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017

ON THE COMPUTATION OF LYAPUNOV EXPONENTS FOR CONTINUOUS DYNAMICAL SYSTEMS*

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Abstract. In this paper, we consider discrete and continuous QR algorithms for computing all of the Lyapunov exponents of a regular dynamical system. We begin by reviewing theoretical results for regular systems and present general perturbation results for Lyapunov exponents. We then present the algorithms, give an error analysis of them, and describe their implementation. Finally, we give several numerical examples and some conclusions.

Key words. Lyapunov exponents, regular systems, exponential dichotomy, point spectrum, orthogonalization techniques, error analysis

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1. Introduction.

Lyapunov exponents (or characteristic numbers) were first introduced by Lyapunov [Ly] in order to study the stability of nonstationary solutions of ordinary differential equations (ODEs) and have since been extensively studied in the literature (e.g., see [Ce, NS, SC]). The Lyapunov exponent of a real valued function $f(t)$ defined for $t \geq 0$ is

$$\lambda = \limsup_{t\to\infty} \frac{1}{t} \log(|f(t)|). \tag{1.1}$$

Thus, λ characterizes the long-time exponential behavior of $f(t)$. For an n-dimensional linear system

$$\dot{\mathbf{y}}(t) = A(t)\mathbf{y}(t) \tag{1.2}$$

with a bounded coefficient matrix $A(t)$, the characteristic number λ of the norm of a solution trajectory is well defined. More generally, consider n linearly independent solutions of (1.2) in the form $\mathbf{y}_i = Y(t)\mathbf{p}_i$, where $Y(t)$ is a fundamental solution matrix with $Y(0)$ orthogonal, and $\{\mathbf{p}_i\}$ is an orthonormal basis of $\mathbb{R}^n$. Then, the corresponding characteristic numbers

$$\lambda_i = \limsup_{t\to\infty} \frac{1}{t} \log(\|Y(t)\mathbf{p}_i\|) \tag{1.3}$$

are well defined; here, and throughout, $\|\cdot\|$ refers to the 2-norm. When the sum of the characteristic numbers is minimized, the orthonormal basis $\{\mathbf{p}_i\}$ is called **normal** and the λ_i are called the **Lyapunov exponents**.

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The Lyapunov exponents associated with a normal basis satisfy

$$\sum_{i=1}^{n} \lambda_i \geq \limsup_{t\to\infty} \frac{1}{t} \int_0^t \operatorname{trace}(A(s))ds = \limsup_{t\to\infty} \frac{1}{t} \log|\det Y(t)|. \tag{1.4}$$

When equality holds for a fundamental solution $Y(t)$ with respect to some normal basis, the linear system is called **regular**.

It can be readily seen that Lyapunov exponents are fixed under a change of variables of the type $X(t) = T(t)Y(t)$ if T and T^{-1} are uniformly bounded. Furthermore, Perron and Diliberto show (see [Le, C]) that for bounded continuous $A(t)$, there exists an orthogonal change of variables $Q(t)$ such that $X(t) = Q^T(t)Y(t)$ satisfies

$$\dot{X}(t) = \tilde{A}(t)X(t), \tag{1.5}$$

where $\tilde{A}(t)$ is upper triangular. The following theorem indicates the importance of such systems.

THEOREM 1.1 (see [Pe, Ly]). *If $A(t) \in \mathbb{R}^{n\times n}(t)$ is upper triangular with all entries continuous and bounded, then a necessary and sufficient condition for regularity of* (1.2) *is that*

$$\limsup_{t\to\infty} \frac{1}{t} \int_0^t A_{ii}(s)ds + \limsup_{t\to\infty} \frac{1}{t} \int_0^t (-A_{ii}(s))ds = 0, \quad i = 1,\dots,n. \tag{1.6}$$

This condition is equivalent to the existence of the limit

$$\mu_i = \lim_{t\to\infty} \frac{1}{t} \int_0^t A_{ii}(s)ds, \; i = 1,\dots,n,$$

in which case $\mu_i \equiv \lambda_i$. □

Lyapunov exponents for (1.2) serve the same role in asymptotic stability analysis as the real parts of the eigenvalues for the constant coefficient case $A(t) \equiv A$, and indeed they are the same in this case. In the case of a periodic system, if $A(t) \equiv A(t+\omega)$ for positive period ω, then

$$\lambda_i = \mathbb{R}\mathrm{e}(\rho_i),$$

where the ρ_i are the Floquet exponents of the monodromy matrix (e.g., see [H]). Given their fundamental importance, it is not surprising that Lyapunov exponents have received a great deal of attention both theoretically and computationally.

Henceforth, unless stated otherwise, we assume that the system (1.2) is regular. However, verifying regularity for a given system is difficult. An alternate approach of Sacker and Sell [SaSe] uses the concept of the **spectrum**. The linear system (1.2) is said to have *exponential dichotomy* if there exist constants $K, L \geq 1$, $\alpha, \beta > 0$, and an orthogonal projection P such that

$$\begin{aligned} \|Y(t)PY^{-1}(s)\| &\leq Ke^{-\alpha(t-s)}, t \geq s, \\ \|Y(t)(I-P)Y^{-1}(s)\| &\leq Le^{-\beta(s-t)}, s \geq t. \end{aligned} \tag{1.7}$$

Exponential dichotomy implies, for example, that k fundamental solution components are exponentially decreasing and $n-k$ are exponentially increasing, where $\operatorname{rank}(P) =$

k. The Sacker–Sell spectrum of (1.2) is the set of real values γ for which the translated systems

$$\dot{\mathbf{x}} = [A(t) - \gamma I]\mathbf{x} \tag{1.8}$$

do not have exponential dichotomy. Equivalently, the spectrum of (1.2) is the complement of the **resolvent**, which is the set of values γ for which (1.8) does have an exponential dichotomy. In general, the spectrum is a collection of at most n compact intervals. When each of these intervals is a point γ_i, $i = 1, \ldots, n$ (not necessarily distinct), then the spectrum is termed **point spectrum**. In such case, each γ_i equals a Lyapunov exponent λ_i (see [SaSe, Theorem 3, p. 338]); moreover, the system is regular, as is shown below.

Consider the system (1.2) and its adjoint

$$\dot{Y} = A(t)Y, \tag{1.9}$$

$$\dot{V} = -A^T(t)V, \qquad \text{where} \qquad V(t) = Y^{-T}(t). \tag{1.10}$$

LEMMA 1.2. *The value $\lambda \in \mathbb{R}$ is in the resolvent of* (1.9) *if and only if $-\lambda$ is in the resolvent of* (1.10)*.*

Proof. We prove only the sufficiency, as the necessity is proven in the same way. Let λ be in the resolvent of (1.9), and let $Y_\lambda(t)$ be the fundamental solution of the translated system $\dot{Y}_\lambda = (A(t) - \lambda I)Y_\lambda(t)$. Thus,

$$\|Y_\lambda(t)PY_\lambda^{-1}(s)\| \le Ke^{-\alpha(t-s)}, t \ge s,$$
$$\|Y_\lambda(t)(I-P)Y_\lambda^{-1}(s)\| \le Ke^{-\alpha(s-t)}, s \ge t,$$

or, equivalently,

$$\|Y(t)PY^{-1}(s)\| \le Ke^{(\lambda-\alpha)(t-s)}, t \ge s,$$
$$\|Y(t)(I-P)Y^{-1}(s)\| \le Ke^{(-\lambda-\alpha)(s-t)}, s \ge t,$$

for appropriate projection P and positive constants K, α. Since we are using the 2-norm, we have

$$\|Y(t)PY^{-1}(s)\| = \|Y^{-T}(s)P^TY^T(t)\| = \|V(s)PV^{-1}(t)\|\,.$$

By letting $\tilde{P} := I - P$, $s =: \tilde{t}$, and $t =: \tilde{s}$, we see that $-\lambda$ is in the resolvent of (1.10) since

$$e^{-\lambda(t-s)}\|Y(t)PY^{-1}(s)\| = \|V_{-\lambda}(\tilde{t})(I-\tilde{P})V_{-\lambda}^{-1}(\tilde{s})\| \le Ke^{-\alpha(\tilde{s}-\tilde{t})}\,,\ \tilde{s} \ge \tilde{t}\,,$$

and, similarly,

$$\|V_{-\lambda}(\tilde{t})\tilde{P}V_{-\lambda}^{-1}(\tilde{s})\| \le Ke^{-\alpha(\tilde{t}-\tilde{s})}\,,\ \tilde{t} \ge \tilde{s}\,. \qquad \square$$

COROLLARY 1.3. *Let system* (1.9) *have spectrum $[a_1, b_1] \cup \cdots \cup [a_p, b_p]$, where $a_i \le b_i$, $i = 1, \ldots, p$, and $b_i < a_{i+1}$, $i = 1, \ldots, p-1$. Then, the spectrum of* (1.10) *is given by $[-b_p, -a_p] \cup \cdots \cup [-b_1, -a_1]$.* $\square$

COROLLARY 1.4. *If the system* (1.9) *has point spectrum, given by the values $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$, then* (1.10) *has point spectrum given by $-\lambda_1 \le -\lambda_2 \le \cdots \le -\lambda_n$. In particular,* (1.2) *and* (1.5) *are regular, and*

$$\lim_{t-s\to\infty} \frac{1}{t-s} \int_s^t \tilde{A}_{ii}(\tau)d\tau$$

exist for $i = 1, \ldots, n$, where $\tilde{A}(t)$ is defined in (1.5)*.*

Proof. The first statement is an immediate consequence of Lemma 1.2. The statement about regularity follows directly from a theorem by Perron [A, Theorem 3.6.1] stating that a given system is regular if and only if the Lyapunov exponents of the system and those of its adjoint are symmetric with respect to the origin. ∎

Below we let $\lambda[f]$ denote the Lyapunov exponent of the function $f(t)$ and use a similar notation for Lyapunov exponents of vectors. We have the following.

