Title: Lyapunov Exponents: Computation

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History and Scope

In 1892, in his doctoral thesis *The general problem of the stability of motion* (reprinted in its original form in [33]), Lyapunov introduced several groundbreaking concepts to investigate stability in differential equations. These are collectively known as Lyapunov Stability Theory. Lyapunov was concerned with the asymptotic stability of solutions with respect to perturbations of initial data. Among other techniques (e.g., what are now known as first and second Lyapunov methods), he introduced a new tool to analyze the stability of solutions of linear time-varying systems of differential equations, the so-called *characteristic numbers*, now commonly and appropriately called *Lyapunov exponents.*

Simply put, these characteristic numbers play the role that the (real parts of the) eigenvalues play for time invariant linear systems. Lyapunov considered the n-dimensional linear system

$$\dot{x} = A(t)x\,, \tag{1}$$ {aeqn}

where A is continuous and bounded: $\sup_t \|A(t)\| < \infty$. He showed that, "if all characteristic numbers (see below for their definition) of (1) are negative, then the zero solution of (1) is asymptotically (in fact, exponentially) stable." He further proved an important characterization of stability relative to the perturbed linear system

$$\dot{x} = A(t)x + f(t,x)\,, \tag{2}$$ {PertLin}

where $f(t,0)=0$, so that $x=0$ is a solution of (2), and further $f(t,x)$ is assumed to be "small" near $x=0$ (this situation is what one expects from a linearized analysis about a bounded solution trajectory). Relative to (2), Lyapunov proved that, "if the linear system (1) is *regular*, and all its characteristic numbers are negative, then the zero solution of (2) is asymptotically stable." About 30 years later, it was shown by Perron in [38] that the assumption of regularity cannot generally be removed.

Definition

We refer to the monograph [1] for a comprehensive definition of Lyapunov exponents, regularity, and so forth. Here, we simply recall some of the key concepts.

Consider (1) and let us stress that the matrix function $A(t)$ may be either given, or obtained as the linearization about the solution of a nonlinear differential equation; e.g., $\dot{y} = f(y)$ and $A(t) = Df(y(t))$ (note that in this case, in general, A will depend on the initial condition used for the nonlinear problem). Now, let X be a fundamental matrix solution of (1), and consider the quantities

$$\lambda_i = \limsup_{t\to\infty} \frac{1}{t} \ln ||X(t)e_i|| \ , \ i=1,\dots,n, \tag{3}$$ {les}

where e_i denotes the i-th standard unit vector, $i=1,\dots,n$. When $\sum\limits_{i=1}^{n} \lambda_i$ is minimized with respect to all possible fundamental matrix solutions, then the λ_i are called the characteristic numbers, or Lyapunov exponents, of the system. It is customary to consider them ordered as: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Similar definitions can be given for $t \to -\infty$ and/or with $\liminf$ replacing the $\limsup$, but the description above is the prevailing one. An important consequence of *regularity* of a given system is that in (3) one has limits instead of limsups.

More Recent Theory

Given that the condition of regularity is not easy to verify for a given system, it was unclear what practical use one was going to make of the Lyapunov exponents in order to study stability of a trajectory. Moreover, even assuming that the system is regular, it is effectively impossible to get a handle on the Lyapunov exponents except through their numerical approximation. It then becomes imperative to have some comfort that what one is trying to approximate is robust; in other words, it is the Lyapunov exponents themselves that will need to be stable with respect to perturbations of the function A in (1). Unfortunately, regularity is not sufficient for this purpose.

Major theoretical advances to resolve the two concerns above took place in the late 1960's, thanks to the work of Oseledec and Millionshchikov (e.g., see [36] and [34]). Oseledec was concerned with stability of trajectories on a (bounded) attractor, on which one has an invariant measure. In this case, Oseledec's *Multiplicative Ergodic Theorem* validates regularity for a broad class of linearized systems; the precise statement of this theorem is rather technical, but its practical impact is that (with respect to the invariant measure) almost all trajectories of the nonlinear system will give rise to a regular linearized problem. Millionshchikov introduced the concept of *integral separation*, which is the condition needed for stability of the Lyapunov exponents with respect to perturbations in the coefficient matrix, and further gave important results on the prevalence of this property within the class of linear systems.

