the second case, we calculated not only the Lyapunov spectral intervals, but also the Sacker-Sell intervals.

Example 34 Our first example is a Lyapunov-regular DAE system which is constructed similar to the ODE examples in [17, 20]. We have constructed a DAE system of the form (4) by beginning with an upper triangular implicit ODE system, applying appropriate kinematic equivalence transformations and then adding additional algebraic variables. In this way we have obtained a semi-implicit DAE system of the form (17) which was then transformed again to obtain a DAE system of the form (4), whose spectral information is the same as that of original implicit ODE system.

The original triangular implicit ODE system had the form $\bar{E}_{1,1}(t)\dot{\bar{x}}_1 = \bar{A}_{1,1}(t)\bar{x}_1$, where

$$\bar{E}_{1,1}(t) = \begin{bmatrix} 1+\frac{1}{t+1} & 1 \\ 0 & 1 \end{bmatrix}, \quad \bar{A}_{1,1}(t) = \begin{bmatrix} \lambda_1 - \frac{1}{t+1} & \omega \sin t \\ 0 & \lambda_2 + \cos(t+1) \end{bmatrix}, \quad t \in \mathbb{I},\ \lambda_i \in \mathbb{R} \quad (i = 1,2),$$

where $\lambda_i, i = 1,2,\ (\lambda_1 < \lambda_2)$ are given real parameters. We then performed a transformation transformed to get the implicit ODE system $\tilde{E}_{1,1}(t)\dot{\tilde{x}}_1 = \tilde{A}_{1,1}(t)\tilde{x}_1$ given by

$$\tilde{E}_{11} = U_1\bar{E}_{1,1}V_1^T, \quad \tilde{A}_{11} = U_1\bar{A}_{1,1}V_1^T + U_1\bar{E}_{1,1}V_1^T\dot{V}_1V_1^T,$$

with $U_1(t) = G_{\gamma_1}(t),\ V_1(t) = G_{\gamma_2}(t)$, where $G(\gamma_i)$ is a Givens rotation

$$G_\gamma(t) = \begin{bmatrix} \cos\gamma t & \sin\gamma t \\ -\sin\gamma t & \cos\gamma t \end{bmatrix}$$

with some real parameters γ_1, γ_2. We choose additional blocks $\tilde{E}_{12} = U_1, \tilde{A}_{12} = V_1, \tilde{A}_{22} = U_1V_1$ and finally

$$\tilde{E} = \begin{bmatrix} \tilde{E}_{11} & \tilde{E}_{12} \\ 0 & 0 \end{bmatrix}, \quad \tilde{A} = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix}.$$

Using a 4×4 orthogonal matrix

$$G(t) = \begin{bmatrix} \cos\gamma_3 t & 0 & 0 & \sin\gamma_3 t \\ 0 & \cos\gamma_4 t & \sin\gamma_4 t & 0 \\ 0 & -\sin\gamma_4 t & \cos\gamma_4 t & 0 \\ -\sin\gamma_3 t & 0 & 0 & \cos\gamma_3 t \end{bmatrix},$$

with real values γ_3, γ_4 we obtained a strangeness-free DAE system of the form (4) with coefficients $E = \tilde{E}G^T,\ A = AG^T + \tilde{E}G^T\dot{G}G^T$. Furthermore, because Lyapunov-regularity together as well Lyapunov exponents are invariant under orthogonal change of variables, this system is Lyapunov-regular with the Lyapunov exponents λ_1, λ_2.

For our numerical tests we have used the values

$$\omega = 3,\ \lambda_1 = 5,\ \lambda_2 = 1,\ \gamma_1 = \gamma_4 = 2,\ \gamma_2 = \gamma_3 = 1.$$

In the following two tables the described discrete and continuous QR method for computing the Lyapunov exponents are compared. We present the interval length T, the step size h, the computed Lyapunov exponents, the relative error in % and the CPU-time. The last column shows the computing time if only one spectral interval (the larger one) is computed, i.e., we have the case $p = 1$. As integrator in the continuous QR method we have used the classical fourth order explicit Runge-Kutta method with projection, see [16], applied to

$$\begin{aligned} \dot{Q} &= \bar{E}^{-1}\big(\bar{A}Q - \bar{E}QB\big), \\ W &= Q^T(\bar{E}^{-1}\bar{A})Q, \\ B &= \mathrm{upp}(W) + \mathrm{low}(W)^T, \end{aligned}$$

where for the solution of the linear systems with $\bar{E}$ we use an LU factorization with partial pivoting.