LEMMA 1.5. *Consider the system*

$$\dot{\mathbf{x}} = L(t)\mathbf{x}\,, \tag{1.11}$$

where $L(t)$ *is a triangular matrix with integrable coefficients. Let*

$$l_i^+ = \limsup_{t\to\infty} \frac{1}{t}\int_0^t L_{ii}(s)ds\,, \quad l_i^- = \liminf_{t\to\infty} \frac{1}{t}\int_0^t L_{ii}(s)ds\,.$$

Then, l_i^+ *and* l_i^- *lie in the same spectral interval of* (1.11).

Proof. Without loss of generality, we assume that $L(t)$ is lower triangular. Let $X(t,0)$ be the fundamental matrix solution of (1.11) such that $X(0,0) = I$, obtained by successive forward integration. Although $X(t,0)$ is in general not normal, a theorem by Lyapunov (see [A, Theorem 2.4.2]) guarantees the existence of a unit lower triangular matrix C such that $X(t) := X(t,0)C = \{\mathbf{x}_1(t),\ldots,\mathbf{x}_n(t)\}$ is normal. If $\alpha_k := \lambda[\mathbf{x}_k]$, $k = 1,\ldots,n$, then clearly $\lambda[X_{kk}] = l_k^+ \le \alpha_k$ where $X_{kk}(t)$ is the kth diagonal element of $X(t)$. Let now $Y(t) = \{\mathbf{y}_1(t),\ldots,\mathbf{y}_n(t)\}$ be the basis of the adjoint system to (1.11) such that $Y^T(t)X(t) = I$, and let $\lambda[\mathbf{y}_k] = \beta_k, k = 1,\ldots,n$. Notice that

$$\lambda[Y_{kk}] = \lambda[1/X_{kk}] = \limsup_{t\to\infty}\frac{1}{t}\log|1/X_{kk}| = -\liminf_{t\to\infty}\frac{1}{t}\log|X_{kk}| = -l_k^-\,,$$

so that $\lambda[\mathbf{y}_k] = \beta_k \ge -l_k^-$. Since $l_k^- \le l_k^+$, we have

$$-\beta_k \le l_k^- \le l_k^+ \le \alpha_k\,.$$

It follows from [SaSe, Theorem 3] and Corollary 1.3 that $\alpha_k \in [a_k, b_k]$, and $\beta_k \in [-b_k, -a_k]$, so $[-\beta_k, \alpha_k]$ is contained in a spectral interval of (1.11), and the result follows. ∎

One of the key theoretical tools for determining Lyapunov exponents is the continuous QR factorization of $Y(t)$,

$$Y(t) = Q(t)R(t)\,, \tag{1.12}$$

where $Q(t)$ is orthogonal and $R(t)$ is upper triangular with positive diagonal elements R_{ii}, $i = 1,\ldots,n$. This factorization is crucial in both [O] and [JPS]. The following lemma underlies its importance.

LEMMA 1.6. *Consider the system* (1.2)*, and let* $Q(t)$ *be a differentiable orthogonal matrix for all* t*. Then the Lyapunov exponents of the system*

$$\dot{\mathbf{z}} = \tilde{A}(t)\mathbf{z}, \tag{1.13}$$

where

$$\tilde{A}(t) = Q(t)^T A(t)Q(t) - Q(t)^T\dot{Q}(t), \tag{1.14}$$

are the same as the Lyapunov exponents of the original system (1.2). *Moreover, the spectra of* (1.13) *and* (1.2) *are identical.*

Proof. If $Y(t)$ is a fundamental solution of (1.2), then $Z(t) = Q^T(t)Y(t)$ is a fundamental solution of (1.13). Thus, the invariance of the Lyapunov exponents follows from (1.3) and the norm-preserving property of $Q(t)$. The equivalence of the spectra is also a direct consequence of this orthogonality of $Q(t)$. ∎

Note that from (1.12)

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \log ||Y(t)\mathbf{p}_i|| = \lim_{t\to\infty} \frac{1}{t} \log ||R(t)\mathbf{p}_i||. \tag{1.15}$$

$Q(t)$ in (1.14) is an example of a *Lyapunov* or *kinematic similarity transformation*, and it has been known since Lyapunov [Ly] that regularity of a system is preserved under such a transformation, so by Theorem 1.1

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \log |R_{ii}(t)|, 1 \le i \le n\,. \tag{1.16}$$

The factorization (1.12) also proves to be a fundamental computational tool since from (1.16) a change of variables

$$\mathbf{z}(t) \,=\, Q(t)^T \mathbf{y}(t),$$

with differentiable $Q(t)$, chosen so that $\tilde{A}(t)$ in (1.14) has a triangular structure, greatly simplifies the computation of the Lyapunov exponents.

After giving some results on exponential dichotomy and its relation to Lyapunov exponents in section 2, we describe two techniques to achieve this change of variables and then give a partial error analysis of these techniques in sections 3 and 4. To our knowledge, ours are the first convergence results for these algorithms, which are the most widely used techniques for computing Lyapunov exponents. One technique involves performing a *continuous* QR decomposition of the fundamental solution matrix $Y(t)$; the other is a *discrete* QR method, where $Y(t)$ is computed first and then an orthogonal factorization is formed.

Remark 1.7. In this introduction and in the next section, we consider continuous dynamical systems (i.e., differential equations). On the other hand, Lyapunov exponents, as well as the concepts of regularity, exponential dichotomy, and point spectrum, have immediate extensions to discrete dynamical systems, and only minor modifications to our exposition are needed. Some of these modifications are in [DV]. In particular, results analogous to Theorem 1.1, Lemmas 1.2 and 1.5, and Corollary 1.4 hold, as well as discrete analogues of the results of the next section. We will make use of these discrete extensions.

2. Some perturbation results.

We now consider the effect of perturbations of the matrix $A(t)$ on the Lyapunov exponents of the linear problem (1.2). We shall henceforth assume that (1.2) has point spectrum, which is given by its Lyapunov exponents $\{\lambda_i\}_{i=1}^n$.

Consider the perturbed system

$$\dot{\mathbf{z}} \,=\, [A(t) + E(t)]\,\mathbf{z}, \tag{2.1}$$

where for the moment we assume that $E(t)$ is a continuous matrix function such that $\sup_t \|E(t)\| < \delta$ for some small $\delta > 0$. A relation between bounds on perturbations of the Lyapunov exponents and perturbations in $A(t)$ is given in the following perturbation theorem of Sacker and Sell [SaSe] and then quantified in Theorem 2.3 below.

THEOREM 2.1. *For each neighborhood V of the spectrum of* (1.2)*, there exists a neighborhood M of $A(t)$ such that all linear systems whose coefficient matrices lie in M have spectrum in V.* □

Let $\{\Lambda_i\}_{i=1}^p$ be the distinct Lyapunov exponents of (1.2), with respective multiplicities $n_1, \ldots, n_p$. Suppose that the $\{\Lambda_i\}_{i=1}^p$ are in ascending order, and let $\Lambda_0 := -\infty$ and $\Lambda_{p+1} := +\infty$. Given Λ_i, for any positive η_1 and ϵ_1 satisfying $\eta_1 > \epsilon_1 > 0$, $\Lambda_{i+1} > \Lambda_i + \epsilon_1$, and $\Lambda_{i+1} > \Lambda_i + \eta_1 - \epsilon_1$, it is possible to show that there exist bounded constants $K_1 \geq 1$ and $L_1 \geq 1$ (depending on ϵ_1, η_1), and a projection matrix P_1 with $\text{rank}(P_1) = n_1 + \cdots + n_i$, such that

$$\begin{aligned} \|X_{\Lambda_i+\epsilon_1}(t)P_1X^{-1}_{\Lambda_i+\epsilon_1}(s)\| &\leq K_1, t \geq s, \\ \|X_{\Lambda_i+\epsilon_1}(t)(I-P_1)X^{-1}_{\Lambda_i+\epsilon_1}(s)\| &\leq L_1 e^{-(\Lambda_{i+1}-\Lambda_i-\eta_1)(s-t)}, s \geq t, \end{aligned} \tag{2.2}$$

where $X_\gamma(t)$ denotes a fundamental solution matrix of the translated system (1.8). Analogously, given Λ_k, for any positive η_2 and ϵ_2 satisfying $\eta_2 > \epsilon_2 > 0$, $\Lambda_k > \Lambda_{k-1} + \epsilon_2$, and $\Lambda_k > \Lambda_{k-1} + \eta_2 - \epsilon_2$, there exist bounded constants $K_2 \geq 1$ and $L_2 \geq 1$ (depending on ϵ_2, η_2), and a projection matrix P_2 with $\text{rank}(P_2) = n_1 + \cdots + n_{k-1}$, such that

$$\begin{aligned} \|X_{\Lambda_k-\epsilon_2}(t)P_2X^{-1}_{\Lambda_k-\epsilon_2}(s)\| &\leq K_2 e^{-(\Lambda_k-\Lambda_{k-1}-\eta_2)(t-s)}, t \geq s, \\ \|X_{\Lambda_k-\epsilon_2}(t)(I-P_2)X^{-1}_{\Lambda_k-\epsilon_2}(s)\| &\leq L_2, s \geq t. \end{aligned} \tag{2.3}$$

To determine an interval containing a Lyapunov exponent of the perturbed system (2.1), we consider the dichotomy as a function of the translate γ and locate where a change in the rank of the projection occurs.

