Computing Lyapunov spectra with continuous
Gram–Schmidt orthonormalization

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Abstract. We present a straightforward and reliable continuous method for computing the full
or partial Lyapunov spectrum associated with a dynamical system specified by a set of dif-
terential equations. We do this by introducing a stability parameter $\beta > 0$ and augmenting
the dynamical system with an orthonormal $k$-dimensional frame and a Lyapunov vector such
that the frame is continuously Gram–Schmidt orthonormalized and at most linear growth of the
dynamical variables is involved. We prove that the method is strongly stable when $\beta > -\lambda_k$
where $\lambda_k$ is the $k$th Lyapunov exponent in descending order and we show through examples
how the method is implemented. It extends many previous results.

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1. Introduction

One of the most striking coordinate-independent characterizations of a compact dynamical
system of dimension $d$ is its Lyapunov spectrum. It associates a set of $d$ real values to
each orbit of the system which describes exponential instabilities of infinitesimal deviations
from the orbit. Furthermore, for an ergodic dynamical system this set almost surely (in the
measure theoretical sense) does not depend on which orbit you consider. More precisely,
given a smooth vector field $v$ in $\mathbb{R}^d$ we look at the $d$-dimensional evolution equation
$\dot{x} = v(x)$. For an initial condition $x(0) = x_0$ we integrate this to obtain a corresponding
orbit $x(t) = \phi_t(x_0)$. The stability of such an orbit can then be examined by looking at the
evolution of a nearby orbit $x(t) + u(t)$ and linearizing the equations of motion in $u$:

$$\dot{u}(t) = \frac{\partial v}{\partial x}(x(t))u(t) \equiv J(x(t))u(t).$$

(1)

Integrating this along the orbit we obtain the tangent map $u(t) = M_{x_0}(t)u_0$ in which the
transition matrix $M_{x_0}(t) = \partial \phi^t(x_0)/\partial x_0$ is a $d \times d$ matrix-valued function of time. The
exponential instabilities of a trajectory are now reflected in its eigenvalue spectrum or
rather the spectrum of the symmetric product

$$M^T_{x_0}(t)M_{x_0}(t).$$

(2)

The spectrum of this matrix is real and positive and we order it as follows:

$$\mu_1^T(t) \geq \mu_2^T(t) \geq \cdots \geq \mu_d^T(t) \geq 0.$$

(3)

Although the values $a$ priori depend on the initial point $x_0$ chosen, one has the following.
**Theorem (Oseledec [1, 2]).** If \( \mu \) is an ergodic probability measure for the dynamical system then for \( \mu \) almost every \( x_0 \)

\[
\lambda_k = \lim_{t \to \infty} \frac{1}{t} \log \mu_k(t) \tag{4}
\]

exists and is independent of the initial point.

In other words taking an arbitrary (with respect to an ergodic measure) initial point and calculating the above limits, with probability 1 you will obtain its unique Lyapunov spectrum, \( \{\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d\} \). From its definition it is not difficult to show that the spectrum is independent of the choice of coordinate system and thus being intrinsic invariants, their existence and the above theorem is of fundamental importance in the theory of dynamical systems. Determining the spectrum (or part of it) has in fact grown into a small industry in modern nonlinear physics.

From the practical or numerical point of view the above description is insufficient as the matrix \( M(t)^T M(t) \) becomes singular rather fast since its eigenvalues separate exponentially in time (assuming that not all Lyapunov exponents are equal) thus making it difficult to measure the spectrum. Now, several methods have been developed in order to overcome this problem. Frøyland [3] used a systematic but rather complicated evolution equation for comatrices which still has exponential growth, although in a controllable way. Meyer [4] used symplectic transformations to derive the spectrum for Hamiltonian systems also involving exponential growth. Habib and Ryne [5] used a particular representation of the Lie algebra so(2) to obtain an evolution equation for a Hamiltonian system in two dimensions (which appears to work also in four dimensions) which only involves linear growth but which is rather complicated and depends on the Hamiltonian form of the dynamical system. Bennetin et al [6] (for one exponent) and later Shimada and Nagashima [7] (for the whole spectrum) suggested renormalizing (Gram–Schmidt) at regular intervals of time a set of stability vectors picking up the exponents during the renormalization procedure. This method works well and is often used in practice when calculating the spectrum (an example is Gong [8] in which the author considered the Lyapunov spectrum for a compact lattice Yang–Mills SU(2) theory). Goldhirsch et al [9] presented a continuous version of this procedure (cf below) and they developed a set of differential equations for the eigenvalues and eigenvectors of the stability matrix \( M_{so}(t) \) itself, a method, however, unsuited in the presence of a degeneracy of eigenvalues.