For the discrete QR algorithm we have employed a 6-th order BDF method, see e.g., [7].

Example 35 (A DAE system which is not Lyapunov regular.) With the same transformations as in Example 34, we also constructed a DAE that is not Lyapunov regular by changing the matrix $\bar{A}(t)$ in Example 34 to

$$\bar{A}(t) = \begin{bmatrix} \sin(\ln(t+1)) + \cos(\ln(t+1)) + \lambda_1 & \omega \sin t \\ 0 & \sin(\ln(t+1)) - \cos(\ln(t+1)) + \lambda_2 \end{bmatrix}, \quad t \in \mathbb{I}.$$

Table 1: Lyapunov exponents with discrete QR algorithm for Ex. 34.

T	h	$\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}$	rel. error in %	CPU-time in s	CPU-time in $s,\ p=1$
1000	0.12	$\begin{bmatrix} 5.0258 \\ 0.9937 \end{bmatrix}$	$\begin{bmatrix} 0.5170 \\ 0.6285 \end{bmatrix}$	2.8079	2.5262
1000	0.10	$\begin{bmatrix} 5.0144 \\ 0.9948 \end{bmatrix}$	$\begin{bmatrix} 0.2878 \\ 0.5184 \end{bmatrix}$	3.4583	3.0750
1000	0.05	$\begin{bmatrix} 4.9875 \\ 0.9975 \end{bmatrix}$	$\begin{bmatrix} 0.2510 \\ 0.2538 \end{bmatrix}$	6.8130	6.2326
1000	0.01	$\begin{bmatrix} 4.9675 \\ 0.9996 \end{bmatrix}$	$\begin{bmatrix} 0.6502 \\ 0.0442 \end{bmatrix}$	33.5097	30.6883
5000	0.12	$\begin{bmatrix} 5.0544 \\ 0.9934 \end{bmatrix}$	$\begin{bmatrix} 1.0888 \\ 0.6556 \end{bmatrix}$	12.8217	11.9376
5000	0.10	$\begin{bmatrix} 5.0429 \\ 0.9945 \end{bmatrix}$	$\begin{bmatrix} 0.8572 \\ 0.5499 \end{bmatrix}$	15.4020	14.3763
5000	0.05	$\begin{bmatrix} 5.0156 \\ 0.9971 \end{bmatrix}$	$\begin{bmatrix} 0.3125 \\ 0.2859 \end{bmatrix}$	31.0260	28.6265
10000	0.12	$\begin{bmatrix} 5.0588 \\ 0.9935 \end{bmatrix}$	$\begin{bmatrix} 1.1769 \\ 0.6499 \end{bmatrix}$	25.4112	23.6348
10000	0.10	$\begin{bmatrix} 5.0472 \\ 0.9946 \end{bmatrix}$	$\begin{bmatrix} 0.9448 \\ 0.5433 \end{bmatrix}$	30.7016	28.3451
10000	0.05	$\begin{bmatrix} 5.0200 \\ 0.9972 \end{bmatrix}$	$\begin{bmatrix} 0.3990 \\ 0.2792 \end{bmatrix}$	60.8064	56.7574

Table 2: Lyapunov exponents with continuous QR algorithm for Ex. 34.