LEMMA 2.2 (see [SaSe, Lemma 9]). *Suppose $\mu_1 < \mu_2$ are such that the translated system* (1.8) *has exponential dichotomy for $\gamma = \mu_1$ and $\gamma = \mu_2$. Then, there exists a value $\mu \in (\mu_1, \mu_2)$ such that* (1.8) *does not have exponential dichotomy for $\gamma = \mu$ if and only if the rank of the projection onto the stable subspace (P in* (1.7)*) for $\gamma = \mu_1$ is less than the rank of the corresponding projection for $\gamma = \mu_2$.* □

We are now prepared for the main perturbation result.

THEOREM 2.3. *Assume that* (1.2) *has point spectrum given by $\{\lambda_i\}_{i=1}^n$. Let $\{\Lambda_i\}_{i=1}^p$ be the distinct Lyapunov exponents of* (1.2)*, with respective multiplicities $n_1, \ldots, n_p$, arranged in ascending order, and let $\Lambda_0 := -\infty$ and $\Lambda_{p+1} := +\infty$. Suppose that $\delta > 0$ is a bound on the perturbation $E(t)$ in* (2.1)*. For a given $k = i$, consider $\epsilon_j, \eta_j, K_j, L_j$ defined for $j = 1, 2$ in* (2.2) *and* (2.3) *with $k = i$. Let constants α_1, α_2 such that $\alpha_1 > \delta \cdot 4K_1^2$ and $\alpha_2 > \delta \cdot 4L_2^2$ be given. If $\alpha_1 < \Lambda_{i+1} - \Lambda_i - \epsilon_1$, $\beta_1 := (\Lambda_{i+1} - \Lambda_i - \eta_1 - \alpha_1) > \delta \cdot 4L_1^2$, and $\alpha_2 < \Lambda_i - \Lambda_{i-1} - \epsilon_2$, $\beta_2 := (\Lambda_i - \Lambda_{i-1} - \eta_2 - \alpha_2) > \delta \cdot 4K_2^2$, then the Lyapunov exponent μ_i of* (2.1) *lies in the interval $(\Lambda_i - \epsilon_2 - \alpha_2, \Lambda_i + \epsilon_1 + \alpha_1)$.*

Proof. If $\gamma_i = \Lambda_i + \epsilon_1 + \alpha_1$, then $\gamma_i < \Lambda_{i+1}$ and

$$\begin{aligned} \|X_{\gamma_i}(t)P_1X^{-1}_{\gamma_i}(s)\| &\leq K_1 e^{-\alpha_1(t-s)}, t \geq s, \\ \|X_{\gamma_i}(t)(I-P_1)X^{-1}_{\gamma_i}(s)\| &\leq L_1 e^{-\beta_1(s-t)}, s \geq t; \end{aligned} \tag{2.4}$$

i.e., the translated system (1.8) has exponential dichotomy for $\gamma = \gamma_i$ with constants $\alpha_1, K_1, \beta_1, L_1$. By the roughness theorem for exponential dichotomy (see [C, p. 34]), the perturbed translated system

$$\dot{\mathbf{w}} = [A(t) + E(t) - \gamma I]\mathbf{w} \tag{2.5}$$

has exponential dichotomy for $\gamma = \gamma_i$; i.e.,

$$\begin{aligned} \|W_{\gamma_i}(t)Q_1W_{\gamma_i}^{-1}(s)\| &\le \frac{5}{2}K_1^2 e^{-(\alpha_1-2K_1\delta)(t-s)}, t \ge s, \\ \|W_{\gamma_i}(t)(I-Q_1)W_{\gamma_i}^{-1}(s)\| &\le \frac{5}{2}L_1^2 e^{-(\beta_1-2L_1\delta)(s-t)}, s \ge t, \end{aligned} \tag{2.6}$$

where $\text{rank}(Q_1) = \text{rank}(P_1)$ and $W_\gamma(t)$ is the fundamental solution matrix for (2.5). Similarly, if $\rho_i = \Lambda_i - \epsilon_2 - \alpha_2$, then $\rho_i > \Lambda_{i-1}$ and

$$\begin{aligned} \|X_{\rho_i}(t)P_2X_{\rho_i}^{-1}(s)\| &\le K_2 e^{-\beta_2(t-s)}, t \ge s, \\ \|X_{\rho_i}(t)(I-P_2)X_{\rho_i}^{-1}(s)\| &\le L_2 e^{-\alpha_2(s-t)}, s \ge t. \end{aligned} \tag{2.7}$$

The roughness theorem implies that (2.5) has exponential dichotomy for $\gamma = \rho_i$, so

$$\begin{aligned} \|W_{\rho_i}(t)Q_2W_{\rho_i}^{-1}(s)\| &\le \frac{5}{2}K_2^2 e^{-(\beta_2-2K_2\delta)(t-s)}, t \ge s, \\ \|W_{\rho_i}(t)(I-Q_2)W_{\rho_i}^{-1}(s)\| &\le \frac{5}{2}L_2^2 e^{-(\alpha_2-2L_2\delta)(s-t)}, s \ge t, \end{aligned} \tag{2.8}$$

where $\text{rank}(Q_2) = \text{rank}(P_2)$. Since $\text{rank}(Q_1) = n_1 + \cdots + n_i$ and $\text{rank}(Q_2) = n_1 + \cdots + n_{i-1}$, Lemma 2.2 gives the result. ∎

Remark 2.4

(i) The terms ϵ_1 and ϵ_2 are necessary only if there is some type of subexponential growth in the solution. For example, the function $f(t) = t^p$ for integer $p > 0$ has a zero Lyapunov exponent, and for any $\epsilon > 0$ there exists a $K \ge 1$ such that $f(t) \le Ke^{\epsilon t}$ for $t \ge 0$.

(ii) Theorem 2.3 relies on there being sufficient gaps between distinct Lyapunov exponents of (1.2). Subject to the constraints $\alpha_1 < \Lambda_{i+1} - \Lambda_i - \epsilon_1$, $\beta_1 > 4\delta L_1^2$, and $\alpha_2 < \Lambda_i - \Lambda_{i-1} - \epsilon_2$, $\beta_2 > 4\delta K_2^2$, one should choose $\eta_1 > \epsilon_1 > 0$ and $\eta_2 > \epsilon_2 > 0$ to minimize $\epsilon_2 + \alpha_2$ and $\epsilon_1 + \alpha_1$. Notice that, since $\alpha_1 > 0$, we must have $\Lambda_{i+1} > \Lambda_i + \eta_1$ and, similarly, $\Lambda_i > \Lambda_{i-1} + \eta_2$ for the assumptions in Theorem 2.3 to hold.

The following consequence of Theorem 2.3, showing that if several (distinct) Lyapunov exponents of (1.2) are close together, then so are the Lyapunov exponents of (2.1), is immediate.

COROLLARY 2.5. *Let the assumptions of Theorem* 2.3 *be satisfied, except let* $k < i$ *in* (2.3). *Then the Lyapunov exponents* $\mu_k, \dots, \mu_i$ *of the perturbed equation* (2.1) *lie in the interval* $(\Lambda_k - \epsilon_2 - \alpha_2, \Lambda_i + \epsilon_1 + \alpha_1)$. ∎

Remark 2.6. The assumption of $E(t)$ being continuous in Theorem 2.3, and Corollary 2.5, enable us to use the roughness theorem from the original formulation given by Coppel. However, such an assumption is not necessary (see [J] and [Pa]). All that is needed is that $E(t)$ be a matrix of small norm with locally integrable entries; for example, the roughness theorem holds when $E(t)$ is a matrix of small norm with essentially bounded entries. Under this weaker assumption, the explicit form of the constants is changed, but the qualitative result is unchanged.

Nonlinear systems. As described in the seminal work of Oseledec [O], Lyapunov exponents provide a meaningful way to characterize the asymptotic behavior of a nonlinear dynamical system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t),\ \mathbf{x}(0) = \mathbf{x}_0,\ \mathbf{x} \in \mathbb{R}^n, \tag{2.9}$$

where $\mathbf{f}(\mathbf{x}, t)$ is continuously differentiable. They provide a generalization of the linear stability analysis for perturbations of steady state solutions to time-dependent solutions. One of the most important consequences of the work of Oseledec is that for ergodic dynamical systems, the Lyapunov exponents are the same for almost all initial conditions $\mathbf{x}_0$ with respect to any invariant measure for the flow; i.e., their values do not depend on a particular trajectory.

