Supplementary material to the ms "Transport barriers in geophysical flows: a review"

S.V. Prants

1 Finite-time Lyapunov exponents

1.1 Finite-time Lyapunov exponents for a n-dimensional vector field

We describe in this section a general method to compute Lyapunov exponents which is valid for n-dimensional vector fields. Let us start with a n-dimensional set of nonlinear ordinary differential equations in the vector form

$$\begin{gathered}\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t), \quad \mathbf{x} = (x_1, \dots, x_n), \\ \mathbf{f}(\mathbf{x}, t) = (f_1(x_1, \dots, x_n, t), \dots, f_n(x_1, \dots, x_n, t)).\end{gathered} \tag{1}$$

The Lyapunov exponent at a point $\mathbf{x_0}$ is given by

$$\Lambda(\mathbf{x_0}) = \lim_{t\to\infty} \lim_{\|\delta\mathbf{x}(0)\|\to 0} \frac{\ln(\|\delta\mathbf{x}(t)\|/\|\delta\mathbf{x}(0)\|)}{t}, \tag{2}$$

where $\delta\mathbf{x}(t) = \mathbf{x_1}(t) - \mathbf{x_0}(t)$, $\mathbf{x_0}(t)$, and $\mathbf{x_1}(t)$ are solutions of the set (1), $\mathbf{x_0}(0) = \mathbf{x_0}$. The limit (2) exists, is the same for almost all the choices of $\delta\mathbf{x}(0)$ and has a clear geometrical sense: trajectories of two nearby particles diverge (converge) in time exponentially (in average) with the coefficients given by the Lyapunov exponents.

Due to smallness of $\delta\mathbf{x}$, one can linearize the set (1) in a vicinity of a given trajectory $\mathbf{x_0}(t)$ and obtain a set of time-dependent linear equations

$$\begin{pmatrix} \delta\dot{x}_1 \\ \dots \\ \delta\dot{x}_n \end{pmatrix} = J(t) \begin{pmatrix} \delta x_1 \\ \dots \\ \delta x_n \end{pmatrix}, \tag{3}$$

where $J(t)$ is the Jacobian matrix of the set (1) along the trajectory $\mathbf{x_0}(t)$

$$J(t) = \begin{pmatrix} \dfrac{\partial f_1(\mathbf{x_0}(t), t)}{\partial x_1} & \dots & \dfrac{\partial f_1(\mathbf{x_0}(t), t)}{\partial x_n} \\ \dots & \dots & \dots \\ \dfrac{\partial f_n(\mathbf{x_0}(t), t)}{\partial x_1} & \dots & \dfrac{\partial f_n(\mathbf{x_0}(t), t)}{\partial x_n} \end{pmatrix}. \tag{4}$$

Solution of the linear set (3) can be found with the help of the evolution matrix $G(t, t_0)$

$$\begin{pmatrix} \delta x_1(t) \\ \dots\dots \\ \delta x_n(t) \end{pmatrix} = G(t, t_0) \begin{pmatrix} \delta x_1(t_0) \\ \dots\dots \\ \delta x_n(t_0) \end{pmatrix}. \tag{5}$$

The evolution matrix obeys the differential equation which can be obtained after substituting (5) into (3)

$$\dot{G} = JG, \tag{6}$$

with the initial condition $G(t_0, t_0) = I$, where I is the unit matrix. Any evolution matrix has the important multiplicative property

$$G(t, t_0) = G(t, t_1)G(t_1, t_0). \tag{7}$$

One can decompose the evolution matrix as follows:

$$G(t, t_0) = U(t, t_0)\Sigma(t, t_0)V^T(t, t_0), \tag{8}$$

which is known as "a singular-value decomposition". Here U, V are orthogonal matrices, and $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ is a diagonal matrix. The quantities $\sigma_1, \ldots, \sigma_n$ are called singular values of the matrix G.

