

Detecting Exponential Dichotomy on the real line: SVD and QR algorithms

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Abstract In this paper we propose and implement numerical methods to detect exponential dichotomy on the real line. Our algorithms are based on the singular value decomposition and the QR factorization of a fundamental matrix solution. The theoretical justification for our methods was laid down in the companion paper [15].

Keywords Exponential Dichotomy · Sacker-Sell spectrum · Lyapunov exponents

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1 Introduction

Consider the n -dimensional linear system of ODEs

$$\dot{x} = A(t; \lambda)x, \quad (1)$$

where $A : \mathbb{R} \times \mathbb{C} \rightarrow \mathbb{C}^{n \times n}$ is continuous and bounded in t , and smooth in the complex parameter λ (often, A depends analytically on λ).

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Typically, (1) arises as the variational equation associated to a nonlinear system with vector field depending on a parameter λ :

$$\dot{x} = f(x; \lambda). \quad (2)$$

To study stability of a solution of (2) with respect to (variations of) the parameter, we are lead to investigate whether or not (1) possesses exponential dichotomy. Furthermore, systems like (1) arise also when studying orbital stability of traveling waves ([42]) and more in general when studying the spectrum of a linear differential operator L : $Lx = \dot{x} - A(t)x$ ([36]). Indeed, the property of exponential dichotomy (hyperbolicity) is ubiquitous in dynamical systems studies; e.g., see [37, 38] for its importance in the shadowing of dynamical systems and [9, 23, 24, 41] for the central role it plays in invariant manifold theory. But, in spite of its theoretical relevance, general numerical methods to ascertain whether or not a certain system possesses exponential dichotomy are still lacking, with the exception of stability studies for traveling waves, where an extensive and sophisticated literature exist (e.g., see [6–8, 27, 28, 42]).

Our contribution in this paper is to develop robust computational techniques for the detection of exponential dichotomy (ED for short) on the real line for linear n -dimensional systems that depend on a complex parameter. The underlying mathematical assumption which we need is that both two half lines problems (that is, $t \leq 0$ and $t \geq 0$) have Lyapunov exponents that are continuous with respect to perturbations. This is a generic conditions for linear system, and it is much weaker than requiring convergence of the coefficient matrix A to constant values as $t \rightarrow \pm\infty$; the latter condition is effectively the one required by studies on stability of connecting orbits. Indeed, our work provides for the first time a computationally realizable technique for determining exponential dichotomy on the real line, under essentially generic conditions, using information from a finite time interval. Moreover, we also show in this paper that our technique is numerically stable and we also obtain approximations of both the stable and the unstable subspaces.

To verify if (1) possesses exponential dichotomy (ED for short) in \mathbb{R} , in this paper we implement, and test, algorithms which follow the theoretical development we laid down in [15]. In that work, we gave theoretical justification for two different techniques to detect whether or not (1) admits ED in \mathbb{R} . These techniques are based on the singular value decomposition (SVD) and on the QR factorization of a fundamental matrix solution of (1), respectively. Although in [15] we considered the case of real valued coefficient matrix (in (1), $A \in \mathbb{R}^{n \times n}$), the extension to the complex case (which is the case considered in this paper) is straightforward and appropriate comments will be made here below as needed.

The fundamental result on which we developed our analysis in [15] is the following one of Coppel (see [12]): “A given linear system possesses ED in \mathbb{R} if and only if it possesses ED in the two half-lines, and the forward stable subspace and the backward stable subspace¹ are complementary”. So, there are two different tasks: (i) To check whether a system has ED in \mathbb{R}^+ and \mathbb{R}^- , and for this task the techniques in [13], [18], [21] can be used, and (ii) To check complementarity of the forward and backward stable subspaces. This last topic we addressed in [15]. In line with this previous work of ours, in the present paper we base our numerical algorithms on the SVD and QR factorizations of a fundamental matrix solution. However, it should be appreciated that

¹ This is called the *unstable subspace* by Sacker and Sell in [39]

in order to obtain numerically stable techniques, the QR and SVD factorization cannot be implemented in the standard ways, as otherwise the necessary stable/unstable subspaces will not be well approximated. See below for details. As far as we know, our effort is the first general computational effort for detecting ED for continuous dynamical systems. The recent work [26] addresses computation of the exponential dichotomy spectrum for discrete dynamical systems by completely different techniques than those we consider here.

A plan of the paper is as follows. In the remainder of this Introduction we review the relevant spectral concepts and give a high level description of how to detect ED. The key issue of how to detect complementarity of forward and backward stable subspaces for parameter dependent systems is discussed at some length, and the tool of the Evans function is reviewed as well. In Section 2, we discuss SVD and QR techniques and give some new results related to smoothness in the case of parameter dependent systems. In Section 3 we give algorithmic details, and in Section 4 we present results of some numerical experiments.

Notation. Henceforth, we will typically omit writing explicitly the dependence on λ in (1), and simply write $A(t)$. The principal matrix solution of (1) will be written as $\Phi(\cdot, 0)$, or simply $\Phi(\cdot)$, so that $\dot{\Phi} = A(t)\Phi$, $\Phi(0, 0) = \Phi(0) = I$. Analogously, we will employ the notation $\Phi(t_{j+1}, t_j)$ to denote the transition matrix on $[t_j, t_{j+1}]$, that is the solution at time t_{j+1} of the problem

$$\frac{d}{dt}\Phi(t, t_j) = A(t)\Phi(t, t_j), \quad \Phi(t_j, t_j) = I.$$

The Hermitian of a complex valued matrix A will be denoted as A^* (that is, $A^* = \bar{A}^T$).

1.1 Spectra of dynamical systems.

The following concepts will be needed.

The Lyapunov spectrum: Σ_L . The Lyapunov spectrum is typically defined on the half-line, and we review it for the case of $t \geq 0$. It is defined in terms of upper and lower Lyapunov exponents (LEs for short). Given a fundamental matrix X , $\dot{X} = A(t)X$ with $X(0)$ invertible, one defines μ_j , $j = 1, \dots, n$, as

$$\mu_j = \limsup_{t \rightarrow +\infty} \frac{1}{t} \log \|X(t)e_j\|, \quad (3)$$

where the e_j 's are the standard unit vectors. When the sum of the numbers μ_j is minimized as we vary over all possible initial conditions $X(0)$, the μ_i 's are called (upper) Lyapunov exponents of the system, and the initial condition $X(0)$ is called a *normal basis*. We will write λ_j^s , $j = 1, \dots, n$, for the ordered upper LEs. By working with the adjoint system, $\dot{z} = -A^T(t)z$, one analogously defines its ordered upper LEs, which are also called lower LEs of the original system, call them λ_j^i , $j = 1, \dots, n$. The Lyapunov spectral intervals can now be defined as

$$\Sigma_L^+ := \bigcup_{j=1}^n [\lambda_j^i, \lambda_j^s]. \quad (4)$$

In case in which $\lambda_j^i = \lambda_j^s = \lambda_j$, for all $j = 1, \dots, n$, the system is called *regular*. Similar definitions hold for the case of $t \leq 0$, and we write Σ_L^- for the Lyapunov spectrum in this case.

The Exponential Dichotomy, or Sacker-Sell, spectrum: Σ_{ED} . This is defined in terms of exponential dichotomy (see [12]). Recall that (1) has Exponential Dichotomy on J , ($J = \mathbb{R}, \mathbb{R}^+, \mathbb{R}^-$) if there exist constants $K \geq 1$, $\alpha > 0$, and a projection P such that

$$\begin{aligned} \|X(t)PX^{-1}(s)\| &\leq Ke^{-\alpha(t-s)}, \quad t \geq s, \\ \|X(t)(I-P)X^{-1}(s)\| &\leq Ke^{\alpha(t-s)}, \quad t \leq s, \end{aligned} \quad (5)$$

where X is a fundamental matrix solution, and $t, s \in J$. Σ_{ED} is defined to be the set of values $\mu \in \mathbb{R}$ for which the shifted systems $\dot{y} = [A(t) - \mu I]y$ do not have exponential dichotomy.

Remark 1 We remark that by virtue of the roughness theorem for exponential dichotomies (see [11]), Σ_{ED} is stable, that is it is continuous with respect to perturbation in the coefficient matrix A .

We also recall (see [39]) that, for some $k \leq n$, Σ_{ED} is given by a collection of disjoint subintervals

$$\Sigma_{ED} := [a_1, b_1] \cup \dots \cup [a_k, b_k]. \quad (6)$$

Now, let us denote with Σ_{ED}^\pm the exponential dichotomy spectrum for $J = \mathbb{R}^+$ and $J = \mathbb{R}^-$, respectively, and with Σ_{ED} the ED spectrum for $J = \mathbb{R}$. Clearly (1) has ED on \mathbb{R} iff $0 \notin \Sigma_{ED}$, and so—in principle—we should compute Σ_{ED} and verify that $0 \notin \Sigma_{ED}$. However, direct approximation of Σ_{ED} is not a very convenient approach and we rather verify that $0 \notin \Sigma_{ED}$ indirectly, based on the previously recalled result of Coppel ([12]), which we reiterate once more: *System (1) has ED in \mathbb{R} if and only if it has ED in \mathbb{R}^+ and \mathbb{R}^- , and the forward and backward stable subspaces are complementary.*

The forward stable subspace \mathcal{S}^+ is the set of initial conditions leading to decreasing solutions in forward time:

$$\mathcal{S}^+ = \{x \in \mathbb{R}^n : \|\Phi(t)x\| \rightarrow 0 \text{ as } t \rightarrow +\infty\}. \quad (7)$$

The backward stable subspace \mathcal{S}^- is the set of initial conditions leading to decreasing solutions in backward time:

$$\mathcal{S}^- = \{x \in \mathbb{R}^n : \|\Phi(t)x\| \rightarrow 0 \text{ as } t \rightarrow -\infty\}. \quad (8)$$

Remark 2 If the system has ED on \mathbb{R} then the solutions in \mathcal{S}^+ will decrease exponentially in forward time (and increase exponentially in backward time), while the solutions in \mathcal{S}^- will decrease exponentially in backward time (and increase exponentially in forward time).

