TC PR Lecture 4 - Singular vectors and normal modes

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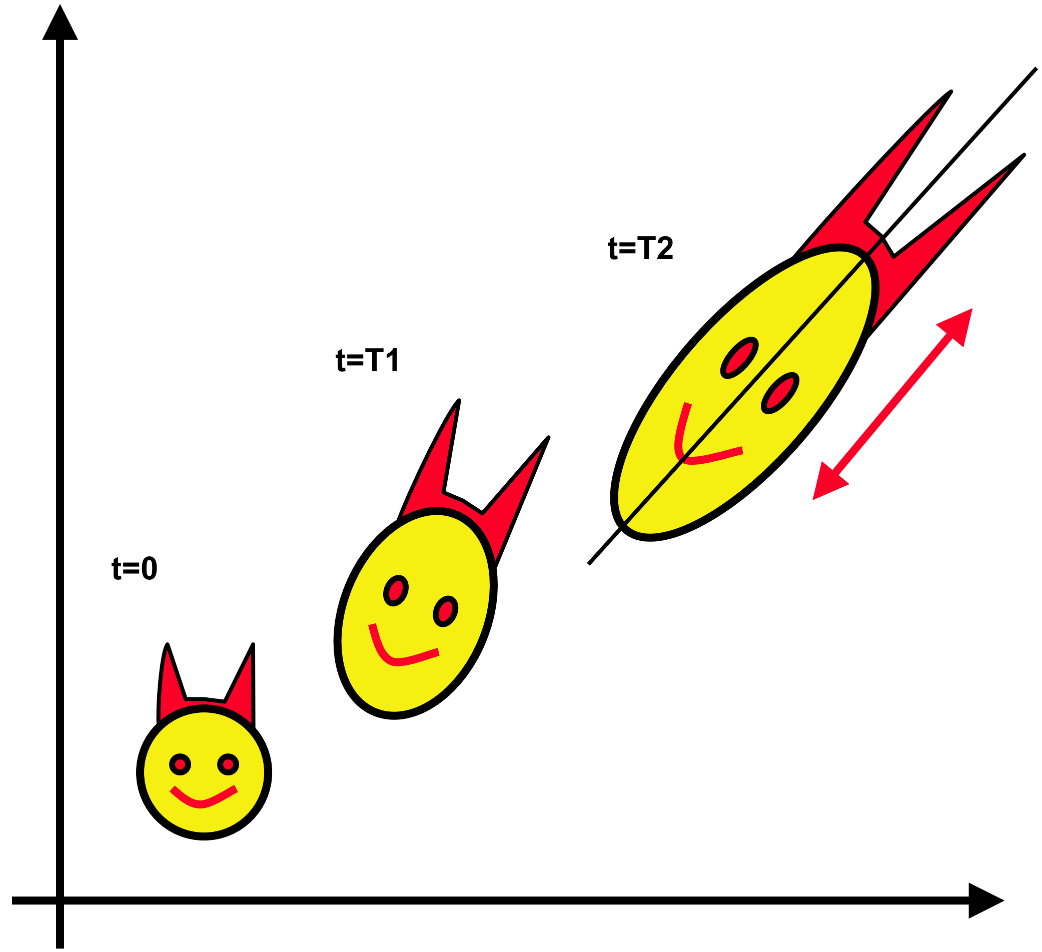
Outline

- Definition of singular vectors.
- Singular vectors and normal modes.
- Matrix decomposition: the SVD theorem.

How should initial uncertainties be defined?

Perturbations pointing along different axes in the phase-space of the system are characterized by different amplification rates. As a consequence, **the initial PDF is stretched principally along directions of maximum growth**.

The component of an initial perturbation pointing along a direction of maximum growth amplifies more than a component along another direction.



Total-energy metric (and norm) definition

Given two state-vectors ***x*** and ***y*** expressed in terms of vorticity ζ, divergence ***D***, temperature ***T***, specific humidity ***q*** and surface pressure π, the total energy metric (and the associated norms) is defined (<..,..> is the Euclidean inner product) as:

$$< x; E_{TE} y >= \frac{1}{2} \iint (\nabla\Delta^{-1}\zeta_x \cdot \nabla\Delta^{-1}\zeta_y + \nabla\Delta^{-1}D_x \cdot \nabla\Delta^{-1}D_y + \frac{C_p}{T_r} T_x T_y) d\Sigma \frac{\partial p}{\partial \eta} d\eta$$

$$+ \int (R_d \frac{T_r}{p_r} \ln \pi_x \ln \pi_y) d\Sigma$$

The adjoint operator

Given any two vectors ***x*** and ***y***, the adjoint operator $\boldsymbol{L}^*$ of the linear operator ***L*** with respect to the Euclidean norm <..,..> is the operator that satisfies the following property:

$$< L^* x; y > = < x; Ly >$$

Using the adjojnt operator $\boldsymbol{L}^*$ the time-t E-norm of z' can be written as:

$$\| z'(t) \|^2 = < L z'_0 ; E L z'_0 > = < z'_0 ; L^* E L z'_0 >$$

Singular vector definition

Consider an N-dimensional system:

$$\frac{\partial y}{\partial t} = A(y)$$

Denote by ***z'*** a small perturbation around a time-evolving trajectory ***z***:

$$\frac{\partial z'}{\partial t} = A_l(z)z' \qquad A_l(z) = \left.\frac{\partial A(z)}{\partial z}\right|_z$$

$$\frac{\partial z}{\partial t} = A(z)$$

The time evolution of the small perturbation ***z'*** is described to a good degree of approximation by the linearized system ***$A_l(z)$*** defined by the trajectory. Note that the trajectory is not constant in time.