T	h	$\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}$	rel. error in %	CPU-time in s	CPU-time in $s,\ p=1$
1000	0.12	$\begin{bmatrix} 4.9631 \\ 0.9999 \end{bmatrix}$	$\begin{bmatrix} 0.7383 \\ 0.0096 \end{bmatrix}$	3.6563	3.5198
1000	0.10	$\begin{bmatrix} 4.9629 \\ 1.0001 \end{bmatrix}$	$\begin{bmatrix} 0.7428 \\ 0.0061 \end{bmatrix}$	4.3888	4.2186
1000	0.05	$\begin{bmatrix} 4.9627 \\ 1.0001 \end{bmatrix}$	$\begin{bmatrix} 0.7463 \\ 0.0134 \end{bmatrix}$	8.7218	8.4196
1000	0.01	$\begin{bmatrix} 4.9627 \\ 1.0001 \end{bmatrix}$	$\begin{bmatrix} 0.7460 \\ 0.0092 \end{bmatrix}$	43.5736	42.1863
5000	0.12	$\begin{bmatrix} 4.9909 \\ 0.9997 \end{bmatrix}$	$\begin{bmatrix} 0.1829 \\ 0.0319 \end{bmatrix}$	16.7958	16.4449
5000	0.10	$\begin{bmatrix} 4.9907 \\ 0.9998 \end{bmatrix}$	$\begin{bmatrix} 0.1870 \\ 0.0217 \end{bmatrix}$	20.1520	19.9026
5000	0.05	$\begin{bmatrix} 4.9905 \\ 0.9998 \end{bmatrix}$	$\begin{bmatrix} 0.1893 \\ 0.0168 \end{bmatrix}$	40.2386	39.3086
10000	0.12	$\begin{bmatrix} 4.9951 \\ 0.9997 \end{bmatrix}$	$\begin{bmatrix} 0.0976 \\ 0.0270 \end{bmatrix}$	33.0881	32.5306
10000	0.10	$\begin{bmatrix} 4.9949 \\ 0.9998 \end{bmatrix}$	$\begin{bmatrix} 0.1017 \\ 0.0156 \end{bmatrix}$	39.7260	39.0194
10000	0.05	$\begin{bmatrix} 4.9948 \\ 0.9999 \end{bmatrix}$	$\begin{bmatrix} 0.1038 \\ 0.0104 \end{bmatrix}$	79.7169	77.7178

Table 3: Bohl exponents computed with discrete QR algorithm Ex. 35.

T	h	H	$\begin{bmatrix} \kappa_1^\ell & \kappa_1^u \\ \kappa_2^\ell & \kappa_2^u \end{bmatrix}$	rel. error in %	CPU-time in s	CPU-time in s, $p=1$
1000	0.12	100	$\begin{bmatrix} -1.2004 & 1.3728 \\ -6.3538 & -4.8750 \end{bmatrix}$	$\begin{bmatrix} 15.1172 & 2.9289 \\ 0.9425 & 35.9545 \end{bmatrix}$	3.6339	2.9289
5000	0.12	100	$\begin{bmatrix} -1.2004 & 1.4051 \\ -6.3538 & -3.5938 \end{bmatrix}$	$\begin{bmatrix} 15.1172 & 0.6475 \\ 0.9425 & 0.2241 \end{bmatrix}$	17.0300	15.4671
10000	0.12	100	$\begin{bmatrix} -1.2004 & 1.4051 \\ -6.3538 & -3.4824 \end{bmatrix}$	$\begin{bmatrix} 15.1172 & 0.6475 \\ 0.9425 & 0.0941 \end{bmatrix}$	33.2838	30.4316
10000	0.12	500	$\begin{bmatrix} -0.7338 & 1.3949 \\ -6.1660 & -3.5829 \end{bmatrix}$	$\begin{bmatrix} 48.1142 & 1.3653 \\ 3.8701 & 0.0808 \end{bmatrix}$	34.3723	31.5720
10000	0.075	100	$\begin{bmatrix} -1.2022 & 1.4079 \\ -6.3719 & -3.5837 \end{bmatrix}$	$\begin{bmatrix} 14.9948 & 0.4474 \\ 0.6600 & 0.0581 \end{bmatrix}$	53.2889	48.7271
50000	0.12	100	$\begin{bmatrix} -1.4065 & 1.4051 \\ -6.3538 & -3.5824 \end{bmatrix}$	$\begin{bmatrix} 0.5461 & 0.6475 \\ 0.9425 & 0.0941 \end{bmatrix}$	152.3445	152.3445
50000	0.12	500	$\begin{bmatrix} -1.4065 & 1.3949 \\ -6.1660 & -3.5829 \end{bmatrix}$	$\begin{bmatrix} 0.5482 & 1.3653 \\ 3.8701 & 0.0808 \end{bmatrix}$	166.3611	151.8304
50000	0.5	100	$\begin{bmatrix} -1.3846 & 1.3812 \\ -6.2225 & -3.5703 \end{bmatrix}$	$\begin{bmatrix} 2.0963 & 2.3376 \\ 2.9893 & 0.4321 \end{bmatrix}$	39.6996	36.0344
100000	0.12	100	$\begin{bmatrix} -1.4065 & 1.4051 \\ -6.3538 & -3.5824 \end{bmatrix}$	$\begin{bmatrix} 0.5482 & 0.6475 \\ 0.9425 & 0.0941 \end{bmatrix}$	331.4083	299.8992
100000	0.12	500	$\begin{bmatrix} -1.4065 & 1.3949 \\ -6.3149 & -3.5829 \end{bmatrix}$	$\begin{bmatrix} 0.5482 & 1.3653 \\ 1.5491 & 0.0808 \end{bmatrix}$	331.5006	301.4223
100000	0.5	100	$\begin{bmatrix} -1.3846 & 1.3812 \\ -6.2259 & -3.5703 \end{bmatrix}$	$\begin{bmatrix} 2.0963 & 2.3376 \\ 2.9893 & 0.4321 \end{bmatrix}$	79.3260	72.1256