As a consequence, to verify if (1) has ED in \mathbb{R} , we will check that (see [15])

- (ED-1) It has ED in \mathbb{R}^+ and \mathbb{R}^- . [That is, $0 \notin \Sigma_{ED}^\pm$.]
- (ED-2) The stable and the unstable subspaces of (7) and (8) are complementary. [That is, they form a basis for \mathbb{R}^n .]

The first task in our method will be to compute Σ_{ED}^+ and Σ_{ED}^- as well as bases for \mathcal{S}^+ and \mathcal{S}^- , respectively, for a given value of λ in (1). Let us for the moment assume that these bases are known.

Algorithm 3 Detect ED in \mathbb{R} , given Σ_{ED}^{\pm} and bases for \mathcal{S}^{\pm} .

Step 1 First, we check whether or not **(ED-1)** is verified. If not, (i.e., $0 \in \Sigma_{\text{ED}}^+$ or $0 \in \Sigma_{\text{ED}}^-$), then $0 \in \Sigma_{\text{ED}}$ and (1) does not admit ED in \mathbb{R} . If **(ED-1)** is verified, we proceed to **Step 2**.

Step 2 Let v_1^+, \dots, v_k^+ , and v_1^-, \dots, v_m^- be the computed bases for \mathcal{S}^+ and for \mathcal{S}^- , respectively (of course, these bases will depend on λ). If $m \neq n - k$, then **(ED-2)** is violated and once again $0 \in \Sigma_{\text{ED}}$ and there is no ED in \mathbb{R} .

Step 3 If $m + k = n$, we need to verify whether \mathcal{S}^+ and \mathcal{S}^- are complementary. To this purpose, we introduce a tool analogous to the Evans function which is routinely used in the analysis of orbital stability of traveling waves ([42]). It is convenient to make explicit the dependence on λ . We let

$$d(\lambda) = \det(v_1^+(\lambda), \dots, v_k^+(\lambda), v_1^-(\lambda), \dots, v_{n-k}^-(\lambda)), \quad \lambda \in \mathbb{C}. \quad (9)$$

(a) If for some value of λ , say $\lambda = \hat{\lambda}$, $d(\hat{\lambda}) = 0$, then $0 \in \Sigma_{\text{ED}}(\hat{\lambda})$ and (1) does not have ED in \mathbb{R} for $\lambda = \hat{\lambda}$.

(b) If $d(\hat{\lambda}) \neq 0$, then $0 \notin \Sigma_{\text{ED}}(\hat{\lambda})$ and (1) has ED in \mathbb{R} for $\lambda = \hat{\lambda}$.

Notice that **Step 1** and **Step 2** can be addressed solely with the information coming from Σ_{ED}^{\pm} , for which existing algorithms can be used (e.g., see [13, 18, 21]). However, new techniques are required for **Step 3**.

Remark 4 When $A = A(t; \lambda)$ in (1) is analytic in λ , then a fundamental matrix solution $X(t; \lambda)$ is also analytic in λ , and analytic bases for $\mathcal{S}^+(\lambda)$ and $\mathcal{S}^-(\lambda)$ exist as well ([30]). It follows that the function d in (9) could be taken as analytic function of λ , and this would allow use of the Cauchy Theorem to detect zeros of d in the complex plane. This issue has been extensively investigated in the context of computing the Evans function to infer orbital stability of traveling waves (e.g., see [28]); for example, in [28] (using a method different from ours) the authors recover an analytic Evans function d , the caveat being that they need to know the dimensions of the stable subspaces ahead of time. We favor different techniques, whereby the dimensions of the stable subspaces $\mathcal{S}^+(\lambda)$ and $\mathcal{S}^-(\lambda)$, as well as bases for them, are recovered at once from the SVD or QR factorizations of a fundamental matrix solution X : $X = U\Sigma V^*$ and $X = QR$, respectively, with U, V, Q unitary, R upper triangular and Σ diagonal. However—in general—we do not obtain analytic bases (in λ) for these subspaces. This is simply because with our algorithms we will obtain real valued (and generally non-constant) diagonal entries for the triangular factor R in the QR factorization of X and real valued Σ in the SVD. As a consequence, the Cauchy-Riemann conditions in general will not hold and so there is no analyticity. Nevertheless, we will be able to ascertain whether or not $d(\hat{\lambda})$ is zero by using two different approaches. As we will see below, Proposition 1, with our methods $d(\lambda)$ will be a continuous function of λ ; when λ is restricted to be real, this will allow us to check for sign changes of $d(\lambda)$ to locate its zeroes. Furthermore, we will introduce a modified function (see (13)), $\tilde{d}(\lambda)$, whose real and imaginary parts turn out to be smooth in $\text{Real}(\lambda)$ and $\text{Im}(\lambda)$; therefore, we will be able to apply Newton's method to the 2-dimensional (real valued) nonlinear systems in $\text{Real}(\lambda)$ and $\text{Im}(\lambda)$ to find its roots.

2 SVD and QR techniques

The results summarized in Sections 2.1 and 2.2, unless otherwise specified, apply to both forward and backward time. We will state them just in forward time.

2.1 SVD method

SVD techniques use the information emerging from the smooth SVD of a fundamental matrix solution X . One seeks the smooth decomposition $X(t) = U(t)\Sigma(t)V^*(t)$, with $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$, the σ_i 's being the singular values of X , and U and V unitary. Under the assumption of distinct singular values, U , V and Σ retain same degree of regularity of X (with respect to time t) and the equations for the SVD can be written as ([13])

$$\begin{aligned}\dot{U} &= UH(U, \Sigma, t); \\ \dot{V} &= VK(U, \Sigma, t); \\ \dot{\Sigma} &= \text{Real}(C)\Sigma,\end{aligned}\tag{10}$$

where $C = (U^*AU)$. The matrix valued function H and K are skew-Hermitian with entries specified by

$$\begin{aligned}H_{ij} &= C_{ij} + \frac{C_{ij} + \bar{C}_{ji}}{\sigma_j^2/\sigma_i^2 - 1}, \quad H_{ji} = -\bar{H}_{ij}, \quad i < j \\ K_{ij} &= \frac{C_{ij} + \bar{C}_{ji}}{\sigma_j^2/\sigma_i^2 - 1} + \frac{C_{ij} + \bar{C}_{ji}}{\sigma_j^2/\sigma_i^2 + 1}, \quad K_{ji} = -\bar{K}_{ij}, \quad i < j \\ H_{jj} - K_{jj} &= \text{Im}(C_{jj}), \quad j = 1, \dots, n.\end{aligned}\tag{11}$$

In our implementations, we resolved the n degrees of freedom in the last equation of (11), imposing $K_{jj} = 0$, $H_{jj} = \text{Im}(C_{jj})$, for $j = 1, \dots, n$; see **(SVD-3)** below.

We now recall some results from [13, 14, 18] which will be needed to understand our techniques. Although the results in these cited works are given for real-valued A , they easily extend to the complex case; some details will be given below as needed.

Below, the underlying **standing assumption** is that (1) has distinct and stable Lyapunov exponents. [This is a generic property in the Banach space of continuous matrix functions endowed with the sup norm ([36]).]

(SVD-1) (See [13, Proposition 4.1] and [18, Lemma 7.1].) After a finite time $\hat{t} > 0$, the singular values of any fundamental matrix solution X are distinct so that the differential equations for U , Σ and V in (10) apply.

(SVD-2) (See [13, Theorem 4.2 and Theorem 4.6], [14] and [18, Theorem 8.4].) Given any fundamental matrix solution X (i.e., any initial condition $X(0)$ for it), Σ_L^+ and Σ_{ED}^+ can be recovered from knowledge of the diagonal of C . Let

$$\lambda_j^i = \liminf_{t \rightarrow +\infty} \frac{1}{t} \log \sigma_j(t), \quad \lambda_j^s = \limsup_{t \rightarrow +\infty} \frac{1}{t} \log \sigma_j(t), \quad j = 1, \dots, n,$$

and for $S > 0$ sufficiently large

$$\alpha_j^S = \inf_{t \geq 0} \frac{1}{S} \int_t^{t+S} \text{Real}(C_{jj}(\tau)) d\tau, \quad \beta_j^S = \sup_{t \geq 0} \frac{1}{S} \int_t^{t+S} \text{Real}(C_{jj}(\tau)) d\tau.$$

Then: $\Sigma_L^+ = \bigcup_{j=1}^n [\lambda_j^i, \lambda_j^s]$ and $\Sigma_{\text{ED}}^+ = \bigcup_{j=1}^n [\alpha_j^S, \beta_j^S]$.