Here we shall present a unified approach in which we augment the dynamical system with an orthonormal frame and a Lyapunov vector such that the augmented system is dynamically strongly stable and involves at most linear growth such that the Lyapunov spectrum is obtained almost surely (in the measure sense of choosing an arbitrary initial point and frame). The method is not constrained to Hamiltonian systems, it applies to any finite-dimensional dynamical system and is straightforward to implement on a computer.

2. Continuous Gram–Schmidt orthonormalization

We define a time-dependent orthonormal \( k \)-frame to be a set of \( k(k \leq d) \) orthonormal vectors:

\[
\mathcal{E}(t) = \{e_1(t), \ldots, e_k(t)\} \quad (e_i, e_j) = \delta_{ij} \quad 1 \leq i, j \leq k \tag{5}
\]

where \((\cdot, \cdot)\) is the usual Euclidian product in \( \mathbb{R}^d \). Using this frame we let \( J_{lm} = (e_j, J e_m) \) denote the matrix elements of the Jacobian matrix \( J \) and we note that these matrix elements depend on time both through the Jacobian and the frame. We introduce a stability parameter.
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Let $\beta > 0$ and define the (symmetric) stabilized matrix elements $L_{mm} = J_{mm} + \beta((e_m, e_m) - 1)$ and $L_{lm} = J_{lm} + J_{ml} + 2\beta(e_l, e_m)$. Finally, let $\Lambda = \{\Lambda_1(t), \ldots, \Lambda_k(t)\}$ be a $k$-dimensional real vector.

The augmented dynamical system is now given by the following set of differential equations (of which the first two are vector equations)

$$
\dot{x} = v(x) \\
\dot{e}_m = J_{em} - \sum_{l \geq m} e_l L_{lm} \\
\dot{\Lambda}_m = J_{mm} \\
\text{for } m = 1, \ldots, k.
$$

(6)

For the dynamical evolution of these equations we have the following.

**Theorem.** Let $x_0$ be an initial point for which the associated Lyapunov spectrum (cf equation (4)) $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$ exists. Set $\Lambda(t = 0) = 0$. Choosing the stability parameter $\beta > -\lambda_k$ then for almost any (i.e. with probability 1 when choosing randomly) initial frame $E(t = 0)$ the time evolution of the dynamical system (6) yields:

$$
\lim_{t \to \infty} \frac{1}{t} \Lambda_m(t) = \lambda_m \\
\text{for } m = 1, \ldots, k.
$$

(7)

Thus, by following a trajectory of the augmented system we obtain almost surely the $k$ first elements in the Lyapunov spectrum for the given orbit. The somewhat peculiar condition on the stability parameter is satisfied, for example by setting $\beta > \max_{|e| = 1} (-e, Je)$ where the maximum is over all unit-length vectors $e$ and over the relevant region of phase space. Dynamically such a choice corresponds to finding the strongest local contraction.

The proof of this theorem is given in the appendix where in particular, it is shown that the dynamics preserve the orthonormality of the frame. When the elements of $J$ are assumed to be bounded in phase space we see that the above dynamical system only involves at most linear growth of the dynamical variables (through the $\Lambda_m$’s). Given a dynamical system with an ergodic measure we see by combining the Oseledec theorem and the above that the Lyapunov spectrum is obtained almost surely by choosing an arbitrary initial point and an arbitrary initial frame.

An interesting case is when $k = d$, i.e. when we want to calculate the complete spectrum. In this case, our orthonormal frame is complete and we may expand $Je_m$ in equation (6) in terms of the basis vectors themselves. Setting $\beta = 0$ we obtain

$$
\dot{e}_m = \sum_{l > m} e_l J_{lm} - \sum_{l < m} e_l J_{ml} \equiv \sum_l e_l A_{lm}
$$

(8)

where $A_{lm}$ is antisymmetric and thus by construction a generator of orthonormal transformations (of our frame). A straightforward linear analysis shows that the resulting dynamical system is marginally stable.