Here we have used $\omega = 3,\ \lambda_1 = 0,\ \lambda_2 = -5$. Since Lyapunov and Sacker-Sell spectra are invariant with respect to global kinematical equivalence transformation, it is easy to compute the Lyapunov spectral intervals as $[-1, 1]$ and $[-6, -4]$ and the Sacker-Sell spectral intervals as $[-\sqrt{2}, \sqrt{2}]$ and $[-5-\sqrt{2}, -5+\sqrt{2}]$.

The examples show that the discrete QR algorithm delivers results of good accuracy. Even for short intervals with large step-sizes the Lyapunov exponents are computed with a small relative error similar to the results in [40]. For large intervals T the exponents are well determined, even for large step-size as $h = 0.5$. The results of the continuous QR algorithm are usually more accurate than those of the discrete QR algorithm with a cost that is comparable or sometimes a little higher.

6 Conclusion

In this paper we have developed QR methods for computing all or just a few spectral intervals for linear time-varying DAEs. Unlike the method previously proposed in [40], the methods presented here are applied directly to the DAE. Furthermore, we have derived the perturbation and error analysis. It has been shown that, under certain natural assumptions, the spectral intervals can be approximated with an accuracy that is of the same magnitude as that of the local integration scheme.

As future work, we suggest the investigation of block-versions of the QR methods and their error analysis, where the integral separation holds between several blocks which contain the equal

Table 4: Bohl exponents computed with continuous QR algorithm Ex. 35.

T	h	H	$\begin{bmatrix} \kappa_1^\ell & \kappa_1^u \\ \kappa_2^\ell & \kappa_2^u \end{bmatrix}$	rel. error in %	CPU-time in s	CPU-time in $s,\ p=1$
1000	0.12	100	$\begin{bmatrix} -1.2049 & 1.3801 \\ -6.4039 & -4.8928 \end{bmatrix}$	$\begin{bmatrix} 14.7974 & 2.4138 \\ 0.1604 & 36.4500 \end{bmatrix}$	4.7465	4.5688
5000	0.12	100	$\begin{bmatrix} -1.2049 & 1.4121 \\ -6.4039 & -3.5983 \end{bmatrix}$	$\begin{bmatrix} 14.7974 & 0.1473 \\ 0.1604 & 0.3484 \end{bmatrix}$	22.0405	21.0872
10000	0.12	100	$\begin{bmatrix} -1.2049 & 1.4121 \\ -6.4039 & -3.5860 \end{bmatrix}$	$\begin{bmatrix} 14.7974 & 0.1473 \\ 0.1604 & 0.0057 \end{bmatrix}$	43.6055	41.8855
10000	0.12	500	$\begin{bmatrix} -0.7336 & 1.4020 \\ -6.2131 & -3.5864 \end{bmatrix}$	$\begin{bmatrix} 48.1257 & 0.8624 \\ 3.1350 & 0.0181 \end{bmatrix}$	45.2865	43.3202
10000	0.075	100	$\begin{bmatrix} -1.2049 & 1.4125 \\ -6.4043 & -3.5858 \end{bmatrix}$	$\begin{bmatrix} 14.8008 & 0.1204 \\ 0.1544 & 0.0006 \end{bmatrix}$	69.6667	66.9073
50000	0.12	100	$\begin{bmatrix} -1.4141 & 1.4121 \\ -6.4039 & -3.5860 \end{bmatrix}$	$\begin{bmatrix} 0.0057 & 0.1473 \\ 0.1604 & 0.0057 \end{bmatrix}$	213.0068	207.9180
50000	0.12	500	$\begin{bmatrix} -1.4141 & 1.4020 \\ -6.2131 & -3.5864 \end{bmatrix}$	$\begin{bmatrix} 0.0071 & 0.8624 \\ 3.1350 & 0.0181 \end{bmatrix}$	213.8641	209.0700
100000	0.12	100	$\begin{bmatrix} -1.4141 & 1.4121 \\ -6.4039 & -3.5860 \end{bmatrix}$	$\begin{bmatrix} 0.0057 & 0.1473 \\ 0.1604 & 0.0057 \end{bmatrix}$	424.3621	415.0898

Lyapunov exponents. Furthermore, a direct implementation of the QR methods for some special classes of DAEs such as DAEs of Hessenberg form would be of interest.