(SVD-3) (See [13, Theorem 5.4].) By using $K_{jj} = 0$ in (11), $j = 1, \dots, n$, then, as $t \rightarrow +\infty$, $K \rightarrow 0$ exponentially fast and $V \rightarrow \widehat{V}^+$, with \widehat{V}^+ constant unitary matrix. Further, V converges to \widehat{V}^+ exponentially fast and the rate of convergence can be estimated as follows. Let v_i be the i -th column of V and \widehat{v}_j^+ the j -th column of \widehat{V}^+ , then

$$\limsup_{t \rightarrow +\infty} \frac{1}{t} \log |v_i(t)^* \widehat{v}_j^+| \leq A |\lambda_i^s - \lambda_j^s|, \quad (12)$$

with $-1 \leq A < 0$, and $A = -1$ for regular systems. The columns of $X(0)\widehat{V}^+$ span the growth subspaces associated to Σ_{ED}^+ . It follows that, if k is the number of negative Lyapunov exponents, then the last k columns of $X(0)\widehat{V}^+$ span \mathcal{S}^+ .

Notice that with a different choice for the K_{jj} 's in the last equation of (11), the new solution of (10) will not generally converge to a constant matrix, but would behave for large t as $\tilde{V}(t)^+ \simeq \widehat{V}^+ D(t)$, with $D(t) = \text{diag}(e^{i\theta_1(t)}, \dots, e^{i\theta_n(t)})$, where \widehat{V}^+ is the one in **(SVD-3)**. (So, practically speaking, for large t the columns of \tilde{V}^+ and \widehat{V}^+ span the same subspaces.)

It must be appreciated that, as long as the system has stable and distinct Lyapunov exponents, with SVD techniques we can obtain Σ_{ED}^+ without requiring the fundamental matrix solution X to be normal, and any initial condition $X(0)$ will do. For this reason, we will just use the principal matrix solution Φ to characterize all desired quantities. Clearly in this case the growth subspaces (which are those in (7) and (8)) are given by the columns of \widehat{V} ([13, Theorem 5.8]).

Remark 5 Exponential convergence of V to \widehat{V}^+ together with the bound (12) implies that for $\epsilon = \text{eps}$, the machine accuracy, we can estimate the time $T^+ > 0$ such that

$$\|V(t; \lambda) - \widehat{V}^+(\lambda)\| \leq \text{eps}, \quad t \geq T^+,$$

as $T^+ = \log(\text{eps}) / (A \max_{j=1, \dots, n-1} (\lambda_j^s - \lambda_{j+1}^s))$. From the numerical point of view, it is therefore reasonable to use the columns of $V(T^+; \lambda)$ to approximate \mathcal{S}^+ , which is what we will do.

Similar results to those above apply to the case of $t \leq 0$, and to the limiting behavior as $t \rightarrow -\infty$. In particular, by the SVD method we will obtain a matrix \widehat{V}^- and from its last m columns we can obtain a basis for \mathcal{S}^- (as above, we will actually use the last m columns of $V(T^-; \lambda)$ to approximate \mathcal{S}^-).

2.1.1 A modified Evans' function

Now, let $A = A(t; \lambda)$ in (1) be analytic in λ . As already pointed out in Remark 4, in general X does not have an analytic SVD in λ . Then, we do not expect $\widehat{V}^\pm(\lambda)$ to be analytic functions of λ , nor of course $V(T^\pm; \lambda)$. However, we can reason differently. Let $\lambda = \lambda_R + i\lambda_I$, and view the coefficient matrix as $A(t; \lambda_R, \lambda_I) : \mathbb{R}^2 \rightarrow \mathbb{C}^{n \times n}$, for each given t . Obviously this is differentiable in (λ_R, λ_I) , and so is a fundamental matrix solution of (1), $X(t; \lambda_R, \lambda_I)$. Therefore, under the assumption of distinct singular values, also $U(t; \lambda_R, \lambda_I)$, $\Sigma(t; \lambda_R, \lambda_I)$ and $V(t; \lambda_R, \lambda_I)$, are smooth functions with respect to (λ_R, λ_I) , for any t . In particular, $V(T^\pm; \lambda_R, \lambda_I)$ are differentiable with respect to (λ_R, λ_I) , where T^\pm are chosen as in Remark 5.

Now, let **(ED-1)** hold, and assume that $\dim(\mathcal{S}^+) = k$, $\dim(\mathcal{S}^-) = m = n - k$, so that the function d in (9) is well defined. Denote with $\tilde{v}_1^+, \dots, \tilde{v}_k^+$ the last k columns of

$V(T^+; \lambda_R, \lambda_I)$ and with $\tilde{v}_1^-, \dots, \tilde{v}_m^-$ the last m columns of $V(T^-; \lambda_R, \lambda_I)$ and observe that these columns approximate to machine precision the corresponding columns of \hat{V}^\pm . We then consider the function

$$\tilde{d}(\lambda_R, \lambda_I) = \det(\tilde{v}_1^+(\lambda_R, \lambda_I), \dots, \tilde{v}_k^+(\lambda_R, \lambda_I), \tilde{v}_1^-(\lambda_R, \lambda_I), \dots, \tilde{v}_m^-(\lambda_R, \lambda_I)) , \quad (13)$$

which is differentiable with respect to (λ_R, λ_I) . This is the function we will use in our numerical method. So doing, we will be able to use root finding techniques, such as Newton's method, to approximate the zeros of \tilde{d} (and hence of d).

We conclude this section with a result showing that we always have continuity of \hat{V}^\pm with respect to λ .

Proposition 1 *Assume system (1) has distinct and stable Lyapunov exponents. Then \hat{V}^\pm are continuous functions of λ . In particular, d in (9) is a continuous function of λ .*

Proof First consider the case of $t \geq 0$. Let $p = 0, 1, 2, \dots$, and consider the sequence of functions $V_p(\lambda) = V(p; \lambda)$. These are continuous functions of λ . Moreover, by (12) and the assumption of distinct Lyapunov exponents, there exists $\alpha(\lambda) > 0$ bounded away from 0, such that for p sufficiently large $\|V_p(\lambda) - \hat{V}^+(\lambda)\| \leq e^{-\alpha(\lambda)p}$. Let $a > 0$ be such that $\alpha(\lambda) \geq a > 0$. Then, for all $\epsilon > 0$ there exists $N > 0$ such that for all $p > N$, $e^{-ap} < \epsilon$ so that the sequence $\{V_p\}$ is uniformly convergent to \hat{V}^+ implying continuity of \hat{V}^+ with respect to λ . Similarly for $t \leq 0$.

2.2 QR method

QR techniques are based on the (unique) decomposition of a *normal* fundamental matrix solution $X = QR$, where Q is unitary and R is upper triangular with positive diagonal. It is well known that X admits a smooth QR decomposition whose factors obey the following differential equations

$$\dot{Q} = QH(Q, D, t) \quad (14)$$

$$\dot{R} = B(Q, t)R . \quad (15)$$

Here, H is a skew-hermitian matrix whose entries are given by

$$H_{ij} = (Q^*AQ)_{ij}, \quad H_{ji} = -\bar{H}_{ij}, \quad i > j, \quad H_{jj} = \text{Im}(Q^*AQ)_{jj} , \quad (16)$$

and B is upper triangular with entries

$$B_{ij} = (Q^*AQ)_{ij} + \overline{(Q^*AQ)_{ji}}, \quad i < j, \quad B_{jj} = \text{Real}((Q^*AQ)_{jj}) .$$

We now recall some results from [15, 18, 21] which are needed to justify QR-based techniques. Below, the **standing assumption** is that the diagonal elements of B satisfy one of the conditions (i) or (ii) below:

(i) B_{ii} and B_{jj} are integrally separated, i.e. there exist $a, d > 0$ such that

$$\int_s^t (B_{ii}(\tau) - B_{jj}(\tau)) d\tau \geq a(t - s) - d, \quad t \geq s \geq 0, \quad i < j, \quad (17)$$

- (ii) B_{ii} and B_{jj} are not integrally separated, but $\forall \epsilon > 0$ there exists $M_{ij}(\epsilon) > 0$ such that

$$\left| \int_s^t (B_{ii}(\tau) - B_{jj}(\tau)) d\tau \right| \leq M_{ij}(\epsilon) + \epsilon(t-s), \quad t \geq s \geq 0, \quad i < j. \quad (18)$$

Note that condition (17) is equivalent to requiring that (1) has distinct and stable Lyapunov exponents, [18, Theorem 3.4 and Corollary 5.1], while (18) implies that the Lyapunov exponents of the system are stable but not necessarily distinct, [21].

The following properties hold (we state them for $t \geq 0$, but the case of $t \leq 0$ is analogous).

- (QR-1)** (See [21, Theorem 5.5], [18, Theorem 8.1].) The Lyapunov and exponential dichotomy spectra can be recovered from the diagonal elements of B as follows. Let

$$\lambda_j^i = \liminf_{t \rightarrow +\infty} \int_0^t B_{jj}(\tau) d\tau, \quad \lambda_j^s = \limsup_{t \rightarrow +\infty} \int_0^t B_{jj}(\tau) d\tau, \quad (19)$$

then $\Sigma_L^+ = \bigcup_{j=1}^n [\lambda_j^i, \lambda_j^s]$. Also, for S sufficiently large, let

$$\alpha_j^S = \inf_{t \geq 0} \frac{1}{S} \int_t^{t+S} B_{jj}(\tau) d\tau, \quad \beta_j^S = \sup_{t \geq 0} \frac{1}{S} \int_t^{t+S} B_{jj}(\tau) d\tau, \quad (20)$$

and one has $\Sigma_{ED}^+ = \bigcup_{j=1}^n [\alpha_j^S, \beta_j^S]$.