For a given solution trajectory $\mathbf{x}(t)$, one considers the linear variational equation

$$\dot{Y} = D\mathbf{f}(\mathbf{x})Y = A(t)Y, \; Y(0) = I, \tag{2.10}$$

where $A(t) = (\partial \mathbf{f}/\partial \mathbf{x})$ is the Jacobian at $\mathbf{x}(t)$. Then, for a fundamental solution matrix $Y(t)$ the symmetric positive definite matrix

$$\Lambda = \lim_{t\to\infty} \Lambda_{\mathbf{x}_0}(t) := \lim_{t\to\infty} (Y^T(t)Y(t))^{\frac{1}{2t}} \tag{2.11}$$

is well defined [O]. If $\{\mathbf{p}_i, \mu_i\}_1^n$ denote the eigenvectors and associated eigenvalues of Λ such that $\Lambda \mathbf{p}_i = \mathbf{p}_i \mu_i$, or $\mathbf{p}_i^T \Lambda \mathbf{p}_i = \mu_i$, then the Lyapunov exponents with respect to the trajectory $\mathbf{x}(t)$ of (2.9) (or the linear system (2.10)) are given by

(2.12)
$$\lambda_i = \log(\mu_i) = \log(\lim_{t\to\infty} < Y(t)\mathbf{p}_i, Y(t)\mathbf{p}_i >^{\frac{1}{2t}}) = \lim_{t\to\infty} \frac{1}{t} \log ||Y(t)\mathbf{p}_i||, i = 1, \ldots, n,$$

where $\langle \mathbf{z}, \mathbf{y} \rangle := \mathbf{z}^T \mathbf{y}$ and $\|\mathbf{z}\| := \langle \mathbf{z}, \mathbf{z} \rangle^{1/2}$. Thus, λ_i is a measure of the mean logarithmic growth rate of perturbations in the subspace $Eig(\Lambda, \mu_i) = \{\mathbf{p}_i \in \mathbb{R}^n : \Lambda \mathbf{p}_i = \mu_i \mathbf{p}_i\}$, and $\{\lambda_i\}$ describes how nearby trajectories for the dynamical system (2.9) converge or diverge from $\mathbf{x}(t)$.

In this work, we only consider the linear system (2.10) and neglect the errors involved in computing it from (2.9). The perturbation results of Theorem 2.3 and Corollary 2.5 apply to the nonlinear system (2.9) if the Jacobian of the computed trajectory is uniformly close to the Jacobian of some exact trajectory, although (at best) one approximates the Lyapunov exponents of some solution trajectory. In the ergodic case in which the Lyapunov exponents are almost everywhere independent of initial conditions with respect to an ergodic measure, however, the perturbation results ensure that the approximations are close by. It is important to note that this is an ergodic result, which means that it holds in the limit as $t \to \infty$. But different initial conditions can, and generally do, produce different finite time approximations to the Lyapunov exponents. To have the Jacobians close, we need some restrictions on the systems. One important case is for systems in which the Lipschitz constant for Df is small and shadowing results hold (e.g., see [CVV1, E]). Also, an inexact Jacobian with error uniformly small in t occurs when there is noise in the original nonlinear system or noise in the Jacobian, or when only a finite difference approximation of the Jacobian is available.

3. Basic numerical methods.

In theory, one simply needs to perform a QR (or SVD) decomposition of $Y(T)$ for T sufficiently large, but in practice the columns of $Y(t)$ become numerically linearly dependent (each component eventually undergoes exponential growth as determined by the largest Lyapunov exponent), and it is necessary to keep the columns linearly independent by periodically factoring $Y(t)$.

Discrete *QR* method. The most popular method for computing Lyapunov exponents is some variation of the discrete QR algorithm. It is suggested by Benettin, Galgani, Giorgilli, and Strelcyn [BGGS], who use a Gram–Schmidt algorithm to compute the QR decompositions, and it is implemented in [WSSV]. This algorithm is modified by Eckmann and Ruelle [ER], who implement the approach used theoretically in [JPS], using Householder transformations.

Algorithm description. The gist of the approach is to indirectly compute the QR factorization of $Y(t)$ at the points $t_0 < t_1 < \cdots < t_j < t_{j+1} < \cdots$. Specifically, given

$$Y_0 := Q_0 = I, \tag{3.1}$$

for $j = 0, 1, \ldots$, one solves

$$\dot{Z}_j = AZ_j, Z_j(t_j) = Q_j, \quad t_j \leq t \leq t_{j+1}, \tag{3.2}$$

for $Z_j(t)$, and then takes the QR decomposition

$$Z_j(t_{j+1}) = Q_{j+1}R_{j+1}, \tag{3.3}$$

where R_{j+1} has positive diagonal entries. Since $Q_0 = I$, by letting $Y_j := Y(t_j)$ one has

$$\begin{aligned} Y_{j+1} &= Z_j(t_{j+1})Q_j^T Y_j = Q_{j+1}R_{j+1}Q_j^T Y_j = \cdots \\ &= Q_{j+1}R_{j+1}\ldots R_1 Q_0 = Q_{j+1}\prod_{k=j+1}^{1} R_k. \end{aligned}$$

From (1.16), the Lyapunov exponents can thus be obtained as

$$\lambda_i = \lim_{j\to\infty}\frac{1}{t_j}\log\|(R_j)_{ii}\cdots(R_1)_{ii}\| = \lim_{j\to\infty}\frac{1}{t_j}\sum_{k=1}^{j}\log\|(R_k)_{ii}\|. \tag{3.4}$$

Note that R_k expresses the local growth rates of the fundamental solution components on $[t_k, t_{k+1}]$. □

Continuous *QR* method. The continuous QR method is considered in [BGGS, GSO, GPL]. Various difficulties with the method are reported, and, in fact, in [GPL] it is found to be not competitive with the discrete QR approach. However, we shall see that, properly implemented, it is often much better than the discrete QR method.

Algorithm description. We have

$$Y(t) = Q(t)R(t)\,, \quad \dot{Y} = \dot{Q}R + Q\dot{R} = AQR, \tag{3.5}$$

so

$$Q^T\dot{Q} - Q^TAQ = -\dot{R}R^{-1}. \tag{3.6}$$

Since $\dot{R}R^{-1}$ is upper triangular, the skew symmetric matrix $H(t,Q) := Q^T\dot{Q}$ satisfies

$$H_{ij} = \begin{cases} (Q^TAQ)_{ij}, i > j, \\ 0, i = j, \\ -(Q^TAQ)_{ji}, i < j\ . \end{cases} \tag{3.7}$$

Therefore, the matrix system

$$\dot{Q} = Q\,H(t,Q) \tag{3.8}$$

can be solved for $Q(t)$. From (3.6)

$$\dot{R} = \tilde{A}R\,, \tag{3.9}$$

where $\tilde{A}$ is defined in (1.14), and since $H_{ii} = 0, i = 1, \ldots, n$,

$$\dot{R}_{ii} = (Q^T AQ)_{ii} R_{ii}, i = 1, \ldots, n. \tag{3.10}$$

Thus,

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \log R_{ii}(t) = \lim_{t\to\infty} \frac{1}{t} \int_0^t \tilde{A}_{ii}(s)ds\,, \qquad \tilde{A}_{ii}(t) = (Q^T(t)A(t)Q(t))_{ii}\,. \tag{3.11}$$

The matrix $Q(t)$ with $Q(0) = Y(0)R^{-1}(0)$ and the resulting $\tilde{A}(t)$ are unique. If $Y(0) = Q(0) = I$, this method is the closure of the discrete QR method since (if integrations are done exactly) $R(t_{j+1}) = \prod_{k=j+1}^{1} R_k$. □

In many cases of interest, the fundamental solution matrix $Y(t)$ has both exponentially increasing and decreasing modes; the problem of computing this type of (dichotomic) solution matrix arises also when solving boundary value problems for ODEs (e.g., see [AMR]). Not surprisingly, there has been a parallel development of the discrete and continuous QR methods in this area. The discrete QR algorithm has been examined extensively, and there is reliable software (see [G, SW]). While the continuous QR algorithm has also been investigated, its numerical properties are not as well understood [Me, Da, DRV].

4. Error analysis.

The two chief sources of error to consider are (a) the error from truncation of the infinite time problem to a finite one and (b) the discretization errors from numerical integration of the differential equations.

Truncated time exponents. In practice, computation of Lyapunov exponents is done for finite time, and we need the following.

