

Phase space, Tangent-Linear and Adjoint Models, Singular Vectors, Lyapunov Vectors and Normal Modes

Assume a phase space of dimension N where $\mathbf{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_N \end{bmatrix}$ is a state vector.

Autonomous governing equations with initial state:

$$\frac{d\mathbf{X}}{dt} = \mathbf{F}(\mathbf{X}); \mathbf{X}(t_0) = \mathbf{X}_0; \mathbf{F} = \begin{bmatrix} F_1 \\ \vdots \\ F_N \end{bmatrix}$$

Unique solution for an arbitrary time $t > t_0$: $\mathbf{X}(t) = \mathbf{M}(\mathbf{X}_0)$; *i.e. the trajectory*.

Conditions for stability with respect to small perturbations of the initial state are investigated by adding small increments to \mathbf{X}_0 , integrate forward in time and neglect non-linear terms:

$$\begin{aligned} \frac{d}{dt} [\mathbf{X} + \delta\mathbf{x}] &= \mathbf{F}(\mathbf{X} + \delta\mathbf{x}); \delta\mathbf{x}(t_0) = \delta\mathbf{x}_0 \\ \Leftrightarrow \frac{d\mathbf{X}}{dt} + \frac{d}{dt} \delta\mathbf{x} &\approx \mathbf{F}(\mathbf{X}) + \mathbf{J} \cdot \delta\mathbf{x}; \delta\mathbf{x}(t_0) = \delta\mathbf{x}_0; \end{aligned}$$

where the jacobian is evaluated along the non-linear solution trajectory:

$$\mathbf{J} = \left[\frac{\partial \mathbf{F}}{\partial \mathbf{X}} \right]_{\mathbf{X}(t)} = \begin{bmatrix} \frac{\partial F_1}{\partial X_1} & \dots & \frac{\partial F_1}{\partial X_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_N}{\partial X_1} & \dots & \frac{\partial F_N}{\partial X_N} \end{bmatrix}_{\mathbf{X}(t)}$$

The *Tangent-Linear Model (TL)*, is then:

$$\frac{d}{dt} \delta\mathbf{x} = \mathbf{J} \cdot \delta\mathbf{x}; \quad \delta\mathbf{x}(t_0) = \delta\mathbf{x}_0$$

and the solution is: $\delta\mathbf{x}(t) = \mathbf{L}(t_0, t) \cdot \delta\mathbf{x}_0$, where the *propagator or resolvent* is:

$$\mathbf{L}(t_0, t) = \left[\frac{\partial \mathbf{M}}{\partial \mathbf{X}} \right]_{\mathbf{X}(t)} = \begin{bmatrix} \frac{\partial M_1}{\partial X_1} & \dots & \frac{\partial M_1}{\partial X_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial M_N}{\partial X_1} & \dots & \frac{\partial M_N}{\partial X_N} \end{bmatrix}_{\mathbf{X}(t)}$$

If $\mathbf{X}(t)$ is a fixed point (a constant), then \mathbf{J} is a constant, and we can formally write:

$$\mathbf{L}(t_0, t) = e^{\mathbf{J}(t-t_0)}$$

If the eigenvalues of \mathbf{J} are μ_i , then the eigenvalues of \mathbf{L} are $\Lambda_i = e^{\mu_i(t-t_0)}$, $i=1, \dots, N$.

and for non-constant $\mathbf{X}(t)$ and \mathbf{J} , this can be generalized to:

$$\mathbf{L}(t_0, t) = e^{\int_{t_0}^t \mathbf{J} dt}$$

For numerical integrations, time is stepped forward in K steps, Δt , and we can define:

$$\mathbf{L}(t_0, t) = \mathbf{L}_{K-1} \cdot \dots \cdot \mathbf{L}_k \cdot \dots \cdot \mathbf{L}_0 = \prod_{k=0}^{K-1} \mathbf{L}_k = \exp \left[\sum_{k=0}^{K-1} \mathbf{J}_k \Delta t \right]$$

where $\mathbf{L}_k = \mathbf{L}(t_k, t_k + \Delta t)$.