3. Numerical results

In the following we apply the above method in order to calculate the Lyapunov spectrum for two standard systems; the Lorenz system and a three degrees of freedom Hamiltonian system with a quartic potential. In order to obtain good statistics on the Lyapunov exponents we determine a time over which to integrate the systems in order to obtain reasonable convergence and then make 1000 runs of each system with random initial conditions.
The Lorenz system [10] is given by:

\[
\begin{align*}
\dot{x} &= -\sigma x + \sigma y \\
\dot{y} &= r x - y - x z \\
\dot{z} &= x y - b z 
\end{align*}
\]  

(9)

with the usual choice of parameter \(\sigma = 10, r = 28\) and \(b = \frac{8}{3}\). In figure 1 we present the resulting Lyapunov exponents of a single run for the Lorenz system. The result of 1000 runs is given in table 1.

Next we apply our method to a Hamiltonian system with a quartic potential:

\[
H = \frac{p_x^2 + p_y^2 + p_z^2}{2} + \frac{x^2 y^2 + y^2 z^2 + z^2 x^2}{2} + \frac{x^4 + y^4 + z^4}{32}.
\]

(10)

The last term is added in order to have a compact phase space and avoid having to deal with problems of convergence related to near-integrable motion along the coordinate axes, but still chosen with a sufficiently small prefactor in order to not stabilize the dynamics. A single

Table 1. The average of the Lyapunov exponents of 1000 runs of the Lorenz system and their root mean square deviations (rms dev.). The sum of the exponents is \(-13.6667 = -\sigma - 1 - b\) as expected from equation (9).

| \(k\) | \(\lambda_k\) | rms dev. |
|------|---------------|----------|
| 1    | 0.9057        | 4.7 \times 10^{-3} |
| 2    | 1.4 \times 10^{-5} | 8.3 \times 10^{-4} |
| 3    | -14.5724      | 4.6 \times 10^{-3} |

Figure 1. The three (finite-time) Lyapunov exponents from a single run of the Lorenz system.
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Figure 2. The three positive (finite-time) Lyapunov exponents from a single run of (10). We present only the positive exponents since, due to the symplectic structure of the equations, the absolute value of the negative exponents are exactly equal to the positive ones.

Table 2. The average of the Lyapunov exponents of 1000 runs of the Hamiltonian system (10) and their root mean square deviations.

| k | $\lambda_k$ | rms dev. |
|---|-------------|----------|
| 1 | 0.2374      | $3.6 \times 10^{-3}$ |
| 2 | 0.1184      | $3.6 \times 10^{-3}$ |
| 3 | $3.90 \times 10^{-4}$ | $7.0 \times 10^{-5}$ |

run of the resulting six-dimensional system is presented in figure 2 and the corresponding averages of 1000 runs are given in table 2.

Looking at the results for the two systems there is one striking difference which is apparent both for the single run results shown in the figures and in the averages given in the tables. Whereas the (finite-time) exponent $\lambda_2$ for the Lorenz system, corresponding to the marginally stable direction along the flow, fluctuates around zero, the equivalent (finite-time) exponent, $\lambda_3$, for the Hamiltonian system is clearly different from zero although converging for increasing $t$. The difference can be made even more apparent when plotting $e^{\lambda t}$, as in figure 3. $e^{\lambda t}$ is the stability eigenvalue for the marginally stable direction over the entire integration. For the Lorenz system this remains constantly close to one as expected for a marginal eigenvalue. For the Hamiltonian system, however, it grows linearly. The explanation lies in the degeneracy of this eigenvalue. The Hamiltonian (10) has another marginally stable direction associated with $\text{grad } H$. In local coordinates the Jacobian for the flow will in general take on a Jordan normal form for the two marginally stable directions, i.e. we cannot expect to find a full set of eigenvectors for the Jacobian. One may consider the possibility of factoring out the marginally stable directions and not include them in the
integration, but here we just note that we know that the corresponding exponents equal zero exactly for infinite time.