- (QR-2)** (See [15, Theorems 10, 15, and 22].) Let k be the number of negative Lyapunov exponents of (1) (for $t \geq 0$) and let $Y = R^{-1} \text{diag}(R)$. Rewrite $Y = (Y_u, Y_s)$, where Y_s comprises the last k columns of Y . Then the subspace spanned by the columns of Y_s converges: if we let $\mathcal{Y}(t) := X(0)Y_s(t)$, then $\text{Span}(\mathcal{Y}(t)) \rightarrow \text{Span}(\hat{\mathcal{Y}}^+)$ as $t \rightarrow +\infty$, exponentially fast. To estimate the convergence speed, let $P(t)$ be the orthogonal projection onto $\text{Span}(\mathcal{Y}(t))$, and \hat{P}^+ be the orthogonal projection onto $\text{Span}(\hat{\mathcal{Y}}^+)$; then,

$$\limsup \frac{1}{t} \log \|P(t)(I - \hat{P}^+)\| \leq G(\lambda_{n-k}^s - \lambda_{n-k+1}^s), \quad -1 \leq G < 0,$$

and moreover $\text{Span}(\hat{\mathcal{Y}}^+) = \mathcal{S}^+$ (and $G = -1$ for regular systems).

Remark 6 If in **(QR-2)** we assume that the Lyapunov exponents are distinct (that is, (17) holds), then Y tends to a constant upper triangular matrix \hat{Y} with 1's on the diagonal. Each column of $X(0)\hat{Y}$ will span the line of initial conditions leading to a certain exponential growth or decay, given by the Lyapunov exponents. If instead (18) holds, and the Lyapunov exponents are not distinct, then the subspaces spanned by the columns of Y still converge to the subspaces associated to the different exponential growths (different Lyapunov exponents) although Y will not converge (see [15, Theorem 15]). Notice that, in order to detect ED in \mathbb{R} , we are just interested in the computation of forward and backward stable spaces, so it does not really matter which one of (17) or (18) hold.

Similar considerations and results hold for $t \leq 0$, although in this case the diagonal elements of B are required to satisfy the following variants of (17) and (18), respectively.

- (i) The diagonal of B is integrally separated: $\int_s^t (B_{ii}(\tau) - B_{jj}(\tau)) d\tau \geq -a(t-s) - d$, for $t \leq s \leq 0$ and $i < j$; or

- (ii) B_{ii} and B_{jj} are not integrally separated, but $\forall \epsilon > 0$ there exists $M_{ij}(\epsilon) > 0$ such that

$$\left| \int_s^t (B_{ii}(\tau) - B_{jj}(\tau)) d\tau \right| \leq M_{ij}(\epsilon) - \epsilon(t - s), \quad t \leq s \leq 0, \quad i < j. \quad (21)$$

With these assumptions, then analogs of **(QR-1)** and **(QR-2)** hold for $t \leq 0$ as well.

Remark 7 The properties in **(QR-2)** ensure exponential convergence of $\text{Span}(X(0)Y_s(t))$ to the forward stable subspace. It follows that there is a finite time $T^+ > 0$ such that $\|P(t)(I - \hat{P})\| \leq \text{eps}$, for all $t \geq T^+$, and $T^+ = \log(\text{eps})/(G(\lambda_{n-k}^s - \lambda_{n-k+1}^s))$. Then it is reasonable to approximate the forward stable subspace by $\text{Span}(X(0)Y_s(T^+))$, which is what we do in our numerical computations. Similarly for $t \leq 0$.

Remark 8 QR-based techniques need a normal initial condition $X(0)$, for which conditions (17) and (18) are verified, in forward time and in backward time respectively. In general, this precludes us from taking $X(0) = I$, and further we may need different initial conditions for the forward and backward integrations (see [15, Remark 2]). In practice, we select random initial conditions, which has worked reliably in all of our numerical experiments.

Similarly to what we observed for the SVD, when A is analytic in λ , an analytic (in λ) QR factorization of X does not generally exist. However, using same reasoning as in Section 2.1.1, we can view Q and R as differentiable functions of (λ_R, λ_I) for given t , and in particular, $\mathcal{Y}(T^\pm; \lambda_R, \lambda_I)$ are differentiable with respect to (λ_R, λ_I) . Now, assume **(ED-1)** is satisfied and that $\dim(\mathcal{S}^+) = k$ and $\dim(\mathcal{S}^-) = m = n - k$. Denote with $\tilde{y}_1^+, \dots, \tilde{y}_k^+$, the last k columns of $X(0)Y_s(T^+)$ and with $\tilde{y}_1^-, \dots, \tilde{y}_m^-$, the last m columns of $X(0)Y_s(T^-)$. We will then approximate d in (9) as (see (13))

$$\tilde{d}(\lambda_R, \lambda_I) = \det(\tilde{y}_1^+, \dots, \tilde{y}_k^+, \tilde{y}_1^-, \dots, \tilde{y}_m^-), \quad (22)$$

which is differentiable with respect to (λ_R, λ_I) and it will be used in our numerical experiments to approximate the zeros of d .

Remark 9 When computing Lyapunov exponents or exponential dichotomy spectrum on the half line, we just need to compute the logarithms of the diagonal elements of R and this allows to overcome underflow or overflow phenomena related to exponential growth or decay. However, to compute also forward and backward stable subspaces, we need to compute all of R . Some ingenuity is required to compute Y . Details will be given in Section 3.

Remark 10 We note that the constants A and G which we have in Remark 5 and Remark 7, respectively, are computable.

3 Algorithms

As usual, our algorithmic description is for $t \geq 0$, the modifications needed for $t \leq 0$ are self explanatory.

We first review the QR algorithms. These are quite well known in the context of approximating Lyapunov exponents (e.g., see [5, 17] and references there).

3.1 Discrete QR

Let $X(0) = X_0 = Q_0 R_0$, and let $t_0 < t_1 < t_2 < \dots$, be the chosen gridpoints during time integration. Denote with $\Phi(t_{j+1}, t_j)$ the transition matrix from t_j to t_{j+1} , i.e. the solution at t_{j+1} of the problem

$$\frac{d}{dt}\Phi(t, t_j) = A(t)\Phi(t, t_j), \quad \Phi(t_j, t_j) = I.$$

In terms of transition matrices, the solution of (1) at time t_{k+1} rewrites as

$$X(t_{k+1}) = \Phi(t_{k+1}, t_k) \cdots \Phi(t_2, t_1) \Phi(t_1, t_0) Q_0 R_0.$$

Thus, to obtain the QR factorization of $X(t_{k+1})$ one can proceed as follows

$$\Phi(t_1, t_0) Q_0 = Q_1 R_1, \quad \Phi(t_2, t_1) Q_1 = Q_2 R_2, \quad \dots,$$

so that

$$X(t_{k+1}) = Q_{k+1} R_{k+1} \cdots R_1 R_0. \quad (23)$$

At the same time we will need to compute Y to approximate forward and backward stable subspaces. Instead of Y , we will actually compute $Z = Y^{-1} = D^{-1} R$, $D = \text{diag}(R)$; see below. Let $D_k = \text{diag}(R_k)$ so that $Z(t_k)$ rewrites as $Z(t_k) = (D_k \cdots D_0)^{-1} (R_k \cdots R_0)$. So, to update Z , we will write

$$Z(t_k) = (D_{k-1} \cdots D_0)^{-1} (D_k^{-1} R_k) (D_{k-1} \cdots D_0) Z(t_{k-1}) = T_k Z(t_{k-1}),$$

where T_k is the unit upper triangular matrix

$$T_k^{ij} = \frac{R_k^{ij}}{R_k^{ii}} \prod_{l=0}^{k-1} \frac{R_l^{jj}}{R_l^{ii}}, \quad i \leq j. \quad (24)$$

Remark 11 If the diagonal elements of B satisfy (17), then $T_k^{ij} \leq \frac{R_k^{ij}}{R_k^{ii}} e^{-at_k} e^d$, and $\frac{R_k^{ij}}{R_k^{ii}} \leq e^{M(t_k - t_{k-1})}$, where $M = \sup_{t \geq 0} \|B\|$. So, for $t_k > \frac{d}{a} + \frac{M}{d} h$, with $h = \min_k (t_k - t_{k-1})$, $T_k^{ij} < 1$ and the algorithm to compute $Z(t_k)$ is stable. Instead, if the diagonal elements of B satisfy (18), then we can only ensure $T_k^{ij} < \frac{R_k^{ij}}{R_k^{ii}} e^{M_{ij}(\epsilon)} e^{\epsilon t_k}$ and there is no guarantee that $T_k^{ij} < 1$ for t_k sufficiently large. This is a difficulty related to the particular problem, not to the algorithm.

To approximate the forward stable subspace from Z we proceed as follows. Let $T > 0$ be sufficiently large (ideally, $T = T^+$), and let $X(0)Y(T) = U(T)L(T)$ be the unique QL factorization of $X(0)Y(T)$, with Q unitary and L lower triangular with positive diagonal, so that $\text{Span}(X(0)(Y_j, \dots, Y_n)) = \text{Span}(U_j, \dots, U_n)$, where Y_j and U_j are j -th columns of Y and U respectively ($j = 1, \dots, n$). To obtain U , we take the unique QR factorization of $(Z(T)X(0)^{-1})^T$, call it UL^{-T} , where L has positive diagonal elements. We next summarize the overall algorithm.

Algorithm 12 *Discrete QR Method on the half-line.*

- Let X_0 be a random initial condition, $X_0 = Q_0 R_0$ be the unique QR decomposition of X where R has positive diagonal elements. Initialize $Z = D_0^{-1} R_0$, and initialize S to the upper triangular matrix of all 1's: $S_{ij} = 1$, for $j \geq i$.