The maximum value $\lim\limits_{\|\delta\mathbf{x}(0)\|\to 0} \dfrac{\|\delta\mathbf{x}(t)\|}{\|\delta\mathbf{x}(0)\|}$ for the set (3) equals to $\sigma_1(G(t))$. It is the maximum singular value of the matrix $G(t)$. If $\lim\limits_{t\to\infty} \dfrac{\sigma_2(G(t))}{\sigma_1(G(t))} = 0$, where $\sigma_2(G(t))$ is the next (smaller) singular value of the matrix $G(t)$ in magnitude, then (2) can be redefined as follows:

$$\Lambda_{\max} = \lim_{t\to\infty} \frac{\ln \sigma_1(G(t))}{t - t_0}. \tag{9}$$

The quantity

$$\Lambda = \frac{\ln \sigma_1(G(t))}{t - t_0} \tag{10}$$

is called the finite-time Lyapunov exponent (FTLE). It is the ratio of the logarithm of a maximal possible stretching of a vector to a time interval $t - t_0$. The "instantaneous" Lyapunov exponent Λ_0 is a Lyapunov exponent of the set of linear equations

$$\begin{pmatrix} \delta\dot{x}_1 \\ \ldots \\ \delta\dot{x}_n \end{pmatrix} = J(0) \begin{pmatrix} \delta x_1 \\ \ldots \\ \delta x_n \end{pmatrix}. \tag{11}$$

It is the rate of exponential diverging of trajectories at a given point and at a given instant of time.

Equation (6) can not be numerically integrated over a large time because the elements of the corresponding evolution matrix grow exponentially, if one of the Lyapunov exponents is positive. However, we can divide a large time interval on subintervals with the duration which is less or order of the Lyapunov timescale, $t_\Lambda = 1/\Lambda$, and represent the whole evolution matrix as a product of the evolution matrices computed on these subintervals using the property (7). We compute this product and the corresponding singular values using the GNU Multiple Precision Arithmetic Library in order to preserve the absolute precision of our representation of the evolution matrix.

1.2 Singular-value decomposition and evolution matrix for two-dimensional case

The singular-value decomposition is a representation of any $m \times n$-matrix in the form

$$M = U\Sigma V, \tag{12}$$

where U and V are $m \times m$ and $n \times n$ unitary matrices, respectively, Σ is a diagonal $m \times n$-matrix. The diagonal elements of Σ are singular values of the matrix M. The eigenvectors u and v, such that $Mv = \sigma u$ and $M^* u = \sigma v$ (σ is a singular value of M), are, respectively, left and right singular vectors of the matrix M. If M is real-valued then its singular values are real as well. U and V are orthogonal matrices. The matrix Σ and its singular-value decomposition are defined to an accuracy of the permutation of singular values. Therefore, one may require to order the singular values of Σ as a nonincreasing sequence, and such a decomposition is unique.

If the matrix M is squared then its singular-value decomposition has a simple geometric meaning. Action of any matrix to a vector can be represented as the following three successive transformations: the first rotation/reflection by the matrix V, a stretching/contraction along the coordinate axis by the matrix Σ and the second rotation/reflection by the matrix U. Thus, the matrix M transforms a sphere of the unit radius in an ellipsoid with the semiaxis to be equal to singular values directed along the left singular vectors. The right singular vectors are correspondingly pre-images of the ellipsoid's semiaxis.

Let us consider now a 2D flow with a 2×2 evolution matrix with the singular-value decomposition

$$G = UDV \Rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \cos\phi_2 & -\sin\phi_2 \\ \sin\phi_2 & \cos\phi_2 \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 \\ \sin\phi_1 & \cos\phi_1 \end{pmatrix}. \tag{13}$$

Transformations of a circle with the unit radius by those matrices and its singular vectors are shown in Fig. 1. Reflection matrices are not used in this decomposition, therefore, singular values can be negative. However, it is clear from general consideration that the evolution matrix of a continuous flow cannot contain reflections.