To illustrate the effect of the stabilizing factor β we consider the time to reach a certain error level on the orthonormality of the basis $E$ with varying β. To be specific, we consider the error $e = \left[ \sum_{i,j=1}^K (e_i, e_j - \delta_{ij})^2 \right]^{1/2}$ and the time $T(\beta)$ it takes for this error to grow to a certain level as a function of β. Since this will depend on the initial conditions we have
taken the average of 10 runs for each of the systems. The result is presented in figure 4. We let the systems run a maximum time before deciding that the chosen error level would not be reached. For the Lorenz system this time was set at 2000 and for the Hamiltonian system at 10,000. The curves of figure 4 therefore saturate at these values. For the Lorenz system $T(\beta)$ increases drastically near $\beta = -\lambda_3$ as expected, whereas for the Hamiltonian system the picture is a little less clear with the large increase of $T(\beta)$ occurring at a slightly larger value than $\beta = -\lambda_6$. The difference is due to the relative high homogeneity of the Lorenz system versus the rather strong dependence of the local finite-time stability exponents on the phase space position in the Hamiltonian system. Based on these results we have chosen to set $\beta = 20$ for the Lorenz system and $\beta = 0.5$ for the Hamiltonian system. The point here is to set $\beta$ sufficiently high to stabilize the given system under integration, but not excessively high since this could easily lead to unnecessarily high requirements on the accuracy of the integration routine. In practice, one simply chooses a reasonable $\beta$ and then checks that orthonormality is fulfilled for a trial run of the system.

The method of calculating Lyapunov exponents of ODEs that we have presented in this paper is nothing but a continuous version of the standard Gram–Schmidt orthonormalization procedure. As mentioned above this was already proposed by Goldhirsch et al. [9, equations (5.12) and (5.26)] but without the crucial stability term. Apart from the aesthetic pleasure of formulating the whole procedure as one set of differential equations, the method will show its usefulness when calculating Lyapunov spectra where the difference between the largest and the smallest exponent is large. In such a case, using standard methods, one rapidly loses accuracy on the eigenvector associated with the lowest exponent and therefore also of the exponent itself. One would therefore have to employ the Gram–Schmidt orthonormalization quite often; the continuous orthonormalization naturally avoids this problem with the $\beta$-term replacing the stabilizing effect of the (nonlinear) Gram–Schmidt procedure. On the other hand, if one is only interested in calculating the largest exponent for a given system there is essentially no difference between standard methods and the method given here since orthonormalization is unnecessary except to avoid a possible numerical overflow. Computationally, the continuous method is somewhat heavier than standard methods. To compute $k$ exponents of a $d$-dimensional system one needs, in addition to the usual $J e_m$ operation ($O(kd^2)$), to compute $e_t J e_m$ and $e_t e_m$, both $O(k^2d)$. For a full spectrum the computation is thus a factor of 3 heavier, whereas for partial spectra it will be somewhat less.

Appendix

A.1. Proof of the theorem

We first remark that when the frame is orthonormal the stabilizing terms vanish identically. We shall show that the resulting equations correspond to a differential version of a Gram–Schmidt orthonormalization of a set of $k$ independent tangent vectors evolving in time according to equation (1).

Thus, consider a time-dependent set of vectors $\{f_1, \ldots, f_k\}$ which are linearly independent and satisfy $f'_m = J(x(t)) f_m$. We expand this set of vectors uniquely into an orthonormal set $\{e_1, \ldots, e_k\}$, i.e.

$e'_m = \sum_{l \leq m} e_l \kappa_{lm}$

where $\{\kappa_{lm}\}_{l \leq m}$ are a set of time-dependent parameters with positive diagonal elements, i.e. $\kappa_{mm} > 0$.

We shall show that the $e_m$’s and the diagonal elements $\kappa_{mm}$ satisfy the differential
equations
\[ \dot{e}_m = J e_m - e_m J_{mm} - \sum_{l<m} e_l (J_{lm} + J_{ml}) \]  
(A1)

\[ \dot{\kappa}_{mm} = J_{mm} \kappa_{mm}. \]

We prove it by induction. So assume it is true for the vectors \( \{e_1, \ldots, e_{m-1}\} \). From \( \dot{f}_m = J f_m \) we obtain:
\[ \sum_{l<m} (\dot{e}_l \kappa_{lm} + e_l \dot{\kappa}_{lm} - J e_l \kappa_{lm}) = 0. \]  
(A2)