Further Uses of Lyapunov Exponents

Lyapunov exponents found an incredible range of applicability in several contexts, and both theory and computational methods have been further extended to discrete dynamical systems, maps, time series, etc.. In particular:

(i) The largest Lyapunov exponent of (2), λ_1, characterizes the rate of separation of trajectories (with infinitesimally close initial conditions). For this reason, a positive value of λ_1 (coupled with compactness of the phase space) is routinely taken as an indication that the system is *chaotic* (see [37]).

(ii) Lyapunov exponents are used to estimate *dimension* of attractors through the Kaplan-Yorke formula (Lyapunov dimension):

$$\mathrm{Dim}_L = k + (\lambda_1 + \lambda_2 + \cdots + \lambda_k)/|\lambda_{k+1}|$$

where k is the largest index i such that $\lambda_1 + \lambda_2 + \cdots + \lambda_i > 0$. See [31] for the original derivation of the formula and [9] for its application to the 2-d Navier Stokes equation.

(iii) The sum of all the positive Lyapunov exponents is used to estimate the entropy of a dynamical system (see [3]).

(iv) Lyapunov exponents have also been used to characterize persistence and degree of smoothness of invariant manifolds (see [26] and see [17] for a numerical study).

(v) Lyapunov exponents have even been used in studies of piecewise-smooth differential equations, where a formal linearized problem as in (1) does not even exist (see [27, 35]).

(vi) Finally, there has been growing interest also in approximating bases for the *growth directions* associated to the the Lyapunov exponents. In particular, there is interest in obtaining representations for the stable (and unstable) subspaces of (1), and in their use to ascertain stability of traveling waves. E.g., see [12, 39].

Factorization Techniques

Many of the applications listed above are related to nonlinear problems, which in itself is witness to the power of linearized analysis based on the Lyapunov exponents. Still, the computational task of approximating some or all of the Lyapunov exponents for dynamical systems defined by the flow of a differential equation is ultimately related to the linear problem (1), and we will thus focus on this linear problem.

Techniques for numerical approximation of Lyapunov exponents are based upon smooth matrix factorizations of fundamental matrix solutions X, to bring it into a form from which it is easier to extract the Lyapunov exponents. In practice, two techniques have been studied: based on the QR factorization of X and based on the SVD (singular value decomposition) of X. Although these techniques have been adapted to the case of incomplete decompositions (useful when only a few Lyapunov exponents are needed), or to problems with Hamiltonian structure, we only describe them in the general case when the entire set of Lyapunov exponents is sought, the problem at hand has no particular structure, and the system is regular. For extensions, see the references.

QR Methods

The idea of QR methods is to seek the factorization of a fundamental matrix solution as $X(t) = Q(t)R(t)$, for all t, where Q is an orthogonal matrix valued function and R is an upper triangular matrix valued function with positive diagonal entries. The validity of this factorization has been known since Perron [38] and Diliberto [25], and numerical techniques based upon the QR factorization date back at least to [4].

QR techniques come in two flavors, continuous and discrete, and methods for quantifying the error in approximation of Lyapunov exponents have been developed in both cases (see [22, 23, 24, 13, 40]).

Continuous QR

Upon differentiating the relation $X = QR$ and using (1), we have

$$AQR = Q\dot{R} + \dot{Q}R \quad \text{or} \quad \dot{Q} = AQ - QB\,, \tag{4}$$ {Qeqns}

where $\dot{R} = BR$, hence B must be upper triangular. Now, let us formally set $S = Q^T\dot{Q}$ and note that since Q is orthogonal then S must be skew-symmetric. Now, from $B = Q^TAQ - Q^T\dot{Q}$ it is easy to determine at once the strictly lower triangular part of S (and from this, all of it), and the entries of B. To sum up, we have two differential equations, for Q and for R. Given $X(0) = Q_0R_0$, we have

$$\dot{Q} \;=\; QS(Q,A)\,, \quad Q(0) = Q_0\,, \tag{5}$$ {QDE}

$$\dot{R} \;=\; B(t)R\,, \quad R(0) = R_0\,,\;\; B := Q^TAQ - S(Q,A)\;, \tag{6}$$ {RDE}