- At the k -th step, form the upper triangular matrix W with elements $W_{ij} = \frac{R_{k-1}^{jj}}{R_{k-1}^{ii}}$, for $j \geq i$. Update S as $S = S \bullet W$, where \bullet denotes the entrywise (Hadamard) product of two matrices: $(A \bullet B)_{ij} = A_{ij} B_{ij}$. Solve (1) on $[t_{k-1}, t_k]$, with initial condition $\Phi(t_{k-1}, t_{k-1}) = I$. Take the QR factorization of the product $\Phi(t_k, t_{k-1}) Q_{k-1} = Q_k R_k$, let $T_k = (D_k^{-1} R_k) \bullet S$, and update Z : $Z = T_k Z$.
- Approximate Σ_{ED}^+ similarly to **(QR-1)** with \inf and \sup replaced by $\min_{\tau \geq t \geq T^+}$ and $\max_{\tau \geq t \geq T^+}$, where T^+ is the final time of integration. Here, $\tau > 0$ is sufficiently large so that transient behavior does not penalize the computation of Σ_{ED}^+ .
- To approximate the directions spanning S^+ , we form the QR factorization $(Z(T^+) X_0^{-1})^T = UL^{-T}$; assuming that there are k negative Lyapunov exponents, then the last k columns of U give the sought directions.

3.2 Continuous QR

In the continuous version of the QR algorithm, we solve differential equations for the unknowns Q , $Z = Y^{-1}$, $\nu_j = \frac{R_{j+1,j+1}}{R_{jj}}$ for $j = 1, \dots, n-1$ and $\nu_n = \log(R_{nn})$. The system of equations to solve is the following

$$\begin{aligned} \dot{Q} &= QH(Q, t), \\ \dot{\nu}_j &= \text{Real}(G_{j+1,j+1}(t) - G_{jj}(t))\nu_j, \quad j = 1, \dots, n-1, \\ \dot{\nu}_n &= \text{Real}(G_{nn}(t)), \\ \dot{Z} &= C(Q, \nu, t)Z, \end{aligned} \quad (25)$$

where $G = (Q^* A Q)$, C is strictly upper triangular with elements $C_{ij} = (G_{ij} + \overline{G_{ji}}) \frac{R_{jj}}{R_{ii}}$, for $i < j$, and H is shew-Hermitian with entries $H_{ij} = G_{ij}$ for $i > j$ and $H_{jj} = i \text{Im}(G_{jj})$, for $j = 1, \dots, n$. Notice that at each step we recover $\frac{R_{jj}}{R_{ii}}$ from the ν_j 's: $\frac{R_{jj}}{R_{ii}} = \prod_{k=i}^{j-1} \nu_k$.

To compute Σ_{ED}^+ we proceed as in **(QR-1)**, where $B_{jj} = \text{Real}(G_{jj})$, approximating the \limsup and \liminf as follows (see [18]), for $\tau > 0$ sufficiently large:

$$\tilde{\alpha}_j^S = \min_{\tau \leq t \leq T^+} \frac{1}{S} \int_t^{t+S} B_{jj}(s) ds, \quad \tilde{\beta}_j^S = \max_{\tau \leq t \leq T^+} \frac{1}{S} \int_t^{t+S} B_{jj}(s) ds. \quad (26)$$

Finally, we observe that to update the ν_j 's at every step we need to approximate $\int_t^{t+h} (B_{j+1,j+1}(s) - B_{jj}(s)) ds$, so we just need to add up the local contributions from t to $t+S$ to approximate the integrals in (26). To approximate directions, instead, we proceed just as we did for the discrete QR algorithm: at the last step, we take the QR factorization of $(Z(T^+) X_0^{-1})^T = UL^{-T}$. The relevant columns of U give the sought directions.

Remark 13 Assume the system has stable and distinct Lyapunov exponents. Then the diagonal elements of B satisfy (17) and $C_{ij} < B_{ij} e^{-at+d}$. It follows that for $t > \frac{d+\log(M)}{a}$, $M = \sup_t \|B(t)\|$, $C_{ij} < 1$ and so Z can be computed with no overflow (see also Remark 13 in [15]). When instead the diagonal elements of B satisfy (18), then as in the discrete algorithm, we can only insure $C_{ij} < B_{ij} e^{M_{ij}(\epsilon) e^{\epsilon t}}$ and we can not guarantee Z to be bounded (see equation (25) in [15] for bounds on exponential growth of Z). Clearly this is a difficulty related to the problem under exam, and not to the algorithm chosen to solve the problem.

3.3 Error Analysis

We next develop an error analysis for the approximation of subspaces. We assume that either the integral separation condition (17) holds or the condition (18) holds that implies the stability of Lyapunov exponents in the non-integrally separated case. In addition, we assume that there exists $\rho_{ij} > 0$ such that for all $t \in [0, T]$, the difference between the exact $Q(t)$ and the computed $\tilde{Q}(t)$ is bounded as

$$|Q_{ij}(t) - \tilde{Q}_{ij}(t)| \leq \rho_{ij}. \quad (27)$$

The existence of the bounds ρ_{ij} follow from the work in [19, 20, 22, 43]. Let I_S denote the index set such that for $i < j$, $(i, j) \in I_S$ if (17) holds and $(i, j) \notin I_S$ if (18) holds.

Let Z be the matrix in (25). We have then that for $i < j$, $C_{ij}(t) = R_{ii}^{-1}(t)B_{ij}(t)R_{jj}(t)$, $C_{jj}(t) = 0$, and

$$\dot{Z}_{ij} = \sum_{k=i+1}^j C_{ik}Z_{kj}, \quad Z_{ij}(t) = Z_{ij}(0) + \int_0^t \sum_{k=i+1}^j C_{ik}(s)Z_{kj}(s)ds. \quad (28)$$

We want to compare Z_{ij} (exact) with \tilde{Z}_{ij} (approximate). Let $G = (Q^*AQ)$ and $\tilde{G} = (\tilde{Q}^*A\tilde{Q})$. We can control the difference between Q and \tilde{Q} and hence the difference for $i < j$ between $B_{ij}(t) = G_{ij} + \overline{G}_{ji}$ and $\tilde{B}_{ij}(t) = \tilde{G}_{ij} + \overline{\tilde{G}}_{ji}$. Similarly we can control the difference between $B_{ii}(t) = \text{Real}(G_{ii})$ and $\tilde{B}_{ii}(t) = \text{Real}(\tilde{G}_{ii})$.

For ease of notation, let $B_{ij}(t) = \beta(t)$, $\tilde{B}_{ij}(t) = \beta(t) + \delta(t)$, $B_{jj}(t) - B_{ii}(t) = \alpha(t)$, and $\tilde{B}_{jj}(t) - \tilde{B}_{ii}(t) = \alpha(t) + \epsilon(t)$. Then for all t ,

$$|\delta(t)| \leq \delta_0, \quad |\epsilon(t)| \leq \epsilon_0, \quad |\beta(t)| \leq M_0$$

where these uniform bounds on $\delta(t)$ and $\epsilon(t)$ follows from the uniform bounds on the difference between $Q(t)$ and $\tilde{Q}(t)$.

We need a fundamental bound on

$$\tilde{C}_{ij}(t) - C_{ij}(t) = \int_0^t [\beta(t) + \delta(t)] e^{\int_0^t \alpha(s) + \epsilon(s) ds} dt - \int_0^t \beta(t) e^{\int_0^t \alpha(s) ds} dt.$$

Under the assumption (17), we have $a > 0$ and $d \geq 0$, $\int_0^t \alpha(s) ds \leq -at + d$. Using the triangle inequality we bound

$$\left| \int_0^t \delta(t) e^{\int_0^t \alpha(s) + \epsilon(s) ds} dt \right| \leq \delta_0 \int_0^t e^{-(a-\epsilon_0)t+d} dt \leq \frac{\delta_0 e^d}{a-\epsilon_0} (1 - e^{-(a-\epsilon_0)t}) \quad (29)$$

provided $a - \epsilon_0 > 0$, and

$$\begin{aligned} \left| \int_0^t \beta(t) \left\{ e^{\int_0^t \alpha(s) + \epsilon(s) ds} - e^{\int_0^t \alpha(s) ds} \right\} dt \right| &\leq M_0 \int_0^t e^{-at+d} \{e^{\epsilon_0 t} - 1\} dt \\ &\leq \frac{M_0 e^d}{a(a-\epsilon_0)} \left\{ a(1 - e^{-(a-\epsilon_0)t}) - (a-\epsilon_0)(1 - e^{-at}) \right\}. \end{aligned} \quad (30)$$

Under the assumption (18), we have for all $\epsilon > 0$ there exists $M > 0$ such that $\int_0^t \alpha(s) ds \leq \epsilon t + M$. Again, using the triangle inequality we bound

$$\left| \int_0^t \delta(t) e^{\int_0^t \alpha(s) + \epsilon(s) ds} dt \right| \leq \delta_0 \int_0^t e^{(\epsilon+\epsilon_0)t+M} dt \leq \frac{\delta_0 e^M}{\epsilon+\epsilon_0} (e^{(\epsilon+\epsilon_0)t} - 1) \quad (31)$$

and

$$\begin{aligned} & \left| \int_0^\tau \beta(t) \left\{ e^{\int_0^t \alpha(s) + \epsilon(s) ds} - e^{\int_0^t \alpha(s) ds} \right\} dt \right| \leq M_0 \int_0^\tau e^{\epsilon t + M} \{e^{\epsilon_0 t} - 1\} dt \\ & \leq \frac{M_0 e^M}{\epsilon(\epsilon + \epsilon_0)} \left\{ \epsilon(e^{(\epsilon + \epsilon_0)\tau} - 1) - (\epsilon + \epsilon_0)(e^{\epsilon\tau} - 1) \right\}. \end{aligned} \quad (32)$$