DEFINITION 4.1. *For given time $T < \infty$, the* truncated time (Lyapunov) exponents *are the exact values obtained by truncating the infinite limits to the value T. For regular systems this reduces to*

$$\lambda_i(T) = \frac{1}{T} \int_0^T \tilde{A}_{ii}(s)ds = \frac{1}{T} \log R_{ii}(T)\,, \tag{4.1}$$

where $\tilde{A}_{ii}(t)$ and $R_{ii}(t)$ are the diagonal entries of upper triangular $\tilde{A}(t)$ and $R(t)$ defined in (1.14) *and* (1.12)*, respectively.* □

Recall that the Lyapunov exponents and the spectra of (1.2) and (1.13) are the same. To analyze the error in a truncated time approximation to λ_i, for $\gamma = \lambda_i$, we consider the diagonal terms of the upper triangular fundamental solution matrix of (1.13). Letting $\phi_{\lambda_i}(t) = e^{-\lambda_i t}\phi_i(t)$ and

$$\phi_i(t) = e^{\int_0^t \tilde{A}_{ii}(s)ds}\,,$$

we have that for any $\xi_i > 0$ and $\rho_i > 0$ there exist K_i, $L_i \geq 1$ such that

$$\begin{aligned} &|\phi_{\lambda_i+\xi_i}(t)\phi^{-1}_{\lambda_i+\xi_i}(s)| \leq K_i, t \geq s, \\ &|\phi_{\lambda_i-\rho_i}(s)\phi^{-1}_{\lambda_i-\rho_i}(t)| \leq L_i, t \geq s\,. \end{aligned} \tag{4.2}$$

Setting $s = 0$ and $t = T > 0$ gives

$$|e^{-(\lambda_i+\xi_i)T}\phi_i(T)| \le K_i, \quad |e^{-(\lambda_i-\rho_i)T}\phi_i(T)| \ge L_i^{-1}. \tag{4.3}$$

From (4.1) we obtain

$$-\rho_i - \frac{1}{T}\log(L_i) \le \frac{1}{T}\int_0^T \tilde{A}_{ii}(s)ds - \lambda_i \equiv \lambda_i(T) - \lambda_i \le \xi_i + \frac{1}{T}\log(K_i), \tag{4.4}$$

which is summarized as follows.

LEMMA 4.2. *Let λ_i be a Lyapunov exponent of* (1.2). *Then, given $\xi_i, \rho_i > 0$, there exist constants $K_i, L_i \ge 1$ such that the error bound* (4.4) *for the truncated time Lyapunov exponents holds.* □

A way to estimate K_i, L_i and the subexponential growth and decay constants ξ_i, ρ_i while computing the Lyapunov exponents is presented in section 5.

Numerical integration error. The first results we have are for the constant and periodic coefficient cases, which are the two simplest instances of systems which have point spectrum (in particular, they are regular; see Corollary 1.4).

Constant and periodic coefficient matrices. We shall show the following.

Claim 1. Let A be constant and let the discrete QR method be used with a fixed stepsize $h > 0$. Let $R(Ah)$ be a rational matrix function approximating e^{Ah} such that $R(Ah)$ is invertible, with no eigenvalues on the negative real axis. Then, in the limit the discrete QR method computes the Lyapunov exponents of the system $\dot{\mathbf{z}} = B\mathbf{z}$ exactly, as real parts of the eigenvalues of a logarithm matrix B, where $R(Ah) = e^{hB}$.

Claim 2. Let $A(t)$ be ω periodic, $A(t + \omega) = A(t)$, and choose the stepsize sequence for the discrete QR algorithm so that $t_J = \omega$ for some index J. Moreover, let the stepsize sequence used over the first period for the approximation of the Z_j matrices be used also for every other time period. Then, in the limit the discrete QR method computes the real parts of the Floquet exponents of the computed approximation to the monodromy matrix exactly. In particular, the significant error is that over one period, and it does not accumulate.

Remark 4.3. There are noteworthy similarities between computing Lyapunov exponents in the two cases above and "orthogonal iteration," a well-known method which is a prototype for computing eigenvalues of a matrix C. It consists of the following: given C and Q_0 (e.g., $Q_0 = I$), let

$$Z_{j+1} = CQ_j,$$

and then form the QR decomposition of Z_{j+1},

$$Z_{j+1} = Q_{j+1}R_{j+1},$$

for $j = 0, 1, 2, \dots$ (cf. (3.2), (3.3)). It is well known (e.g., see [SB]) that the sequence $Q_j^T CQ_j$ (Schur iteration) converges to a Schur decomposition of C if the eigenvalues of C are all real and distinct. If there are multiple eigenvalues (or complex conjugate eigenvalues) the sequence of Q_j may not actually converge, and neither do the $Q_j^T CQ_j$. But in all cases, as $j \to \infty$, $Q_j^T CQ_j$ approaches a quasi-triangular structure whose eigenvalues are the eigenvalues of C. Technically, failure to converge can occur for columns whose eigenvalues have equal modulus. ∎

To show Claim 1, suppose that we use the discrete QR method (3.1)–(3.3) for computing the Lyapunov exponents for a constant coefficient problem. We are really doing the following: given Q_0 (e.g, $Q_0 = I$), we have $Z_j(t_{j+1}) = e^{Ah}Q_j$, and then $Z_j(t_{j+1}) = Q_{j+1}R_{j+1}$ for $j = 0, 1, \ldots$. Note that Ah is a logarithm of e^{Ah}. Thus, we obtain the Lyapunov exponents as

$$\lambda_i = \frac{1}{h} \lim_{j\to\infty} \frac{1}{j} \log |(R_j)_{ii} \cdots (R_1)_{ii}| ,$$

which in the limit converges to the real part of the ith eigenvalue of A. In practice, we compute a rational approximation $R(Ah)$ to e^{Ah}. Under the assumptions, $R(Ah)$ has a real logarithm hB such that $e^{hB} = R(Ah)$. Therefore, in the limit we actually compute the real parts of the eigenvalues of B, as claimed.

The argument for periodic problems is similar. Recall that a monodromy matrix D satisfies $Y(t + \omega) = Y(t)D$, and for periodic problems $Y(t) = P(t)e^{Bt}$, where B has constant coefficients and $P(t)$ has period ω. Thus, without loss of generality we can consider the monodromy matrix $Y(\omega)$ with $Y(0) = I$. Under the assumptions of Claim 2, we are doing the following: given $Q_0 = I$, we form $Z_j(t_{(j+1)J}) = Y(\omega)Q_j$ and then $Z_j(t_{(j+1)J}) = Q_{j+1}R_{(j+1)J}$ for $j = 0, 1, \ldots$. Thus, we obtain the Lyapunov exponents as

$$\lambda_i = \frac{1}{\omega} \lim_{k\to\infty} \frac{1}{k} \log |(R_{kJ})_{ii} \cdots (R_J)_{ii}| ,$$

which in the limit converges to the real part of the ith eigenvalue of B. In practice, one cannot compute $Y(\omega)$ exactly, and this must be replaced by an approximation $W(\omega)$. By periodicity of the system, and the assumption on the stepsize sequence, we obtain as approximate Lyapunov exponents $1/\omega$ times the real parts of the eigenvalues of a logarithm of $W(\omega)$, as claimed.

General matrices. In the case of a general coefficient matrix $A(t)$, the situation is not as well established as in the constant and periodic coefficient cases. We present two types of results. The first is an idealized case assuming no error propagation during numerical integration; this idealized setting is insightful in order to understand the relative merits of discrete and continuous QR techniques. The second type of result relies upon a more realistic interpretation of what the discrete QR algorithm does, for which we can give estimates of the error (assuming that the original system has point spectrum).

Idealized error analysis. In this case we account for the local error on a given step but assume that local errors do not accumulate. More precisely, we assume that we restart with exact values at each new step.

For the discrete QR method, consider the problem

$$\begin{cases} \dot{Y}^i = AY^i, \quad t \in [t_i, t_{i+1}], \quad i = 0, 1, \ldots, \\ Y^i(t_i) = Q(t_i), \end{cases} \tag{4.5}$$

where $Q(t_i)$ is the Q factor in the QR factorization of the exact $Z_{i-1}(t_i)$ defined in the theoretical description of the discrete QR algorithm in (3.1)–(3.4).

THEOREM 4.4. *Given $t_i = t_0 + ih$ for $i = 1, 2, \ldots,$ suppose that $Y^i(t)$ is the fundamental solution matrix of problem* (4.5) *and suppose that $Y_i = Y^{i-1}(t_i) + W_i$ is* *the computed approximation to* $Y^{i-1}(t_i)$ *with* $||W_i|| < \delta$*, where* δ *is a bound on the local error. Then, for* δ *sufficiently small, the computed Lyapunov exponent* $\hat{\lambda}_j$ *using the discrete QR method with* (4.5) *satisfies*

$$|\hat{\lambda}_j - \lambda_j| < C\delta\,,$$

where to first order the constant C *is shown in the proof below.*

Proof. Let $Y^{i-1}(t_i) = Q(t_i)R^{i-1}(t_i)$ denote the unique QR factorization of $Y^{i-1}(t_i)$. By [St, p. 516] we have

$$\|R^{i-1}(t_i) - R_i\| \le \|W_i\| + b(\|Y^{i-1}(t_i)\| + \|W_i\|)$$

with

$$b \le \frac{3||Y^{i-1}(t_i)^{-1}||\,||W_i||}{1 - 2||Y^{i-1}(t_i)^{-1}||\,||W_i||}.$$

Therefore, for appropriately defined C_1, for any i

$$\|R^{i-1}(t_i) - R_i\| < \delta\left(1 + \frac{3[\kappa(Y^{i-1}(t_i)) + ||Y^{i-1}(t_i)^{-1}||\delta]}{1 - 2||Y^{i-1}(t_i)^{-1}||\delta}\right) \le \delta C_1\,,$$

where $\kappa(Y^{i-1}(t_i))$ denotes the condition number of $Y^{i-1}(t_i)$.