By orthonormality \( (e_m, \dot{e}_m) = 0 \) and by the induction hypothesis \( (e_m, \dot{e}_l) = J_{ml} \) for \( l < m \) so we obtain by taking the scalar product with \( e_m \):
\[ \sum_{l<m} (J_{ml} \kappa_{lm}) + \dot{\kappa}_{mm} - \sum_{l<m} J_{ml} \kappa_{lm} = 0 \]  
(A3)

and hence that \( \dot{\kappa}_{mm} = J_{mm} \kappa_{mm} \). Again for \( l < m \) by the induction hypothesis \( \dot{e}_l - J e_l \) and hence also \( \sum_{l<m} (\dot{e}_l \kappa_{lm} + e_l \dot{\kappa}_{lm} - J e_l \kappa_{lm}) \) are in the span of \( e_1, \ldots, e_{m-1} \) (just re-arrange the terms in (A1)) and hence, we may rewrite equation (A2) as follows
\[ \dot{e}_m \kappa_{mm} + e_m J_{mm} \kappa_{mm} - J e_m \kappa_{mm} = \sum_{l<m} e_l c_l \]  
(A4)

where \( c_l \) are some (time-dependent) parameters. For \( l < m \) the scalar product \( (e_l, \dot{e}_m) \) is constant (zero) in time. Whence \( (e_l, \dot{e}_m) = -(e_m, \dot{e}_l) = -J_{ml} \) and we may take the scalar product with \( e_l \) in (A4) to obtain
\[ -(J_{ml} + J_{lm}) \kappa_{mm} = c_l. \]  
(A5)

Finally, inserting this into (A4) and dividing by \( \kappa_{mm} \) we obtain the desired equation for \( \dot{e}_m \).

From (6) and the above we obtain the relationship \( \kappa_{mm}(t) = \exp(3m(t)) \kappa_{mm}(0) \).

\section*{A.2. The Lyapunov spectrum}

Next, we will show that provided the Lyapunov spectrum exists (which we assume hereafter), the limits \( \lim_{t \to \infty} \frac{1}{t} \Lambda_m(t) \) will almost surely give the spectrum (in descending order). In order to do this we take the positive matrix \( M^T M \) from equation (2) and diagonalize it to obtain
\[ M^T M = \sum_m \mu_m^2 a_m \otimes a_m \]  
(A6)

where \( \{a_k\}_{k=1}^n \) is a set of orthonormal vectors and the \( \mu_k \)'s are as in (3). One has \( \|Mu\|^2 = \sum_k \mu_k^2 (a_k, u)^2 \) which geometrically means that the image of a sphere \( \|u\| = 1 \) will be ellipsoidal with principal axes \( \{\mu_k\} \). Now let \( 1 > r > 0 \) be a fixed constant and let \( u \) be a unit length vector. Suppose that \( |(a_1, u)| > r > 0 \) at all times. Then we have
\[ \mu_1^2 \geq \|Mu\|^2 \geq r^2 \mu_1^2 \]  
(A7)

and hence it follows that:
\[ \lim_{t \to \infty} \frac{1}{2t} \log \|Mu\|^2 - \lambda_1 = \lim_{t \to \infty} \frac{1}{t} \log \mu_1 - \lambda_1 + \frac{1}{t} (\log \|Mu\| - \log \mu_1) = 0 \]  
(A8)

since \( \lambda_1 = \lim_{t \to \infty} \frac{1}{t} \log \mu_1 \) and the expression in the parenthesis is uniformly bounded: \( \log(r) \leq \log \|Mu\| - \log \mu_1 \leq 0 \). Now, the vector \( a_1 \) actually depends on time, but since \( u \) is chosen at random we have at any given instant that \( |(a_1, u)| > r > 0 \) with a probability \( p(r) \) which tends to 1 as \( r \) tends to zero. This follows from simple geometrical
considerations on the area of the $d$-ball, compared with the part of it for which the above inequality holds. Hence, the above results holds with probability $p(r)$ and since $r > 0$ was arbitrary it follows that with probability 1 the limit of $1/t \log \|Mu\|$ will exist and be the maximal Lyapunov exponent. Inserting here $u = e_1(0)$ and $Mu = \exp(\Delta(t))e_1(t)$ we obtain the desired result.