Assume that eigenvalue no. i of \mathbf{L}_k and \mathbf{J}_k are Λ_i^k and μ_i^k respectively, and define:

$$\Lambda_i(t) = \prod_{k=0}^{K-1} \Lambda_i^k ; i = 1, \dots, N$$

The Lyapunov exponent no. i is then:

$$\lambda_i = \lim_{t \rightarrow \infty} \frac{1}{t - t_0} \ln |\Lambda_i(t)| = \lim_{t \rightarrow \infty} \frac{1}{t - t_0} \sum_{k=0}^{K-1} \ln |\Lambda_i^k|$$

= the growth-rate of small perturbations averaged over the attractor. This is a **global** property; i.e. it represents an average property for the entire attractor set of the dynamic system. If one or more $\lambda_i > 0$, there are at list some directions in phase-space along which arbitrary initial perturbations will grow.

$\frac{1}{\Delta t} \ln |\Lambda_i^k|$ is the **local Lyapunov exponent no. i at time-step k** .

Definition of the leading **Local Lyapunov Vector – LLV**:

The vector in phase space (i.e. the physical state) at time t that any arbitrary perturbation, $\mathbf{y}(t-s)$ at a very long time-interval s before t , converges to, assuming a tangent-linear development:

$$\mathbf{l}_1(t) = \lim_{s \rightarrow \infty} \mathbf{L}(t - s, t) \mathbf{y}(t - s)$$

Note that the leading local Lyapunov exponent (i.e. no. 1) is $l_1 = \frac{1}{\Delta t} \ln \frac{\|\mathbf{l}_1(t+\Delta t)\|}{\|\mathbf{l}_1(t)\|}$.

Inner products and distances in phase space, the adjoint

Let $\langle \mathbf{X}, \mathbf{Y} \rangle \equiv s$ be an inner product between state vectors \mathbf{X} and \mathbf{Y} , where s is a real number. In general, the phase-space can be based on complex numbers (which is useful for wave and stability theory). Then $s = \langle \mathbf{X}, \mathbf{Y} \rangle = \langle \bar{\mathbf{Y}}, \mathbf{X} \rangle$, where the bar signifies complex conjugation. (If real

only numbers, complex conjugation makes no difference, and the inner product is commutative.) If the inner product is the **Euclidian**, then: $\langle X, Y \rangle_E = \bar{X}^T Y$, where the superscript T means the matrix transpose. It is also customary to write it in terms of *the dot product*: $\langle X, Y \rangle_E = \bar{X} \cdot Y = \sum_{i=1}^N \bar{x}_i y_i$. Frequently one defines general inner products in terms of the euclidian dot product by employing some weights. Inner products can thus be measured in terms of total energy (kinetic + available potential energy) over a portion of the atmosphere (or the global).

A distance between states in phase space can be the length of the inner product of a vector with itself. The vector, X , is then defined as the difference between the two state vectors, and:

$$\|X\| = \sqrt{\langle X, X \rangle}.$$

The adjoint to an operator L with respect to the inner product $\langle X, Y \rangle$ is denoted L^* , and is defined such that *for any arbitrary vectors X and Y*, $\langle LX, Y \rangle \equiv \langle X, L^*Y \rangle$. Note that in the textbook of Kalnay, the notation L^T (i.e. the transpose to L) is used for the adjoint, thus presuming real numbers and a standard Euclidian inner product. Here we continue to use the more general notation, L^* , of adjoints with respect to unspecified inner products.

The solution to the Tangent-Linear model is, as defined above: $\delta x(t) = L(t_0, t) \cdot \delta x_0$. The size of the perturbation is the distance between $x(t) + \delta x(t)$ and $x(t)$, hence:

$$\|\delta x(t)\|^2 = \langle \delta x(t), \delta x(t) \rangle = \langle L(t_0, t) \delta x_0, L(t_0, t) \delta x_0 \rangle = \langle L(t_0, t)^* L(t_0, t) \delta x_0, \delta x_0 \rangle;$$

which clearly demonstrates *the importance of the combined operator* $L(t_0, t)^* L(t_0, t)$.