If $Y^{i-1}(t_i)$ denotes the solution of (4.5), then from (3.4)

$$\lambda_j = \lim_{k\to\infty}\frac{1}{t_k}\sum_{i=1}^{k}\log(R_{jj}^{i-1}(t_i))\,,$$

whereas the computed exponents satisfy

$$\hat{\lambda}_j = \lim_{k\to\infty}\frac{1}{t_k}\sum_{i=1}^{k}\log(R_{jj}^{i-1}(t_i) + C^{(i)}\delta),$$

where $|C^{(i)}| \le C_1$, $i = 1, \ldots.$ Thus, to first order we have

$$|\lambda_j - \hat{\lambda}_j| \approx \frac{C_1\delta}{h}\cdot\lim_{k\to\infty}\frac{1}{k}\sum_{i=1}^{k}\frac{1}{R_{jj}^{i-1}(t_i)}\,. \qquad \square$$

Remark 4.5. Note that $\lim_{k\to\infty}\frac{1}{k}\sum_{i=1}^{k}\frac{1}{R_{jj}^{i-1}(t_i)} \le \frac{1}{R_{jj}^{\min}}$, where $R_{jj}^{\min}$ denotes the minimum value of $R_{jj}^{i-1}(t_i)$, so difficulties can be expected for negative Lyapunov exponents of large magnitude, even if the approximate fundamental solution matrix is accurate. This explains some observations in the literature regarding the difficulty of computing negative Lyapunov exponents with the discrete QR method.

For the continuous QR method we discretize in two steps: (i) compute the Q factor of $Y(t)$ by integrating the matrix system (3.8) and (ii) approximate the Lyapunov exponent using (3.11). Computationally, these two steps are replaced as follows.

(a) To integrate (3.8), we use unitary schemes (see [DRV]), so that the computed approximation remains orthogonal. We assume that the scheme is of order p, with local truncation error $\mathcal{O}(h^{p+1})$, that the stepsize h is constant, and that Q_k is an accurate approximation to $Q(t_k)$, i.e., $\|Q(t_k) - Q_k\| \le \delta$, with δ small. This latter assumption is more unrealistic the longer the interval of integration.

(b) After truncating the time interval at some finite value T, we approximate the integral in (4.1) by the composite trapezoidal rule where the exact values of $\tilde{A}_{ii}(t_k) = (Q^T(t_k)A(t_k)Q(t_k))_{ii}$ are replaced by the approximations $\tilde{A}^c_{ii}(t_k) = (Q_k^T A(t_k)Q_k)_{ii}$.

From the assumptions above, $|\tilde{A}_{ii}(t_k) - \tilde{A}^c_{ii}(t_k)| = O(\delta)$. Let $\lambda_i^c(t_J)$ be the computed approximation obtained using the composite trapezoidal rule, so that

$$\begin{aligned}\lambda_i^c(t_J) &= \frac{1}{t_J}\frac{h}{2}\sum_{j=1}^{J}[(Q_{j-1}^T A(t_{j-1})Q_{j-1})_{ii} + (Q_j^T A(t_j)Q_j)_{ii}] \\ &= \frac{1}{t_J}\frac{h}{2}\sum_{j=1}^{J}[\tilde{A}_{ii}(t_{j-1}) + \tilde{A}_{ii}(t_j)]\,.\end{aligned}$$

Assuming that $A(t) \in C^k$, $k \geq 2$, if $|\tilde{A}''_{ii}|$ denotes the maximum of $|\tilde{A}''_{ii}(t)|$ over $[t_{j-1}, t_j)$, $j = 1, \ldots, J$, we obtain

$$\begin{aligned}|\lambda_i(t_J) - \lambda_i^c(t_J)| &= \frac{1}{t_J}\left|\sum_{j=1}^{J}\left(-\frac{h^3}{12}\right)\tilde{A}''_{ii}(\xi_j)\right| + \mathcal{O}(\delta) \\ &\leq \frac{h^2}{12}|\tilde{A}''_{ii}| + \mathcal{O}(\delta)\,,\end{aligned}$$

which implies

$$|\lambda_i(T) - \lambda_i^c(T)| = O(\delta) + O(h^2)\,.$$

Notice that there is no indication of a deterioration for negative exponents which there is in the discrete QR case. Another advantage of the continuous QR method over its discrete counterpart is that we do not need to integrate the original system, which is often dichotomic. We instead integrate the Lyapunov equation (3.8), which is neutrally stable since the growth behavior of the fundamental solution is in the R factor, which we never explicitly integrate (only a quadrature is needed, and only for the diagonal entries).

General error analysis. Here we use the main perturbation result of section 2 to find bounds on the error in the Lyapunov exponents obtained using the discrete QR method (for systems with point spectrum).

Let a segmentation $0 = t_0 < t_1 < \cdots < t_k < t_{k+1} < \cdots$ with $h_k := t_{k+1} - t_k$ be given. Let $\Phi(t, t_k)$ be the transition matrices of the problems

$$\dot{\Phi}(t, t_k) = A(t)\Phi(t, t_k)\,,\ \ \Phi(t_k, t_k) = I\,, \tag{4.6}$$

and define the matrices B_k by $h_k B_k = \log \Phi(t_k, t_{k+1})$, $k = 1, 2, \ldots$, where we are taking the principal logarithm. The original problem $\dot{Y} = A(t)Y$, $Y(0) = I$, can thus be rewritten as the piecewise constant problem

$$\dot{Y} = B(t)Y\,,\ \ Y(0) = I\,; \quad B(t) = B_k,\ \ t_k \leq t < t_{k+1}\,. \tag{4.7}$$

In exact arithmetic the discrete QR method can be viewed as successively solving the piecewise constant problems

$$\dot{Z}_k(t) = B_k Z_k(t)\,, \qquad Z_k(t_k) = Q_k\,, \tag{4.8}$$

for $t \in [t_k, t_{k+1})$, where $Q_k R_k = Z_{k-1}(t_k^-)$. Of course, in general the transition matrices, and hence the matrices B_k, are not known explicitly.

A numerical implementation of the discrete QR method can also be viewed as solving exactly piecewise constant problems

$$\dot{W}_k(t) = C_k W_k(t)\,, \qquad W_k(t_k) = H_k\,, \tag{4.9}$$

for $t \in [t_k, t_{k+1})$, where $H_k U_k$ is the unique QR factorization of $W_{k-1}(t_k^-)$ and $h_k C_k$ is the principal logarithm of the computed approximation to the transition matrix. In other words, one is using the discrete QR method on piecewise constant problems

$$\dot{Y} = C(t)Y\,,\ \ Y(0) = I\,; \quad C(t) = C_k,\ \ t_k \le t < t_{k+1}\,, k = 0, 1, \ldots. \tag{4.10}$$

We now use Theorem 2.3 (see also Remark 2.6) to obtain bounds on the distance from the Lyapunov exponents of (4.10) to the exact λ_i's for (4.7).

If Y_{k+1} is the exact solution of (4.10) at t_{k+1}^-, then

$$Y_{k+1} = e^{h_k C_k} Y_k = W_k(t_{k+1}^-) H_k^T Y_k = \cdots = H_{k+1} U_{k+1} U_k \cdots U_1\,,$$

and since the matrices H_k are orthogonal, the Lyapunov exponents of (4.10) are the same as those of the (discrete) triangular system

$$\Psi_{k+1} = U_k \Psi_k\,, \quad \Psi_0 = I\,.$$

Moreover, given any $\eta > 0$, there exists a time $T \equiv T(\eta) > 0$ such that for any $t_k > T$,

$$-\eta + \liminf_{j\to\infty} \frac{1}{t_j} \log(U_j \cdots U_1)_{ii} \le \frac{1}{t_k} \log(U_k \cdots U_1)_{ii} \le \limsup_{j\to\infty} \frac{1}{t_j} \log(U_j \cdots U_1)_{ii} + \eta.$$

From Lemma 1.5, the above lim inf and lim sup lie in a spectral interval of (4.10), so in the limit we actually compute an approximation contained in a spectral interval. If (4.10) is a regular system, then these limits coincide, which raises the interesting question of how to guarantee that a chosen numerical method for a regular system (4.7) produces a regular system (4.10).

Precise error bounds, i.e., precise widths of the spectral intervals for (4.10) as related to the point spectrum of (4.7), depend upon the particular formula used to approximate (4.6). To illustrate, we consider the simplest case of Euler's method to integrate (4.6). For different approximations, an appropriate modification of this argument is generally straightforward.

We have

$$h_k C_k = \log(I + h_k A(t_k))\,,$$

from which the error can be quantified as follows: on $[t_k, t_{k+1})$, let $A(t) = A(t_k) + h_k \dot{A}(\xi_k)$, where $\dot{A}(\xi_k)$ is a matrix whose coefficients are the derivatives of those of $A(t)$, evaluated at (different) points ξ_{ij}. Thus, on $[t_k, t_{k+1})$

$$\|C_k - A(t)\| \le (h_k \|\dot{A}(\xi_k)\| + \|C_k - A(t_k)\|)\,. \tag{4.11}$$

For Euler's method, the bound on the perturbation in the coefficient matrix depends on two factors: (i) the first derivative of $A(t)$ and (ii) the first-order approximation to the matrix exponential. If we could compute matrix exponentials exactly, then the first factor shows that the perturbation is small in norm when $A(t)$ is slowly varying.