Multiplying the matrices, one gets the set with four equations and four variables

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \sigma_1 \cos\phi_1 \cos\phi_2 - \sigma_2 \sin\phi_1 \sin\phi_2 & -\sigma_1 \sin\phi_1 \cos\phi_2 - \sigma_2 \cos\phi_1 \sin\phi_2 \\ \sigma_1 \cos\phi_1 \sin\phi_2 + \sigma_2 \sin\phi_1 \cos\phi_2 & -\sigma_1 \sin\phi_1 \sin\phi_2 + \sigma_2 \cos\phi_1 \cos\phi_2 \end{pmatrix}. \tag{14}$$

Let us introduce the following notations:

$$\begin{aligned} &\alpha = a + d, \quad &&\beta = a - d, \quad &&\gamma = c + b, \quad &&\delta = c - b, \\ &\xi = \sigma_1 + \sigma_2, \quad &&\eta = \sigma_1 - \sigma_2, \quad &&\Phi = \phi_1 + \phi_2, \quad &&\Psi = \phi_2 - \phi_1. \end{aligned} \tag{15}$$

Adding and deducting Eqs. 14 and using the notations (15), we get

$$\alpha = \xi \cos\Phi, \quad \beta = \eta \cos\Psi, \quad \gamma = \eta \sin\Psi, \quad \delta = \xi \sin\Phi. \tag{16}$$

Solution of the set (16) is

$$\xi = \sqrt{\alpha^2 + \delta^2}, \quad \eta = \sqrt{\beta^2 + \gamma^2}, \quad \Phi = \operatorname{arctan2}(\delta, \alpha), \quad \Psi = \operatorname{arctan2}(\gamma, \beta), \tag{17}$$

where $\operatorname{arctan2}(y, x)$ is an angle between the vector (x, y) and the axis x which can be defined as

$$\operatorname{arctan2}(y, x) = \begin{cases} \arctan(y/x), & x \geq 0, \\ \arctan(y/x) + \pi, & x < 0. \end{cases} \tag{18}$$

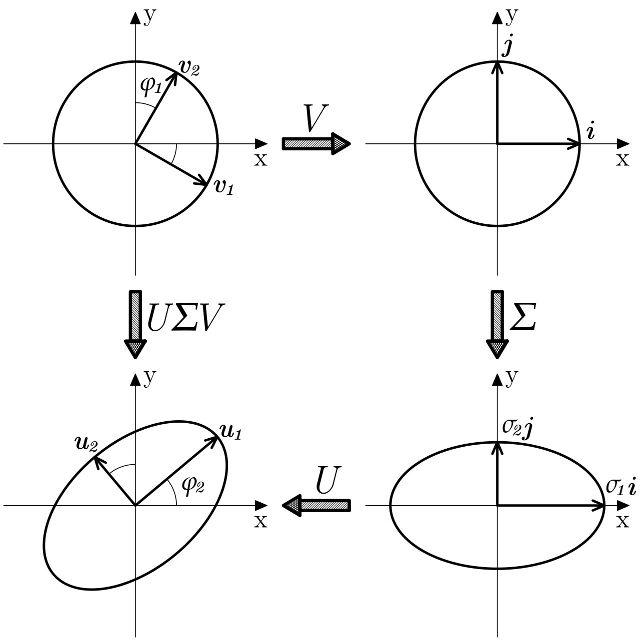

Figure S1: Geometric meaning of the singular-value decomposition of a 2×2 matrix.

The final solution is

$$\begin{aligned}\sigma_1 &= \frac{\sqrt{(a+d)^2+(c-b)^2}+\sqrt{(a-d)^2+(b+c)^2}}{2},\\ \sigma_2 &= \frac{\sqrt{(a+d)^2+(c-b)^2}-\sqrt{(a-d)^2+(b+c)^2}}{2},\\ \phi_1 &= \frac{\operatorname{arctan2}(c-b,\, a+d)-\operatorname{arctan2}(c+b,\, a-d)}{2},\\ \phi_2 &= \frac{\operatorname{arctan2}(c-b,\, a+d)+\operatorname{arctan2}(c+b,\, a-d)}{2}.\end{aligned} \tag{19}$$

It is evident from the solution that the singular values are ordered in a nonincreasing way, i.e., $\sigma_1 \geq \sigma_2$. The product $\sigma_1\sigma_2$ defines the ratio of the final area to the initial and equals to Det M. It follows from the definition of a singular-value decomposition that

$$\sigma_1 \geqslant \frac{\|M\mathbf{x}\|}{\|\mathbf{x}\|} \geqslant \sigma_2, \tag{20}$$

where $\|\cdot\|$ is the Euclidean norm. In other words, the length of any vector $\mathbf{x}$ is changed under the action of the matrix M in σ_2 times as minimum and in σ_1 times as maximum.