Notes

(1) Assume that the resolvent $L(t_0, t)$ can be split into K stepwise sub-intervals over time:

$$L(t_0, t) = L(t_{K-1}, t) L(t_{K-2}, t_{K-1}) \dots L(t_0, t_1) = L_{K-1} L_{K-2} \dots L_0$$

then

$$\begin{aligned} \langle L(t_0, t) \delta x_0, \delta x(t) \rangle &= \langle L_{K-1} L_{K-2} \dots L_0 \delta x_0, \delta x(t) \rangle = \langle \delta x_0, L_0^* \dots L_{K-2}^* L_{K-1}^* \delta x(t) \rangle \\ &= \langle \delta x_0, L(t_0, t)^* \delta x(t) \rangle \end{aligned}$$

The adjoint operator $L(t_0, t)^*$ thus works backwards in time from t to t_0 .

(2) It is also straightforward to show that: $L(t_0, t)^{**} = L(t_0, t)$ and that $L(t_0, t)^* L(t_0, t)$ is self-adjoint (or symmetric, Hermitian):

$$(L(t_0, t)^* L(t_0, t))^* = L(t_0, t)^* L(t_0, t)^{**} = L(t_0, t)^* L(t_0, t)$$

The eigenvalues of this particular self-adjoint operator are real and positive, and the eigenvectors are orthogonal with respect to this particular inner product.

Singular vectors and values

The orthogonal eigenvectors to $L(t_0, t)^* L(t_0, t)$ with respect to the inner product, are $e_i(t_0)$ with eigenvalues σ_i^2 , for $i = 1, \dots, N$, each fulfilling the equations:

$$\mathbf{L}(t_0, t)^* \mathbf{L}(t_0, t) \mathbf{e}_i(t_0) = \sigma_i^2 \mathbf{e}_i(t_0) \text{ for } i = 1, \dots, N.$$

If we define $\mathbf{L}(t_0, t) \mathbf{e}_i(t_0) = \mathbf{e}_i(t)$, i.e. the eigenvector evolved from t_0 to t , the norm evolves according to:

$$\begin{aligned} \|\mathbf{e}_i(t)\|^2 &= \langle \mathbf{e}_i(t), \mathbf{e}_i(t) \rangle = \langle \mathbf{L}(t_0, t) \mathbf{e}_i(t_0), \mathbf{L}(t_0, t) \mathbf{e}_i(t_0) \rangle = \langle \mathbf{L}(t_0, t)^* \mathbf{L}(t_0, t) \mathbf{e}_i(t_0), \mathbf{e}_i(t_0) \rangle \\ &= \sigma_i^2 \|\mathbf{e}_i(t_0)\|^2 \end{aligned}$$

Notice that $\mathbf{e}_i(t_0)$ and $\mathbf{e}_i(t)$ can have different directions in the phase space.

Define:

- $\mathbf{e}_i(t_0)$ are the *initial singular vectors* to the propagator $\mathbf{L}(t_0, t)$ (\mathbf{v} in Kalnay)
- $\mathbf{e}_i(t)$ are the *evolved singular vectors* to the propagator $\mathbf{L}(t_0, t)$ (\mathbf{u} in Kalnay)
- σ_i are the *singular values* vectors to the propagator $\mathbf{L}(t_0, t)$.

The singular values give the ratio between the norm of the evolved and initial singular vectors. If ordered according to the size of the singular values, then singular vector no. 1 defines the direction in phase space at initial time t_0 , which produces the fastest growth of the norm of perturbations over the finite time interval $[t_0, t]$. Notice that there are as many distinct singular vectors as the dimension N of the phase space.