In practice, one can proceed adaptively by monitoring the first derivative of $A(t)$, thereby guaranteeing that $h_k\dot{A}(\xi_k)$ is always small in norm.

The term $\|C_k - A(t_k)\|$ in (4.11) can be bounded as follows. If

$$c_1 := \|I + h_k A(t_k) - e^{h_k A(t_k)}\|\,,$$

then a crude bound on c_1 is given by

$$c_1 \le \frac{1}{2} h_k^2 \|A(t_k)\|^2 e^{h_k\|A(t_k)\|}\,.$$

Letting

$$c_2 = \|\log'(e^{h_k A(t_k)})\|\,,$$

where $\log'(\cdot)$ is the Fréchet derivative of the log matrix function, then using [DMP, Remark 2.2(iii), p. 573] we have

$$\|h_k(C_k - A(t_k))\| \le c_2 c_1 + \mathcal{O}(c_1^2)\,.$$

If h_k is sufficiently small that $c_3 := \|I - e^{h_k A(t_k)}\| < 1$, then $c_2 \le \frac{1}{1-c_3}$ from [DMP, Equation (3.2)]. Therefore, for small h_k, we have

$$\|C_k - A(t_k)\| \le \frac{h_k}{2} \frac{\|A(t_k)\|^2 e^{h_k\|A(t_k)\|}}{1 - c_3}$$

to first order in h_k. If $c_3 \ge 1$, an a priori bound on c_2 can still be obtained but is somewhat more involved [DMP, Equation (3.14)]. Using this in (4.11) we have a full first-order control on the perturbation in the coefficient matrix. Thus, Theorem 2.3 guarantees that as the stepsize goes to zero, the approximate Lyapunov exponents converge to the exact ones.

5. Implementation. In this section we describe our implementations of the discrete and continuous QR methods and present an algorithm for approximating the dichotomy constants used to bound the error in the truncated time exponents. Practically, a nontrivial task is determining a suitable truncation time T over which the solution behavior is revealed, but we simply assume that this has been achieved.

Approximation of dichotomy constants. An interesting side benefit of computing the Lyapunov exponents is that the dichotomy constants, i.e., the values in (4.2), can be approximated at little extra cost. The dichotomy constants are essential, via Theorem 2.3 and (4.4), to obtain quantitative error bounds for the approximations of the Lyapunov exponents. Since we are considering error bounds for individual Lyapunov exponents, it suffices to compute the weak dichotomy constants in (4.4) for each of them. The basic approach is introduced in [CVV2].

Let $\hat{\lambda}$ be the approximation to the Lyapunov exponent λ_i, for which we are computing the dichotomy constants. Below, let $m = 0$ for $\hat{\lambda} < 0$ and $m = 1$ for $\hat{\lambda} > 0$; $a(t) := \tilde{A}_{ii}(t)$; $T := Nh > 0$ for some N and for a fixed stepsize h; and

(5.1) $$M_j := \sup_{\tau - t = jh} e^{(-1)^m I(\tau,t)}\,, \quad 1 \le j \le N\,,$$

where $I(t,\tau)$ is the computed approximation of $\int_t^\tau a(s)ds$. Set $L := M_N e^{-(-1)^m \hat{\lambda} N h}$ and let

(5.2) $$\epsilon := \begin{cases} (-1)^m \frac{\log(M_N)}{hN} - \hat{\lambda}, & \text{if } L \ne 1; \\ 0, & \text{otherwise,} \end{cases} \qquad \text{and} \qquad K := \sup_{1\le j\le N} M_j e^{-(-1)^m(\hat{\lambda}+\epsilon)jh},$$

so for arbitrary $t \leq \tau$ with $\tau - t$ a multiple of h, we have

$$
\begin{aligned}
e^{(-1)^m I(t,\tau)} &= e^{(-1)^m I(t,t+Nh)} \cdots e^{(-1)^m I(t+(k-1)Nh,t+kNh)} e^{(-1)^m I(t+kNh,\tau)} \\
&\leq (M_N)^k e^{(-1)^m I(t+kNh,\tau)} \leq K e^{(-1)^m (\hat{\lambda}+\epsilon)(\tau-t)} .
\end{aligned}
\tag{5.3}
$$

In practice we have found that approximating the dichotomy constants in conjunction with the Lyapunov exponents works well.

Remark 5.1.

(i) The case of a zero Lyapunov exponent may be treated as a stable or an unstable case, i.e., $m = 0$ or 1.

(ii) During numerical integration, several values of N may be considered simultaneously, and then one of them chosen to minimize a given function of K and ϵ subject to (5.3), for instance $\frac{\log(K)}{t} + \epsilon$.

Implementation details: Discrete *QR*. Our implementation of the discrete QR method follows the outline given in (3.1)–(3.4). We integrate the matrix equation (3.2) using either the second-order Runge–Kutta method (Heun's method), the classical fourth-order Runge–Kutta method, or the fourth-order variable step solver RKF45. These are denoted by "Disc RK2," "Disc RK4," and "Disc RKF45," respectively. The QR decomposition (3.3) is done by the modified Gram–Schmidt method (which is stable [GvL]) and, for simplicity, this decomposition is performed for each integration step. We used this Gram–Schmidt procedure because the R factor must be kept "smooth," say by minimizing the variation in the R_{ii}, and the standard implementation of the Householder factorization is not suitable for this (it attempts to minimize roundoff errors and does not generally deliver a slowly changing R). In the nonlinear case, the original problem (2.9) and the variational equation (3.2) are integrated simultaneously with the same numerical integrator.

Implementation details: Continuous *QR*. Our implementation of the continuous QR method follows the approach outlined in (3.5)–(3.11). We integrate the nonlinear skew system (3.8) using either projected or automatic unitary integrators [DRV] in order to preserve orthogonality of the solution. A projected integrator consists of a standard integrator combined with a modified Gram–Schmidt process. We use Heun's method, classical fourth-order Runge–Kutta and RKF45 as the projected integrators, and denote them by "Cont PRK2," "Cont PRK4," and "Cont PRKF45." We use the second-order and fourth-order Gauss Runge–Kutta methods as the automatic unitary integrators and denote them by "Cont GRK2" and "Cont GRK4." For the nonlinear case, we use only the projected unitary integrators because implementation of automatic unitary integrators is less straightforward. The nonlinear and linearized problems are integrated simultaneously, and then the integral in (3.11) is approximated using the composite trapezoidal rule.

6. Numerical examples. In this section, we present numerical results for the continuous and discrete QR methods. We display at least five digits for the computed Lyapunov exponents. The CPU time is recorded in seconds, and all computations have been done in double precision on a Sparc Station 1 with a machine epsilon of approximately $1.E - 16$.

Example 6.1. We construct a linear problem with coefficient matrix $A(t) = Q(t)\tilde{A}(t)Q^T(t) + \dot{Q}(t)Q^T(t)$, where $\tilde{A}(t) = \text{diag}(\lambda_1, \cos(t), -\frac{1}{2\sqrt{t+1}}, \lambda_4)$. Here, $\lambda_1 = 1$,

Table 1
Example 6.1: *Fixed step methods.*

Method	T	Δt	λ_1	λ_2	λ_3	λ_4	CPU
Exact	-	-	1	0	0	−10	-
Cont GRK2	100	0.1	.99981	−.00655	−.08892	−9.99990	268.
Cont GRK4	100	0.1	.999999999	−.00505	−.09051	−9.99999999	323.
Cont PRK2	100	0.1	.99966	−.00776	−.08800	−9.99946	42.4
Cont PRK4	100	0.1	.999999	−.00505	−.09050	−9.99999	56.8
Disc RK2	100	0.1	1.00977	−.00420	−.08965	−7.18290	9.63
Disc RK4	100	0.1	.99995	−.00414	−.09045	−9.83400	17.7
Cont PRK2	100	0.01	.9999999	−.00506	−.09050	−9.9999999	414
Cont PRK4	100	0.01	1	−.00506	−.09050	−10.0000000000	559.
Disc RK2	100	0.01	1.00008	−.00506	−.09051	−9.98317	97.0
Disc RK4	100	0.01	.99999999	−.00506	−.09050	−9.99999	177.
Cont PRK2	1000	0.1	.99965	−.01035	−.01966	−9.99945	418.
Cont PRK4	1000	0.1	.999999	.00082	−.03065	−9.99999	562.
Disc RK2	1000	0.1	1.00974	−.00131	−.02680	−7.18233	99.5
Disc RK4	1000	0.1	.99995	.00086	−.03064	−9.83388	177.

Table 2
Example 6.1: *Variable step methods.*

Method	T	Tol	λ_1	λ_2	λ_3	λ_4	CPU
Exact	-	-	1	0	0	−10	-
Cont PRKF45	100	1E−6	.999999999999	−.00541	−.09052	−9.99999999999	144.
Disc RKF45	100	1E−6	.99975	−.00544	−.09099	−9.97581	1220.
Cont PRKF45	1000	1E−6	.999999999999	.00083	−.03064	−9.99999999999	1420.