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References

[1] L. Ya. Adrianova. *Introduction to linear systems of differential equations.* Trans. Math. Monographs, Vol. 146, AMS, Providence, RI, 1995.

[2] U. M. Ascher and L. R. Petzold. *Computer Methods for Ordinary Differential and Differential-Algebraic Equations.* SIAM Publications, Philadelphia, PA, 1998.

[3] K. Balla and V. H. Linh. Adjoint pairs of differential-algebraic equations and Hamiltonian systems. *Appl. Numer. Math.*, 53:131–148, 2005.

[4] G. Benettin, G. Galgani, L. Giorgilli, and J.M. Strelcyn. Lyapunov exponents for smooth dynamical systems and for hamiltonian systems; a method for computing all of them. Part I: Theory and Part II: Numerical applications. *Meccanica*, 15:9–20, 21–30, 1980.

[5] P. Benner and R. Byers. An arithmetic for matrix pencils: theory and new algorithms. *Numer. Math.*, 103:539–573, 2006.

[6] P. Bohl. Über Differentialungleichungen. *J. f. d. Reine und Angew. Math.*, 144:284–313, 1913.

[7] K. E. Brenan, S. L. Campbell, and L. R. Petzold. *Numerical Solution of Initial-Value Problems in Differential Algebraic Equations.* SIAM Publications, Philadelphia, PA, 2nd edition, 1996.

[8] T. J. Bridges and S. Reich. Computing Lyapunov exponents on a Stiefel manifold. *Phys. D* 156:219–238, 2001.

[9] S. L. Campbell. Linearization of DAE's along trajectories. *Z. Angew. Math. Phys.*, 46:70–84, 1995.

[10] J.-L. Chern and L. Dieci. Smoothness and periodicity of some matrix decompositions. *SIAM J. Matr. Anal. Appl.*, 22:772–792, 2000.

[11] C.J. Chyan, N.H. Du, and V.H. Linh. On data-dependence of exponential stability and the stability radii for linear time-varying differential-algebraic systems. *J. Diff. Equations*, 245:2078–2102, 2008.

[12] N.D. Cong and H. Nam. Lyapunov's inequality for linear differential algebraic equation. *Acta Math. Vietnam*, 28:73–88, 2003.

[13] N.D. Cong and H. Nam. Lyapunov regularity of linear differential algebraic equations of index 1. *Acta Math. Vietnam*, 29:1–21, 2004.

[14] J.L. Daleckii and M.G. Krein. *Stability of solutions of differential equations in Banach spaces.* American Mathematical Society, Providence, RI, 1974.

[15] L. Dieci and T. Eirola. On smooth decompositions of matrices. *SIAM J. Matr. Anal. Appl.*, 20:800–819, 1999.

[16] L. Dieci, R. D. Russell, and E. S. Van Vleck. Unitary integrators and applications to continuous orthonormalization techniques. *SIAM J. Numer. Anal.*, 31:261–281, 1994.

[17] L. Dieci, R. D. Russell, and E. S. Van Vleck. On the computation of Lyapunov exponents for continuous dynamical systems. *SIAM J. Numer. Anal.*, 34:402–423, 1997.

[18] L. Dieci and E. S. Van Vleck. Computation of a few Lyapunov exponents for continuous and discrete dynamical systems. *Appl. Numer. Math.*, 17:275–291, 1995.

[19] L. Dieci and E. S. Van Vleck. Lyapunov and other spectra: a survey. In *Collected lectures on the preservation of stability under discretization (Fort Collins, CO, 2001)*, pages 197–218. SIAM, Philadelphia, PA, 2002.

[20] L. Dieci and E. S. Van Vleck. Lyapunov spectral intervals: theory and computation. *SIAM J. Numer. Anal.*, 40:516–542, 2002.

[21] L. Dieci and E. S. Van Vleck. On the error in computing Lyapunov exponents by QR methods. *Numer. Math.*, 101:619–642, 2005.

[22] L. Dieci and E. S. Van Vleck. Perturbation theory for approximation of Lyapunov exponents by QR methods. *J. Dyn. Diff. Eq.*, 18:815–842, 2006.