Note

The adjoint to the evolved singular vector produces the initial singular vectors in a similar way as the propagator to the initial singular vector produces the evolved:

$$\mathbf{L}(t_0, t)^* \mathbf{e}_i(t) = \mathbf{L}(t_0, t)^* \mathbf{L}(t_0, t) \mathbf{e}_i(t_0) = \sigma_i^2 \mathbf{e}_i(t_0)$$

From this, we also see that:

$$\mathbf{L}(t_0, t) \mathbf{L}(t_0, t)^* \mathbf{e}_i(t) = \sigma_i^2 \mathbf{L}(t_0, t) \mathbf{e}_i(t_0) = \sigma_i^2 \mathbf{e}_i(t)$$

Hence, the evolved singular vectors are eigenvectors to $\mathbf{L}(t_0, t) \mathbf{L}(t_0, t)^*$ with eigenvalues σ_i^2 .

Now, assume that the initial singular vectors are normalized, i.e. $\|\mathbf{e}_i(t_0)\| = 1$ for all $i=1, \dots, N$.

We can use these singular vectors as an orthonormal basis for any vector in the phase space:

$\delta \mathbf{x}_0 = \sum_{i=1}^N \alpha_i \mathbf{e}_i(t_0)$; where $\alpha_i = \langle \delta \mathbf{x}_0, \mathbf{e}_i(t_0) \rangle$. It is straightforward to show that:

$$\|\delta \mathbf{x}(t)\|^2 = \langle \delta \mathbf{x}(t), \delta \mathbf{x}(t) \rangle = \langle \mathbf{L}(t_0, t) \delta \mathbf{x}_0, \mathbf{L}(t_0, t) \delta \mathbf{x}_0 \rangle = \sum_{i=1}^N \alpha_i^2 \sigma_i^2$$

The singular values thus yield the factor by which a component of an initial perturbation is stretched as it rotates in phase space from the direction of the initial singular vector to the evolved. See 6.3.1 and 6.3.2 in Kalnay's book.

Relation to LLV

In the definition of LLV, let $\mathbf{y}(t) = \sum a_i \mathbf{e}_i(t)$; where $\mathbf{e}_i(t) = \mathbf{L}(t-s, t) \mathbf{e}_i(t-s)$

Then for component no.1, choose $\mathbf{y}(t-s) = \mathbf{L}^*(t-s, t) \mathbf{e}_1(t)$, and

$$\mathbf{L}(t-s, t) \mathbf{y}(t-s) = \mathbf{L} \mathbf{L}^* \mathbf{e}_1(t) = \sigma_1^2 \mathbf{e}_1(t)$$

The LLV equals the leading evolved singular vector for infinite past time intervals up to present.

More general inner products

In Kalnay's text-book there is an example on how singular vectors calculated w.r.t. an euclidian inner product can be generalized to other inner products, including local, geographic projections and inner products which differ between initial and final time. The presentation is slightly untraditional, hence the following.

Singular vectors can be defined as the result of finding an initial state vector perturbation $\delta \mathbf{x}(0)$ with unit initial norm: $\langle \delta \mathbf{x}(0), \delta \mathbf{x}(0) \rangle_0 = 1$ such that the norm at final time t is:

$$\langle \delta \mathbf{x}(t), \delta \mathbf{x}(t) \rangle_F = \text{MAXIMUM},$$

where $\delta \mathbf{x}(t) = \mathbf{L}(0, t) \delta \mathbf{x}(0)$ is the solution of the tangent-linear equation. Let \mathbf{C}_0 and \mathbf{C}_F be positiv definit (having only positive eigenvalues), diagonal operators/matrices and \mathbf{P} be a local projection operator. $\mathbf{P} \mathbf{x} = \mathbf{x}$ in all points inside a predefined target domain in physical space, and zero outside. [It is also possible to let \mathbf{P} select some of the state variables as well.] Hence, \mathbf{P} is a diagonal matrix with either 0 or 1 along the diagonal. Now let:

$$\langle \delta \mathbf{x}(t), \delta \mathbf{x}(t) \rangle_F = [\mathbf{P} \mathbf{L} \delta \mathbf{x}(0)]^T \mathbf{C}_F \mathbf{P} \mathbf{L} \delta \mathbf{x}(0) = \text{MAXIMUM},$$

$$\text{with side condition } \langle \delta \mathbf{x}(0), \delta \mathbf{x}(0) \rangle_0 = [\delta \mathbf{x}(0)]^T \mathbf{C}_0 \delta \mathbf{x}(0) = 1$$

In other words, *Singular Vectors defined in this way selects directions in phase space at time t with maximum perturbation \mathbf{C}_F -norm measured inside the target domain, assuming initial perturbations at time 0 of unit \mathbf{C}_0 -norm.* Searching for the maximum while fulfilling the side condition, yields the eigenvalue problem:

$$[\mathbf{P} \mathbf{L}]^T \mathbf{C}_F \mathbf{P} \mathbf{L} \delta \mathbf{x}(0) = \sigma^2 \mathbf{C}_0 \delta \mathbf{x}(0)$$

where σ^2 is the eigenvalue (the lagrangian multiplier from variational analysis).

Scalar multiplication from left with $\mathbf{C}_0^{-1/2}$, and defining $\hat{\mathbf{e}}_0 \equiv \mathbf{C}_0^{1/2} \delta \mathbf{x}(0)$, yields:

$$\hat{\mathbf{L}}^T \hat{\mathbf{L}} \hat{\mathbf{e}}_0 = [\mathbf{C}_0^{-1/2} \mathbf{L}^T \mathbf{P} \mathbf{C}_F \mathbf{P} \mathbf{L} \mathbf{C}_0^{-1/2}] \hat{\mathbf{e}}_0 = \sigma^2 \hat{\mathbf{e}}_0, \text{ where } \hat{\mathbf{L}} \equiv \mathbf{C}_F^{1/2} \mathbf{P} \mathbf{L} \mathbf{C}_0^{-1/2}$$

which is a standard singular value problem with respect to the euclidian inner product. The initial and evolved singular vectors sought after are thus, respectively:

$$\mathbf{e}(0) = \mathbf{C}_0^{-1/2} \hat{\mathbf{e}}_0, \text{ and } \mathbf{e}(t) = \mathbf{L}(0, t) \mathbf{e}(0).$$

Generation of ensembles for medium-range predictions at ECMWF (2015)

Practical procedures for generating SVs

When computing singular vectors and values, the matrices and operators are not explicitly calculated. Instead, an algorithm named *the Lanczos algorithm* is used. This algorithm devices an iterative procedure by which only the impacts of the operators have to be calculated starting from random initial guesses, in order to estimate the eigenvectors and eigenvalues of the combined operators. The Lanczos algorithm can be found described in mathematical textbooks. Here we will only mention that for finding SVs, for which the associated singular values are distinct and positive, the SV with largest singular value is found after few iterations, while SVs with decreasing singular values are gradually found with increasing iteration number. Approximately $2n$ iterations are required to find SV no. n with necessary accuracy. It is absolutely imperative, however, that the adjoint to a tangent-linear operator is computed with full bit-exact accuracy on the computer used in order to achieve this convergence of the Lanczos iteration.

Assume we have the numerical model equations formulated as partial differential equations in physical space. The tangent-linear version to these equations in physical space is estimated assuming that a full solution to the non-linear equations from a given initial condition is calculated and available. That is, the model's estimate of the time-evolution from the initial three-dimensional state is available for every model time-step. This is *the non-linear trajectory*.

By linearizing each term in the non-linear model with respect to perturbations relative to the non-linear trajectory, yields *the tangent-linear model* (TLM) in physical space co-ordinates. The result of computing the numerical tangent-linear model forward in time starting from a given initial perturbation at time 0 and using information from the non-linear trajectory underway, yields the impact of the propagator L valid at a given final time t .