The general case is shown by considering growth rates of exterior products. We shall only show the explicit calculations for the first two Lyapunov exponents, noting that the formulae easily generalize.

We recall that if $\{e_1, \ldots, e_d\}$ is a basis for $V$, then the formal exterior products $\{e_k \wedge e_l\}_{k<l}$ is a basis for the vector space $\wedge^2 V = V \wedge V$. One may define the scalar product:

\[
(u_1 \wedge u_2, v_1 \wedge v_2) = \det \begin{pmatrix} (u_1, v_1) & (u_1, v_2) \\ (u_2, v_1) & (u_2, v_2) \end{pmatrix}
\]

as well as the action of $\wedge^2 A = A \wedge A$:

\[
A \wedge A(u_1 \wedge u_2) = (Au_1) \wedge (Au_2).
\]

Consider now the action of the matrix $\wedge^2 (M^TM)$ as follows

\[
(\mu_1, \mu_2) \mu_1^2 \mu_2^2 a_i \wedge a_j (a_i \wedge a_j, u_1 \wedge u_2).
\]

and using (A11) we deduce the inequality:

\[
\mu_1 \mu_2 |(a_i \wedge a_j, u_1 \wedge u_2)| \leq \| \wedge^2 M(u_1 \wedge u_2) \| \leq \mu_1 \mu_2.
\]

We can then repeat the arguments from above to show that with probability 1

\[
\lim \frac{1}{t} \log \| \wedge^2 M(u_1 \wedge u_2) \| = \lambda_1 + \lambda_2
\]

and by antisymmetry of the wedge the left-hand side will, apart from a uniformly bounded contribution (which almost surely vanishes in the limit), equal

\[
\lim \frac{1}{t} \log \| f_1 \wedge f_2 \| = \lim \frac{1}{t} \log |\kappa_{11}(t)\kappa_{22}(t)| = \lim \frac{1}{t} (\Lambda_1(t) + \Lambda_2(t))
\]
A.3. Linear stability theory

The results obtained above are numerically reliable provided the frame stays orthonormal during the time evolution. In particular the variables \( \Delta_{lm} = (e_l, e_m) - \delta_{lm} \), \( 1 \leq l, m \leq k \) should all vanish. By straightforward differentiation one verifies that they satisfy the following set of differential equations:

\[
\dot{\Delta}_{pm} = -(2\beta + L_{mm} + L_{pp}) - \sum_{l<m} \Delta_{pl}L_{lm} - \sum_{l<p} \Delta_{lm}L_{lp}.
\]  

(A17)

It is clear that \( \Delta_{pm} \equiv 0 \), for all \( p \) and \( m \), is a fixed point of these equations. In order to analyse its stability we substitute \( \Delta_{pm} \rightarrow \Delta_{pm} + \delta_{pm} \) and linearize in the variables \( \delta_{pm} \) to find:

\[
\dot{\delta}_{pm} = -(2\beta + J_{mm} + J_{pp})\delta_{pm} + G(\{\delta_{pl}\}_{l<m}, \{\delta_{lm}\}_{l<p})
\]  

(A18)

where \( G \) is linear in the \( \delta \)'s but depends only on the preceding variables. Here we have used the natural lexicographic ordering: \( (11) < (21) = (12) < (22) < (31) = (13) < (32) = (23) < \cdots \). It follows that the stability of these equations is determined only by the stability of the first term, i.e. of the differential equations (for all \( p \) and \( m \)):

\[
\dot{z} = -(2\beta + J_{mm} + J_{pp})z.
\]  

(A19)

This equation happens to be analytically solvable, surprisingly in terms of our Lyapunov vectors themselves,

\[
z(t) = \exp(-2\beta t - \Lambda_{mm}(t) - \Lambda_{pp}(t))
\]  

(A20)

and we see that stability is ensured provided

\[
\beta > -\lim_{t \rightarrow \infty} \frac{1}{t} \Lambda_{mm}(t) = -\lambda_m
\]  

(A21)

for all \( m = 1, \ldots, k \). As our \( \lambda \)'s are ordered decreasingly it suffices to have \( \beta > -\lambda_k \).

From equation (A19) we also see that stability follows by using the more conservative bound obtained by setting \( \beta > \max_{\|e\|=1} (-(e, Je)) \).

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