Table 3
Example 6.1: *Dich* const $(PRK4, h = 0.1, T = 1000, J = 63)$.

i	ϵ_i	K_i
1	1.E−8	1 + 1.E−6
2	3.5E−3	7.32
3	1.5E−2	1 + 1.E−3
4	1.E−8	1 + 1.E−6

$\lambda_4 = -10$, and

$$Q(t) = \mathrm{diag}(1, Q_\beta(t), 1) \cdot \mathrm{diag}(Q_\alpha(t), Q_\alpha(t)),$$

$$\text{where} \qquad Q_\gamma(t) = \begin{pmatrix} \cos(\gamma t) & \sin(\gamma t) \\ -\sin(\gamma t) & \cos(\gamma t) \end{pmatrix},$$

and $\alpha = 1, \beta = \sqrt{2}$. By construction, $\lambda_2 = 0$ and $\lambda_3 = 0$. Numerical results are summarized in Tables 1 and 2. The accuracy of λ_3 is more sensitive to the length of the integration interval than are the other Lyapunov exponents. The continuous QR method performs well, and the global error is apparently determined by the time truncation factor. The discrete QR method yields poor accuracy for the negative Lyapunov exponent λ_4, as expected. Note the large CPU time and error when a variable stepsize integrator is used with the discrete QR method. The large CPU time can be attributed to the fact that integration for the fundamental matrix solution forces a small step as compared with integration of the neutrally stable Lyapunov equation for the continuous QR method. Table 3 gives the computed values of dichotomy constants with $K_i = \max(L_i, M_i)$ and $\epsilon_i = \max(\xi_i, \rho_i)$ (see (4.4)).

TABLE 4
Example 6.3: *Fixed step methods.*

Method	T	Δt	λ_1	λ_2	CPU
Exact	-	-	0		-
Cont PRK2	100	0.1	.00414	-1.05452	2.40
Cont PRK4	100	0.1	.00099	-1.05729	3.83
Disc RK2	100	0.1	.00249	-1.05020	.79
Disc RK4	100	0.1	.00192	-1.05625	1.12
Cont PRK2	100	0.1	.00104	-1.05730	20.8
Cont PRK4	100	0.1	.00101	-1.05732	33.6
Disc RK2	100	0.01	.00102	-1.05726	7.40
Disc RK4	100	0.01	.00101	-1.05732	11.2
Cont PRK2	100	0.01	.00245	-1.05737	20.8
Cont PRK4	100	0.01	.00026	-1.05866	34.0
Disc RK2	1000	0.1	$-4.5028\text{E}{-5}$	-1.05407	7.35
Disc RK4	1000	0.1	$2.62499\text{E}{-4}$	-1.05869	11.1

TABLE 5
Example 6.3: *Variable step methods.*

Method	T	Tol	λ_1	λ_2	CPU
Exact	-	-	0		-
Cont PRKF45	100	1E−6	$2.30895\text{E}{-4}$	-1.05880	4.23
Disc RKF45	100	1E−6	$1.58738\text{E}{-4}$	-1.05640	17.8
Cont PRKF45	1000	1E−6	$-5.08003\text{E}{-4}$	-1.06020	42.6
Disc RKF45	1000	1E−6	$-5.87591\text{E}{-4}$	-1.05777	178.

The computed dichotomy constants are generally accurate approximations to the exact dichotomy constants $\epsilon_i = 0$ for $i = 1, \ldots, 4$ and $K_1 = 1, K_2 = e^2, K_3 = 1$, $K_4 = 1$, although their accuracy depends on the accuracy of the corresponding approximate exponents. With these values of K_i (for $\epsilon_i = 0$ and exact λ_i), the values corresponding to any other ϵ_i and λ_i may be determined using (4.4) and setting $\epsilon_i = \max\{\rho_i, \xi_i\}$.

Example 6.2. Lyapunov [Ly] presented the nonregular system with coefficient matrix

$$A(t) = \begin{pmatrix} \cos(\log(t+1)) & \sin(\log(t+1)) \\ \sin(\log(t+1)) & \cos(\log(t+1)) \end{pmatrix}.$$

Since nonregular systems do not satisfy (1.16), we cannot expect the QR-based numerical methods to properly compute the Lyapunov exponents. The QR-based methods do approximate the time average of the trace of $A(t)$ for any time T. For this example, the sum of the Lyapunov exponents is $+2$ while

$$\limsup_{t\to\infty} \frac{1}{t}\int_0^t \text{trace}(A(s))ds = \sqrt{2} \quad \text{and} \quad \liminf_{t\to\infty} \frac{1}{t}\int_0^t \text{trace}(A(s))ds = -\sqrt{2},$$

so the computed sum of the Lyapunov exponents oscillates between $-\sqrt{2}$ and $\sqrt{2}$. Our computations for both methods also exhibit this behavior.

Example 6.3. Consider the unforced van der Pol equation $\ddot{u} - k(1-u^2)\dot{u} + u = 0$, $\quad k > 0$. For this problem, every trajectory (except $u = 0$) approaches the attracting limit cycle, so one Lyapunov exponent is zero and the other negative. In Tables 4, 5, and 6 we present some typical results for $k = 1$ and $(u(0), \dot{u}(0)) = (0, 2.1)$.

TABLE 6
Example 6.3: *Dich* const $(PRK4, h = 0.1, T = 1000, J = 1000)$.

i	ϵ_i	K_i
1	.001	1.84
2	.015	5.18

TABLE 7
Example 6.4: *Variable step methods* $(T = 1000)$.

Method	ρ	Tol	λ_1	λ_2	λ_3	CPU
[SN]	40.0	-	1.37	0.0	−22.37	-
Cont PRKF45	40.0	1.E−6	1.36006	.00570	−22.36576	1270.
Disc RKF45	40.0	1.E−6	1.33961	−.01055	−22.30930	6090.
[WSSV]	45.92	-	1.497	0.0	−22.458	-
Cont PRKF45	45.92	1.E−6	1.48804	.00452	−22.52772	1330.
Disc RKF45	45.92	1.E−6	1.47829	−.01086	−22.44645	6030.

Example 6.4. Next, consider the Lorenz equation [Lo]

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} \sigma(y-x) \\ \rho x - xz - y \\ xy - \beta z \end{pmatrix}.$$

Many different algorithms have been used trying to approximate its Lyapunov exponents, but all results ought to be looked at with some caution, since it is not known whether or not the linearized system is regular. Nonetheless, we test our algorithms against previous results. We use the parameter values $\sigma = 16$ and $\beta = 4.0$ and vary ρ. The initial condition is $(x_0, y_0, z_0) = (0, 1, 0)$. We compare with the discrete QR methods of [SN, WSSV] in Table 7.

Note that $\limsup_{t\to\infty} \frac{1}{t}\int_0^t \text{trace}(A(s))ds = -\sigma - \beta - 1 = -21$. The computed Lyapunov exponents satisfy $\sum_1^3 \lambda_i \approx -21$, so their sum attains its minimum possible value.

7. Conclusions. Despite the large body of literature on the computation of Lyapunov exponents, there has been little analysis of the computational error. The need for such analysis is demonstrated by the fact that the computation of Lyapunov exponents is a delicate task. In this work we have considered regular linear systems and concentrated on QR-based methods, which in principle are suitable for such systems. Although regularity has been recognized as a natural condition to have for a long time (see [Ly]), it is not a sufficiently strong condition to guarantee stability of the Lyapunov exponents with respect to perturbations. Our stability result, expressed as the perturbation Theorem 2.3, makes use of a point spectrum assumption, and such assumption appears to us to be essential to make any progress. With this stability result, a backward error analysis can be used to guarantee that the numerical results are reliable.

There are at least two basic difficulties in approximating Lyapunov exponents. The first is intrinsic: do the Lyapunov exponents exist as limits, and if so, how does one find a suitable finite time to truncate the process? The second difficulty is numerical, and it boils down to understanding the effect that the numerical method itself has on the approximation. One should also be aware that the perturbation due to the numerical method might in principle produce nonregular systems, and then there is no longer any guarantee that the QR techniques give accurate approximations to the exponents. As a consequence, it is extremely difficult to say something meaningful about the approximations in the case of a general variable coefficient system without resorting to strong assumptions.

In this paper, we have fully analyzed constant and periodic coefficient problems. For general variable coefficient problems, we have assumed that the original system has point spectrum and then used the perturbation result to obtain some estimates. Also, we have provided some general insight into the relative merits of the discrete and continuous QR methods. Our argument suggests that the discrete QR method performs well for positive Lyapunov exponents but has difficulties for negative (large) Lyapunov exponents. The continuous QR method is shown to be robust when implemented using unitary integrators, which ensure orthogonality of the approximations to $Q(t)$. In both cases, the error in the truncated approximations is given in terms of weak dichotomy constants. These constants also arise in the bounds in the basic perturbation theorem. We give an algorithm for estimating these constants and find it to give accurate estimates of the error.

Our focus on linear problems is partly justified by Theorem 2.3, which shows that the potential change in the Lyapunov exponents due to a perturbation in the linear system is a function of the gap between them. The analysis is thus applicable to nonlinear systems for which some type of global error bounds on the computed solutions are available. Finally, we have only considered the QR methods for finding all Lyapunov exponents; the case where only the first few exponents are computed is treated in [DV].

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