[23] L. Dieci and E. S. Van Vleck. Lyapunov and Sacker-Sell spectral intervals. *J. Dyn. Diff. Eq.*, 19:265–293, 2007.

[24] L. Dieci and E. S. Van Vleck. On the error in QR integration. *SIAM J. Numer. Anal.*, 46:1166–1189, 2008.

[25] M. Diehl, D. B. Leineweber, A. Schäfer, H. G. Bock, and J. P. Schlöder. Optimization of multiple-fraction batch distillation with recycled waste cuts. *AIChE Journal*, 48(12):2869–2874, 2002.

[26] M. Diehl, I. Uslu, R. Findeisen, S. Schwarzkopf, F. Allgöwer, H. G. Bock, T. Bürner, E. D. Gilles, A. Kienle, J. P. Schlöder, and E. Stein. Real-time optimization for large scale processes: Nonlinear model predictive control of a high purity distillation column. In M. Grötschel, S. O. Krumke, and J. Rambau, editors, *Online Optimization of Large Scale Systems: State of the Art*, pages 363–384. Springer Verlag, Heidelberg, Germany, 2001.

[27] E. Eich-Soellner and C. Führer. *Numerical Methods in Multibody Systems*. Teubner Verlag, Stuttgart, Germany, 1998.

[28] K. Geist, U. Parlitz, and W. Lauterborn. Comparison of different methods for computing Lyapunov exponents. *Progr. Theoret. Phys.*, 83:875–893, 1990.

[29] G. H. Golub and C. F. Van Loan. *Matrix Computations*. The Johns Hopkins University Press, Baltimore, MD, 3rd edition, 1996.

[30] J.M. Greene and J-S. Kim. The calculation of Lyapunov spectra. *Physica D*, 24:213–225, 1983.

[31] E. Griepentrog and R. März. *Differential-Algebraic Equations and their Numerical Treatment*. Teubner Verlag, Leipzig, Germany, 1986.

[32] M. Günther and U. Feldmann. CAD-based electric-circuit modeling in industry I. Mathematical structure and index of network equations. *Surv. Math. Ind.*, 8:97–129, 1999.

[33] M. Günther and U. Feldmann. CAD-based electric-circuit modeling in industry II. Impact of circuit configurations and parameters. *Surv. Math. Ind.*, 8:131–157, 1999.

[34] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*. Springer-Verlag, Berlin, Germany, 2nd edition, 1996.

[35] P. Kunkel and V. Mehrmann. Characterization of classes of singular linear differential-algebraic equations. *Electr. J. Lin. Alg.*, 13:359–386, 2005.

[36] P. Kunkel and V. Mehrmann. *Differential-Algebraic Equations. Analysis and Numerical Solution*. EMS Publishing House, Zürich, Switzerland, 2006.

[37] P. Kunkel and V. Mehrmann, Stability properties of differential-algebraic equations and spin-stabilized discretizations. *Electr. Trans. Numer. Anal.* 26:385–420, 2007.

[38] P. Kunkel, V. Mehrmann, W. Rath, and J. Weickert. A new software package for linear differential–algebraic equations. *SIAM J. Sci. Comput.*, 18:115–138, 1997.

[39] P. Kunkel, V. Mehrmann, and S. Seidel. A MATLAB package for the numerical solution of general nonlinear differential-algebraic equations. Technical Report 16/2005, Institut für Mathematik, TU Berlin, Berlin, Germany, 2005. `url: http://www.math.tu-berlin.de/preprints/`.

[40] V.H. Linh and V. Mehrmann. Lyapunov, Bohl and Sacker-Sell spectral intervals for differential-algebraic equations. *J. Dyn. Diff. Eq.*, 21:153–194, 2009.

[41] A. M. Lyapunov. The general problem of the stability of motion. Translated by A. T. Fuller from Edouard Davaux's French translation (1907) of the 1892 Russian original. *Internat. J. Control*, pages 521–790, 1992.

[42] M. Otter, H. Elmqvist, and S. E. Mattson. Multi-domain modeling with modelica. In Paul Fishwick, editor, *CRC Handbook of Dynamic System Modeling*. CRC Press, 2006.

[43] G. W. Stewart. Perturbation bounds for the QR factorization of a matrix. *SIAM J. Numer. Anal.*, 14:509–518, 1977.

[44] E .S. Van Vleck, On the error in the product QR. *Submitted for publication*, 2009.