The diagonal entries of R are used to retrieve the exponents:

$$\lambda_i = \lim_{t\to\infty}\frac{1}{t}\int_0^t (Q^T(s)A(s)Q(s))_{ii}ds\,, \quad i = 1,\dots,n\,. \tag{7}$$ {LEsQR2}

A unit upper triangular representation for the growth directions may be further determined by $\lim_{t\to\infty}\mathrm{diag}(R^{-1}(t))R(t)$ (see [20, 11, 12]).

Discrete QR

Here one seeks the QR factorization of the fundamental matrix X at discrete points $0 = t_0 < t_1 < \cdots < t_k < \cdots$, where $t_k = t_{k-1} + h_k$, $h_k \geq \hat{h} > 0$. Let $X_0 = Q_0R_0$, and suppose we seek the QR factorization of $X(t_{k+1})$. For $j = 0,\dots,k$, progressively define $Z_{j+1}(t) = X(t,t_j)Q_j$, where $X(t,t_j)$ solves (1) for $t \geq t_j$, $X(t_j,t_j) = I$, and Z_{j+1} is the solution of

$$\begin{cases} \dot{Z}_{j+1} = A(t)Z_{j+1}\;, \;\; t_j \leq t \leq t_{j+1} \\ Z_{j+1}(t_j) = Q_j\,. \end{cases} \tag{8}$$ {discQR1}

Update the QR factorization as

$$Z_{j+1}(t_{j+1}) = Q_{j+1}R_{j+1}\,, \tag{9}$$ {discQR2}

and finally observe that

$$X(t_{k+1}) = Q_{k+1}\,[R_{k+1}R_k\cdots R_1R_0] \tag{10}$$ {Y=QR}

is the QR factorization of $X(t_{k+1})$.The Lyapunov exponents are obtained from the relation

$$\lim_{k\to\infty} \frac{1}{t_k} \sum_{j=0}^{k} \log(R_j)_{ii}\,, i = 1, \dots, n\,. \tag{11}$$ {LEsdiscQR}

SVD Methods

Here one seeks to compute the SVD of X: $X(t) = U(t)\Sigma(t)V^T(t)$, for all t, where U and V are orthogonal and $\Sigma = \mathrm{diag}(\sigma_i,\ i = 1\dots, n)$, with $\sigma_1(t) \geq \sigma_2(t) \geq \dots \geq \sigma_n(t)$. If the singular values are distinct, the following differential equations U, V and Σ hold. Letting $G = U^T AU$, they are

$$\dot{U} = UH, \quad \dot{V}^T = -KV^T, \quad \dot{\Sigma} = D\Sigma, \tag{12}$$ {svdfactors}

where $D = \mathrm{diag}(G)$, $H^T = -H$, $K^T = -K$, and for $i \neq j$,

$$H_{ij} = \frac{G_{ij}\sigma_j^2 + G_{ji}\sigma_i^2}{\sigma_j^2 - \sigma_i^2}, \quad K_{ij} = \frac{(G_{ij} + G_{ji})\sigma_i\sigma_j}{\sigma_j^2 - \sigma_i^2}. \tag{13}$$ {handk}

From the SVD of X the Lyapunov exponents may be obtained as

$$\lim_{t\to\infty} \frac{1}{t} \ln \sigma_i(t)\,. \tag{14}$$ {svdles2}

Finally, an orthogonal representation for the growth directions may be determined by $\lim_{t\to\infty} V(t)$ (see [20, 10, 11, 12]).

Numerical Implementation

Although algorithms based upon the above techniques appear deceivingly simple to implement, much care must be exercised in making sure that they perform as one would expect them to. [For example, in the continuous QR and SVD techniques it is mandatory to maintain the factors Q, U, and V, orthogonal]. `Fortran` software codes for approximating Lyapunov exponents of linear and nonlinear problems have been developed and tested extensively and provide a combined state of the knowledge insofar as numerical methods suited for this specific task. See [21, 14, 15].

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