We have from (28) and the analogous formula for $\tilde{Z}_{ij}(t)$ that

$$E_{ij}(t) := Z_{ij}(t) - \tilde{Z}_{ij}(t) = \int_0^t \sum_{k=i+1}^j [C_{ik}(s)Z_{kj}(s) - \tilde{C}_{ik}(s)\tilde{Z}_{kj}(s)] ds$$

and

$$C_{ik}(s)Z_{kj}(s) - \tilde{C}_{ik}(s)\tilde{Z}_{kj}(s) = \tilde{C}_{ik}(s)[Z_{kj}(s) - \tilde{Z}_{kj}(s)] + [C_{ik}(s) - \tilde{C}_{ik}(s)]Z_{kj}(s)$$

Thus,

$$|E_{ij}(t)| \leq \sum_{k=i+1}^j \sup_{0 \leq s \leq t} |\tilde{C}_{ik}(s)| \int_0^t |E_{kj}(s)| ds + \sup_{0 \leq s \leq t} |Z_{kj}(s)| \int_0^t |C_{ik}(s) - \tilde{C}_{ik}(s)| ds$$

Lemma 1 *If the assumptions (17), (18), and (27) hold, and for $i < j$, $\sup_s |\tilde{C}_{ij}(s)| \leq \omega_{ij}$ and $\sup_s |Z_{ij}| \leq \eta_{ij}$, then $E_{ij}(t) = Z_{ij}(t) - \tilde{Z}_{ij}(t)$ may be bounded recursively for $j - i = 1, 2, \dots$, as*

$$|E_{ij}(T)| \leq \sum_{k=i+1}^j \eta_{kj} \int_0^T \delta_{ik}(s) ds + \sum_{k=i+1}^{j-1} \omega_{ik} \int_0^T |E_{kj}(s)| ds \quad (33)$$

where bounds for $\int_0^T \delta_{ij}(s) ds$, $i < j$, are obtained in (29) and (30) for $(i, j) \in I_S$ and in (31) and (32) for $(i, j) \notin I_S$.

Proof We have

$$E_{ij}(T) = \int_0^T \sum_{k=i+1}^j \tilde{C}_{ik}(s)[Z_{kj}(s) - \tilde{Z}_{kj}(s)] + [C_{ik}(s) - \tilde{C}_{ik}(s)]Z_{kj}(s) ds$$

and (33) is obtained in a straightforward way since $E_{kj}(s) = Z_{kj}(s) - \tilde{Z}_{kj}(s)$ and $E_{jj}(s) = 0$. Next, note that when $j = i + 1$, (33) reduces to

$$|E_{i,i+1}(T)| \leq \int_0^T \delta_{i,i+1}(s) ds$$

since we may take $\eta_{jj} = 1$.

In light of this Lemma, in the integrally separated case we have:

Theorem 14 *Suppose assumptions (17) and (27) hold and let $\epsilon > 0$ be given. If $\rho := \max_{i,j} \rho_{ij}$ is sufficiently small, then there exists a time $T > 0$ such that $\|Z^c(T) - Z^e(\infty)\| \leq \epsilon$ where $Z^c(T)$ is the computed Z at time T and $Z^e(\infty)$ is the exact, limiting Z .*

Proof Let T denote the time such that $\|Z^e(t) - Z^e(\infty)\| \leq \epsilon/2$ for all $t \geq T$ as in Remark 7. Next choose ρ small enough so that the bounds obtained in Lemma 1 satisfy $\|Z^c(T) - Z^e(T)\| \leq \epsilon/2$.

Remark 15 *To obtain a computable bound one can further bound $\|Z^{c,q}(T) - Z^c(T)\|$ where $Z^{c,q}(T)$ is a quadrature approximation of $Z^c(T)$ so that the difference $Z^{c,q}(T) - Z^e(\infty)$ between what we can compute, $Z^{c,q}(T)$, and the exact solution in the infinite time limit, $Z^e(\infty)$, may be bounded.*

3.4 Continuous SVD

A continuous SVD algorithm for the approximation of Σ_{ED}^{\pm} , together with the associated directions, have been developed in [13, 14], to which we refer for details. Here we just summarize the main steps.

The following differential equations are solved for the unknowns: U , V and $\nu_j = \frac{\sigma_{j+1}}{\sigma_j}$, for $j = 1, \dots, n-1$, and $\nu_n = \log(\sigma_n)$:

$$\begin{aligned}\dot{U} &= UH, \\ \dot{\nu}_j &= ((\text{Real}(C_{j+1,j+1}) - \text{Real}(C_{jj}))\nu_j, \quad j = 1, \dots, n-1, \\ \dot{\nu}_n &= \text{Real}(C_{nn}(t)), \\ \dot{V} &= VK,\end{aligned}\tag{34}$$

where $C = (U^*AU)$, and H and K are given in (11).

3.5 Exponential Dichotomy spectrum in \mathbb{R}

Once we have computed Σ_{ED}^+ and \mathcal{S}^+ , Σ_{ED}^- and \mathcal{S}^- (see Sections 3.1, 3.2, 3.4), we will proceed as in Algorithm 3 to ascertain ED in \mathbb{R} for the shifted system $\dot{x} = (A(t) - \mu I)x$. Below, we summarize the technique.

- Step 1** Compute Σ_{ED}^+ and Σ_{ED}^- together with $V(T^+)$ and $V(T^-)$ for SVD based techniques, or $Z(T^+)$ and $Z(T^-)$ for QR based techniques. T^{\pm} are the final times reached (see Remarks 5 and 7). If $\mu \in \Sigma_{\text{ED}}^+$ or $\mu \in \Sigma_{\text{ED}}^-$, then $\mu \in \Sigma_{\text{ED}}$.
- Step 2** If $\mu \notin \Sigma_{\text{ED}}^{\pm}$, let k be the number of negative (stable) Lyapunov exponents in forward time and m be the number of positive (stable) Lyapunov exponents in backward time of $\dot{x} = (A(t) - \mu I)x$. If $m \neq n - k$ then $\mu \in \Sigma_{\text{ED}}$.
- Step 3** If $m = n - k$, form a basis of \mathcal{S}^+ with last k columns of $V(T^+)$ for SVD based techniques or last k columns of U^+ with U^+ as in the last step of Algorithm 12 for QR based techniques, and a basis of \mathcal{S}^- with last m columns of $V(T^-)$ or U^- . Compute \tilde{d} as in (13). If $\tilde{d} = 0$ then $\mu \in \Sigma_{\text{ED}}$, else $\mu \notin \Sigma_{\text{ED}}$.

Remark 16 If we just want to ascertain ED in \mathbb{R} for (1) and the whole spectrum is not needed, we can apply the algorithm just to $\mu = 0$.

Remark 17 As previously remarked, it is possible to check if $\tilde{d}(\lambda) = 0$ by exploiting the continuity of \tilde{d} , and its differentiability with respect to (λ_R, λ_I) (see Remarks 5 and 7). For example, we used Newton's method to locate $\hat{\lambda}$ such that $\tilde{d}(\hat{\lambda}) = 0$, approximating the Jacobian of \tilde{d} by centered differences (with stepsize $h = 1.E-5$; exponential notation is adopted to indicate constants used in the computations). Thus, for each Newton iterate \tilde{d} is calculated at four additional values of λ to form an approximation of the Jacobian.

4 Numerical experiments

Below we give numerical results to illustrate performance of our techniques.

Example 18 This is a modification of [15, Example 1, Section 5] and is useful for testing purposes, since we have explicit knowledge of when one has, or does not have, ED. Consider the linear system

$$\dot{X} = A(t)X = \begin{pmatrix} \operatorname{atan}(t) + \frac{t}{1+t^2} + \delta\alpha(t) & (\lambda - 1 - i)\cos(t) \\ 0 & -\frac{1}{2}(\operatorname{atan}(t) + \frac{t}{1+t^2} + \delta\alpha(t)) \end{pmatrix} X, \quad (35)$$

where $\delta = 0.1$ is chosen so that $A_{11}(t)$ and $A_{22}(t)$ are integrally separated and $\alpha(t) = \sin(\log(\frac{t^2+1}{2})) + \frac{2t^2}{t^2+1}\cos(\log(\frac{t^2+1}{2}))$. The principal matrix solution $\Phi(t)$ can be computed explicitly as

$$\begin{aligned} \Phi_{11}(t) &= e^{\beta(t)}, \quad \beta(t) = t \cdot \operatorname{atan}(t) + \delta t \sin(\log(\frac{t^2+1}{2})), \\ \Phi_{12}(t) &= (\lambda - 1 - i)\Phi_{11}(t) \int_0^t (e^{-3/2\beta(s)} \cos(s)) ds, \quad \Phi_{22}(t) = e^{-\frac{1}{2}\beta(t)}, \quad \Phi_{21}(t) = 0. \end{aligned}$$

The diagonal elements of A are independent of λ so by (20), Σ_{ED}^+ and Σ_{ED}^- are independent of λ as well. Moreover, Σ_{ED}^+ and Σ_{ED}^- are continuous spectra (i.e., they are made up by non trivial intervals), because of the oscillatory nature of the function α , and $0 \notin \Sigma_{\text{ED}}^+, \Sigma_{\text{ED}}^-$. So to ascertain ED in \mathbb{R} , we execute **Step 3** of Algorithm 3. Following the same reasoning as in [15, Example 1, Section 5], the forward stable subspace can be computed explicitly as $\mathcal{S}^+ = \operatorname{Span}(v)$, with $v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$ and $v_1 = -(\lambda - 1 - i) \lim_{t \rightarrow +\infty} \int_0^t (e^{-\frac{3}{2}\beta(s)} \cos(s)) ds$, $v_2 = 1$. Similarly, the backward stable subspace is given by $\mathcal{S}^- = \operatorname{Span}(w)$, with $w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$ and $w_1 = -(\lambda - 1 - i) \lim_{t \rightarrow -\infty} \int_0^t (e^{-\frac{3}{2}\beta(s)} \cos(s)) ds$, $w_2 = 1$. It follows that for $\lambda = 1 + i$, the system does not admit ED in \mathbb{R} . Notice that $w_1 \neq v_1$ for $\lambda \neq 1 + i$ so that the system admits ED in \mathbb{R} for $\lambda \neq 1 + i$.