The adjoint model (ADM) to the TLM in physical space co-ordinates with respect to the Euclidian inner product, is also constructed as a numerical model, but steps backwards in time from a final condition at time t . Some terms in the non-linear model is cumbersome to linearize and calculate the adjoint to. These are typically physical terms which involve complex logical procedures (i.e. if-then tests). Some such terms are therefore simplified.

If the ADM is integrated, starting with the result obtained with the TLM at time t , back to time 0, then the result is the effect of applying the combined TLM and ADM to the initial perturbation assumed for time 0 (i.e. $L^T L$). Then the next iteration applies exactly the same procedure on the result of the previous iteration and so on, until the Lanczos algorithm obtain stable results for the number of SVs which are sought after. These are, however, SVs with respect to the Euclidian inner product. In order to generalize to more general inner products, the procedure runs as follows, schematically:

- 1) Assume a set of N initial perturbations at random or according to some assumption;
- 2) Transform this state by multiplying with coefficients as in $C_0^{-1/2}$ and normalize w.r.t. the C_0 inner product;
- 3) Integrate the TLM up to time t ;

- 4) Transform the obtained state by multiplying with 0 or 1 of local projection P;
- 5) Transform this state by multiplying with coefficients as in C_F ;
- 6) Transform the obtained state by multiplying with 0 or 1 of local projection P;
- 7) Integrate the ADM back to time 0
- 8) Transform this state by multiplying with coefficients as in $C_0^{-1/2}$ and normalize w.r.t. the C_0 inner product;
- 9) Apply Lanczos and restart at 3) until satisfied with the accuracy of n SVs.
- 10) Transform the resulting n SVs with coefficients as in $C_0^{-1/2}$.

Generating 50 alternative initial states for the ensemble

At ECMWF initial SVs optimized over 48 hours with the total energy norm ($C_0 = C_F$), are combined with a 10-member ensemble of parallel data assimilation cycles (EDA) to produce alternative initial perturbations to the presumed best, control initial-state analysis. 130 singular vectors (50 targetted (with a projection operator) to the Northern Hemisphere extratropics, 50 targetted to the Southern Hemisphere extratropics, and 30 targetted to six different tropical sub-domains dominated by tropical cyclones) are linearly combined to form 25 SV-based perturbation fields.

Let SV_i , $i=1, \dots, 25$ denote the SV-based preturbation fields, and $E_k = EDA_k - A_0$, $k=1, \dots, 10$ denote the deviation from the control analysis by the EDA-based alternative analyses. The initial states for the n ($n=1, \dots, 50$) alternative ensemble forecasts are:

$$\begin{aligned}
A_1 &= A_0 + [SV_1 + E_1]; & A_2 &= A_0 - [SV_1 + E_1]; \\
& & & \vdots \\
A_{19} &= A_0 + [SV_{10} + E_{10}]; & A_{20} &= A_0 - [SV_{10} + E_{10}]; \\
A_{21} &= A_0 + [SV_{11} + E_1]; & A_{22} &= A_0 - [SV_{11} + E_1]; \\
& & & \vdots \\
A_{39} &= A_0 + [SV_{20} + E_{10}]; & A_{40} &= A_0 - [SV_{20} + E_{10}]; \\
A_{41} &= A_0 + [SV_{21} + E_1]; & A_{42} &= A_0 - [SV_{21} + E_1]; \\
& & & \vdots \\
A_{49} &= A_0 + [SV_{25} + E_5]; & A_{50} &= A_0 - [SV_{25} + E_5];
\end{aligned}$$

Thus, 50 perturbations which are symmetric around the control analysis are obtained.

In addition to pay attention to the initial state uncertainty, also ***the model physics tendencies*** are perturbed at ECMWF. Hence, the model version used for each pair of initial state perturbations are slightly different. In particular the parameterization of deep convection is considered a source of uncertainty which may penetrate upscale.