In our numerical implementations, to find the value of λ for which the system does not admit ED, which we know to be $\lambda_{\text{exact}} = 1 + i$, we use Newton's method with starting value $\lambda_0 = 0.5 + 0.5i$, to find the root of \tilde{d} in (13). We stop the Newton's iteration when the difference of successive iterates is below $1.E - 12$. In Table 1 we show the results obtained with the continuous QR (QRC) and the discrete QR (QRD) methods. The relevant differential equations for both methods are solved with the classic Runge Kutta method of order 4 and constant stepsize $1.E - 3$. The same random initial conditions were used in forward and backward time. In Table 2 we compare the convergence and computational time for QRC, QRD, and the SVD method again using the classical Runge Kutta method of order 4 but with constant stepsize $1.E - 1$. In all the computations for this example, the values of T^+ and T^- were determined as in Remark 5 with $A = -1$. In Table 2, a unit of time was approximately 160 seconds of computation time on the laptop we employed for the computations (done in **Matlab**). A comparison of Tables 1 and 2 illustrate the robustness of the results with respect to stepsize and discretization error.

In Figure 1 we plot the basin of attraction of the Newton method using the discrete QR method, although nearly identical results are obtained with any of the methods. The plot is obtained by checking for convergence on a grid of points in the complex plane.

In Figure 2, we plot the error in approximating the stable subspace of (35) for $\lambda = 0$, both for the discrete QR method and the continuous SVD method as a function of the stepsize h for $h = 1/10, 1/20, 1/40, 1/80, 1/160, 1/320$. Notice that the plot shows $-\log(\text{error})$ vs. $-\log(h)$. Clearly, both methods have order 4.

Table 1 Example 18: Newton method's iterates with $h = 1.E - 3$.

METHOD	$ \lambda_{\text{exact}} - \lambda_k , k = 0, 1, \dots$	$ d(\lambda_{k+1}) $
QRC	$7.1E - 1$	$7.2E - 1$
	$5.2E - 1$	$5.9E - 1$
	$1.3E - 1$	$2.2E - 3$
	$4.4E - 9$	$5.6E - 9$
	$4.0E - 15$	$1.5E - 15$
	$2.9E - 15$	$3.8E - 16$
QRD	$7.1E - 1$	$7.5E - 1$
	$3.6E - 1$	$4.3E - 1$
	$3.8E - 2$	$4.8E - 2$
	$4.5E - 5$	$5.7E - 5$
	$2.9E - 11$	$3.1E - 11$
	$4.4E - 16$	$6.5E - 15$
	$4.8E - 15$	$1.4E - 15$

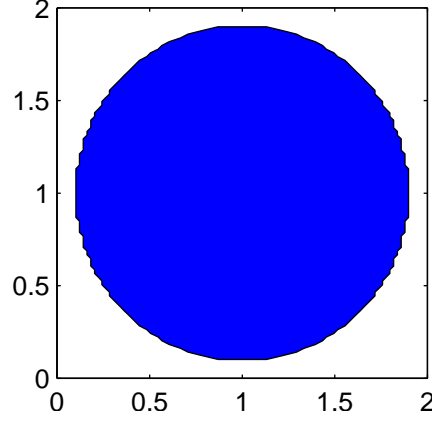
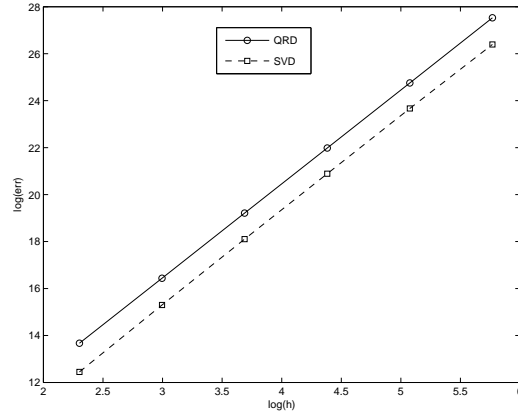
Table 2 Example 18: Newton method's iterates with $h = 1.E - 1$.

METHOD	TIME	$ \lambda_{\text{exact}} - \lambda_k , k = 0, 1, \dots$	$ d(\lambda_{k+1}) $
SVDC	5.5	$7.1e - 1$	$2.8e - 1$
		$1.3e - 1$	$5.5e - 2$
		$1.4e - 3$	$6.0e - 4$
		$1.1e - 7$	$4.2e - 8$
		$1.7e - 7$	$9.3e - 15$
		$1.7e - 7$	$2.0e - 16$
QRC	6	$7.1e - 1$	$7.4e - 1$
		$4.5e - 1$	$5.3e - 1$
		$8.4e - 2$	$1.1e - 1$
		$4.7e - 4$	$6.0e - 4$
		$2.7e - 7$	$6.7e - 10$
		$2.7e - 7$	0
QRD	1	$7.1e - 1$	$7.5e - 1$
		$3.6e - 1$	$4.3e - 1$
		$3.8e - 2$	$4.8e - 2$
		$4.5e - 5$	$5.7e - 5$
		$1.9e - 11$	$2.4e - 11$
		$4.4e - 16$	$2.0e - 15$

Finally, in Table 3 we show the results obtained when approximating Σ_{ED} for $\lambda = 0$ using the discrete QR method. We show only the positive interval of Σ_{ED} ($[\alpha_1, \beta_1]$) and Σ_{ED}^+ ($[\alpha_1^+, \beta_1^+] \cup [\alpha_2^+, \beta_2^+]$), since due to the symmetry of the problem $\Sigma_{\text{ED}}^+ = -\Sigma_{\text{ED}}^-$ and $\Sigma_{\text{ED}} = [\alpha_1, \beta_1] \cup [-\beta_1, -\alpha_1]$. In the Table, the values S and T refer to the values used in (26).

Example 19 We now consider an upper triangular linear system in \mathbb{R}^4 , which is chosen to show how our techniques perform when the coefficient matrix is not asymptotically constant. The diagonal elements of A in (1) are defined as follows

$$\begin{cases} A_{11}(t) = \frac{t^2}{t^2+1} (cb(t) - \lambda + 3 + i) \\ A_{22}(t) = \frac{t^2}{t^2+1} (6 - \lambda + i + \cos(t)) \\ A_{33}(t) = \frac{t^2}{t^2+1} (2 - \lambda + i) \\ A_{44}(t) = \frac{t^2}{t^2+1} (7 - \lambda + i) \end{cases} \quad \text{when } t \leq -1;$$

Fig. 1 Example 18: Basin of attraction of the Newton method.**Fig. 2** Example 18: error on approximation of stable direction.

$$\begin{cases}
 A_{11}(t) = \frac{t^2}{2(t^2+1)} ((t+1)(ca(t) + \lambda - 3 - i) + (1-t)(cb(t) - \lambda + 3 + i)) \\
 A_{22}(t) = \frac{t^2}{2(t^2+1)} ((t+1)(5 - \lambda + i) + (1-t)(6 - \lambda + i + \cos(t))) \\
 A_{33}(t) = \frac{t^2}{2(t^2+1)} ((t+1)(-5 + \lambda + i) + (1-t)(2 - \lambda + i)) \\
 A_{44}(t) = \frac{t^2}{2(t^2+1)} ((t+1)(-2 - \lambda + i) + (1-t)(7 - \lambda + i))
 \end{cases} \quad \text{when } |t| \leq 1;$$

$$\begin{cases}
 A_{11}(t) = \frac{t^2}{t^2+1} (ca(t) + \lambda - 3 - i) \\
 A_{22}(t) = \frac{t^2}{t^2+1} (5 - \lambda + i) \\
 A_{33}(t) = \frac{t^2}{t^2+1} (-5 + \lambda + i) \\
 A_{44}(t) = \frac{t^2}{t^2+1} (-2 - \lambda + i)
 \end{cases} \quad \text{when } t \geq 1.$$

Here $a(t) = \sin(\log(t^2 + 1)) + \frac{2t^2}{t^2+1} \cos(\log(t^2 + 1))$, $b(t) = a(t) + \cos(\log(t^2 + 1)) - \frac{2t^2}{t^2+1} \sin(\log(t^2 + 1))$ and $c = 0.1$.

Table 3 Example 18: Σ_{ED} and Σ_{ED}^+ computed for different values of S and T , with constant stepsize $h = 0.05$.

S	T	$[\alpha_1 \ \beta_1]$	$[\alpha_1^+ \ \beta_1^+]$	$[\alpha_2^+ \ \beta_2^+]$
1.0E+2	1.0E+3	[0.7274 1.7924]	[1.4547 1.7924]	[-0.8962 -0.7274]
1.0E+2	1.0E+4	[0.6736 1.7943]	[1.3473 1.7943]	[-0.8972 -0.6736]
1.0E+3	1.0E+4	[0.6777 1.7924]	[1.3555 1.7924]	[-0.8962 -0.6772]
1.0E+3	1.0E+5	[0.6736 1.7940]	[1.3472 1.7940]	[-0.8970 -0.6736]
1.0E+4	1.0E+5	[0.6744 1.7609]	[1.3488 1.7609]	[-0.8805 -0.6744]

While A_{33} and A_{44} converge quadratically at $\pm\infty$, A_{11} oscillates as $t \rightarrow \pm\infty$ and A_{22} oscillates as $t \rightarrow -\infty$. The precise form of the off-diagonal entries of A is not important in what follows, and we chose them as bounded functions of t and λ , linear in λ . In this example, Σ_{ED}^\pm depend on λ .

Upon inspecting the diagonal elements of A , it is easy to see that in backward time (as $t \rightarrow -\infty$), the Lyapunov exponents are stable for every value of λ , while in forward time (as $t \rightarrow +\infty$) they are not always stable. For example, for $\text{Real}(\lambda)$ in a small neighborhood of 4 and -0.5 , the exponents are not stable. Instead, for $\text{Real}(\lambda) = 3.5$ or 5 there are stable but not distinct Lyapunov exponents (in forward time). For these last two values of λ , SVD techniques are not guaranteed to be reliable. Moreover, for QR methods, in order to obtain proper ordering of the diagonal of B (both in forward and backward time) and satisfy (18) and (21), we cannot select initial condition $X(0) = I$; initial condition chosen randomly worked reliably.

Before reporting on the results of some experiments, we remark that, if for a given value of λ the computed spectra Σ_{ED}^\pm are given by the union of 4 disjoint intervals, stability of the Lyapunov exponents is guaranteed (use [21, Theorem 8.4] and [1, Lemma 5.4.1]). Of course, this is a sufficient condition for stability of the Lyapunov exponents.

The results in Table 4 were obtained with the discrete QR techniques. At every step, we solved the differential equation for $\Phi(t_{k+1}, t_k)$ with a 4-th order explicit Runge Kutta method with constant stepsize $h = 1.0\text{E} - 2$. We approximated directions and spectra up to final time $T = 100$ (this is enough for convergence of directions and to ascertain $0 \notin \Sigma_{\text{ED}}^\pm$). We show the distance between two consecutive iterates and the modulus of \tilde{d} . In Table 4 we show the results obtained when applying Newton's method with initial guess $\lambda_0 = 4.8 + i0.5$, and stopping criterion on the difference of two successive iterates with $\text{tol} = 1.0\text{E} - 15$. Convergence occurs in 6 steps to the root $\hat{\lambda} = 4.1944 + i0.76940$. For $\lambda = \hat{\lambda}$ the two computed half line spectra are $\Sigma_{\text{ED}}^+ = [1.0552 \ 1.3995] \cup [0.8046 \ 0.8055] \cup [-0.8055 \ -0.8046] \cup [-6.1936 \ -6.1867]$ and $\Sigma_{\text{ED}}^- = [-2.1959 \ -2.1900] \cup [-1.5058 \ -0.9910] \cup [1.7476 \ 1.8593] \cup [2.8021 \ 2.8052]$. So, for $\lambda = \hat{\lambda}$, the system admits ED in the two half lines, the dimensions of stable and unstable space sum up to 4, but they are not complementary: the system does not have ED in \mathbb{R} .

Example 20 In this problem, we study the orbital stability of a traveling impulse of the “good” Boussinesq equation

$$u_{tt} = u_{xx} - u_{xxx} - (u^2)_{xx}. \quad (36)$$

Table 4 Example 19: Newton method's iterates.

$ \lambda_{k+1} - \lambda_k , k = 0, 1, \dots$	$ d(\lambda_{k+1}) $
4.6E-1	7.4E-2
1.1E-1	8.2E-3
3.0E-3	5.8E-5
9.1E-5	3.7E-9
4.4E-9	1.2E-13
9.8E-14	5.5E-16

To begin with, we rewrite this as a first order system for $U = \begin{bmatrix} u \\ v \end{bmatrix}$ with $v = u_t$,

$$U_t = \begin{bmatrix} 0 & 1 \\ \partial_{xx} - \partial_{xxxx} & 0 \end{bmatrix} U - \begin{bmatrix} 0 \\ (u^2)_{xx} \end{bmatrix}. \quad (37)$$

Next, consider the traveling wave ansatz $U(x - st, t) = U(z, t)$ which gives

$$U_t = \begin{bmatrix} 0 & 1 \\ \partial_{zz} - \partial_{zzzz} & 0 \end{bmatrix} U + sU_z - \begin{bmatrix} 0 \\ 2(u_z)^2 + 2uu_{zz} \end{bmatrix}. \quad (38)$$

The traveling wave solution $Q(z)$ is the solution of the steady-state problem, and therefore it is given by the vector function $Q(z) = \begin{bmatrix} \hat{u} \\ -s\hat{u}_z \end{bmatrix}$, where \hat{u} solves

$$\hat{u}_{zz} - \hat{u}_{zzzz} - s^2\hat{u}_{zz} - 2(\hat{u}_z)^2 - 2\hat{u}\hat{u}_{zz} = 0. \quad (39)$$

In this case, the exact solution is known:

$$\hat{u}(z) = \frac{3}{2}(1 - s^2)\text{sech}^2\left(\frac{z}{2}\sqrt{1 - s^2}\right),$$

with $|s| < 1$. Linearization of (38) gives the system

$$\begin{bmatrix} u \\ v \end{bmatrix}_t = \begin{bmatrix} v + su_z \\ u_{zz} - u_{zzzz} + sv_z - 4\hat{u}_z u_z - 2\hat{u}u_{zz} - 2u\hat{u}_{zz} \end{bmatrix}. \quad (40)$$

From this, the search for solutions of the type $e^{\mu t}U(z)$ gives the eigenvalue problem

$$\mu \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} v + su_z \\ u_{zz} - u_{zzzz} + sv_z - 4\hat{u}_z u_z - 2\hat{u}u_{zz} - 2u\hat{u}_{zz} \end{bmatrix}, \quad (41)$$

and substituting $v = \mu u - su_z$ in the second equation gives the ODE

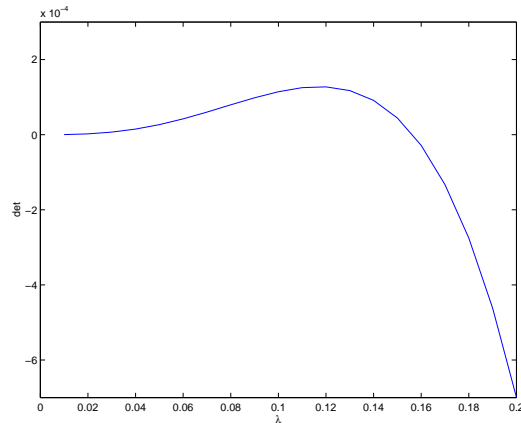
$$u_{zzzz} = (1 - s^2 - 2\hat{u})u_{zz} + (2\mu s - 4\hat{u}_z)u_z - (\mu^2 + 2\hat{u}_{zz})u,$$

which we rewrite as the first order system (1) for the variable $\begin{bmatrix} u \\ u_z \\ u_{zz} \\ u_{zzz} \end{bmatrix}$, obtaining the

coefficient matrix $A(z, \mu) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\mu^2 - 2\hat{u}_{zz} & 2\mu s - 4\hat{u}_z & 1 - s^2 - 2\hat{u} & 0 \end{bmatrix}$. It is relatively to

this system that we search for values of μ for which the system does not admit ED in \mathbb{R} . For $\text{Real}(\mu) > 0$, the system admits ED in both half-lines and the dimensions of forward stable and backward stable spaces sum up to n . It follows that to check whether the system has ED in \mathbb{R} , we will follow **Step 3** in Algorithm 3. To compare our results with the ones in [28], we compute the Evans function $d(\mu)$ for $\mu \in [0, 0.2]$, relatively to computations for the front wave of the (good) Boussinesq equation. The results compare well with those in [28], and show that for a value of μ somewhere in $(0.155, 0.156)$ the linear system does not have ED in \mathbb{R} .

Fig. 3 Example 20: Evans function computation for the Boussinesq equation.



5 Conclusions

In this paper, we have presented robust computational techniques for the detection of ED on the real line. As far as we know, for the first time there are numerically stable algorithms which detect ED on the real line using information from a finite time interval. It is important to stress that our algorithms are justified under generic conditions and do not require asymptotic convergence of the coefficients matrix. Moreover, by our techniques we also obtain approximation of stable and unstable subspaces, and this also appears to be a novelty.

The main tools of our methods are the QR and/or SVD factorizations of the underlying fundamental matrix solution. The theoretical backing for the use of these factorizations rests on our recent work [15]. We emphasize that it is because of these recent theoretical developments (in particular, the subtle issue of convergence for the stable/unstable subspaces) that we have been able to produce general algorithms to detect ED on the real line.

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