Singular vector definition

The solution of the linearized system can be written in terms of the **linear propagator *L(t,0)***:

$$z'(t) = L(t,0)z'_0$$

The linear propagator is defined by the system equations and depends on the trajectory characteristics.

The E-norm of the perturbation at time ***t*** is given by:

$$\left\| z'(t) \right\|^2 = < z'(t); Ez'(t) > = < L(t,0)z'_0; EL(t,0)z'_0 >$$

Singular vector definition

The computation of the directions of maximum growth can be stated as 'finding the directions in the phase-space of the system characterized by the maximum ratio between the time-t and the initial norms':

$$\max_{x_0 \in \Sigma} \frac{\|x(t)\|_E^2}{\|x_0\|_{E_0}^2} = \max_{x_0 \in \Sigma} \frac{< x_0; L^* E L x_0 >}{< x_0; E_0 x_0 >}$$

The problem reduces to solving the following eigenvalue problem:

$$E_0^{-1/2} L^* E L E_0^{-1/2} v = \sigma^2 v$$

Example 1: singular vectors and normal modes

Example 1. Compute and compare the normal modes and the singular vectors with growth measured using the Euclidean inner product (i.e. ***E=Identity***) and for a stationary trajectory (***z=const***):

$$\frac{\partial z'}{\partial t} = A_l(z)z' \qquad A_l(z) = \left.\frac{\partial A(z)}{\partial z}\right|_z$$

$$\frac{\partial z}{\partial t} = A(z) = 0 \qquad z = const$$

For simplicity, suppose that the time integration is done with a forward time scheme:

$$\frac{\partial z'}{\partial t}(t) = \frac{z'(t+dt) - z'(t)}{dt}$$

with the equation right-hand-side computed at time t.

Example 1: singular vectors and normal modes

Then the finite-difference version of the linearized partial differential equation is:

$$z'(t+dt) = [\mathrm{I} + dt \cdot A_l(z(t))]z'(t)$$

and the linear propagator is given by:

$$L(t+dt,t) = \mathrm{I} + dt \cdot A_l(z(t))$$

Suppose that the time integrations from the initial time t_0 to the finite time $t=t_N$ is done in N steps. Then:

$$L(t,0) = \prod_{n=1,N} [\mathrm{I} + dt \cdot A_l(z(t_n))]$$

Ex1 SVs & NMs: normal modes

- **Normal modes.** The normal modes are solutions of the linearized partial differential equation of the form:

$$z'(x,t) = \xi(x)e^{\omega t}$$

Substituting z'(t) into the linearzied partial differential equation shows that the normal modes ξ_i are the eigenvalues of the linear model

$$A_l \xi_i = \omega_i \xi_i$$

Note that, since

$$L(t,0) = \prod_{n=1,N} [\mathrm{I} + dt \cdot A_l(z(t_n))]$$

ξ_i is also an eigenvector of the propagator L(t,0) with eigenvalue:

$$\pi_i = (1 + dt \cdot \omega_i)^N$$

Ex1 SVs & NMs: normal modes

Denote by (μ_l, θ_i) the eigenvectors/eigenvalues of the adjoint operator A_l^*:

$$A_l^* \eta_i = \theta_i \eta_i$$

η_i is also an eigenvector of the adjoint L^* with eigenvalue:

$$\rho_i = (1 + dt \cdot \theta_i)^N$$

Ex1 SVs & NMs: normal modes of L and of L*

Take the inner product of the equation that defines the normal modes of the adjoint operator with the k-th normal mode of $\boldsymbol{A_l}$

$$< A_l^* \eta_i ; \xi_k >=< \theta_i \eta_i ; \xi_k >$$

Applying the adjoint definition the following equation can be deduced:

$$< \eta_i ; A_l \xi_k >=< \theta_i \eta_i ; \xi_k >$$

Since ξ_i is the eigenvector of $\boldsymbol{A_l}$ it follows that the following equation must hold:

$$< \eta_i ; \omega_k \xi_k >=< \theta_i \eta_i ; \xi_k >$$

i.e.:

$$(\omega_k - \theta_i^{cc}) < \eta_i ; \xi_k >= 0$$

Ex1 SVs & NMs: normal modes of L and of L*

Both the normal modes of $\boldsymbol{A_l}$ and of the adjoint operator $\boldsymbol{A_l^*}$ are a complete (but not orthogonal) basis. The equation:

$$(\omega_k - \theta_i^{cc}) < \eta_i ; \xi_k >= 0$$

indicates that one of the following identities must hold:

$$\omega_k = \theta_i^{cc} \qquad\qquad < \eta_i ; \xi_k >= 0$$

The eigenvector η_k of $\boldsymbol{A_l^*}$ for which:

$$< \eta_i ; \xi_k > \neq 0$$

is called the adjoint eigenvector of the eigenvector ξ_l. The adjoint eigenvalue θ_k is equal to the complex-conjugate of the eigenvalue μ_l. The adjoint eigenvector is orthogonal to all but one of the eigenvectors of $\boldsymbol{A_l}$, i.e.:

$$< \eta_i ; \xi_k >= \cos(\alpha)\delta_{i,k}$$

Ex1 SVs & NMs: singular vectors for a self-adjoint L

- **Singular vectors if L is self-adjoint ($L^*L=L^2$).**

By definition, the singular vectors are defined by solving (since ***E=I***):

$$L^* L v_i = \sigma_i^2 v_i$$

Since ***L*** is self-adjoint, the problem reduces to:

$$L^2 v_i = \sigma_i^2 v_i$$

Since for a normal mode

$$L^2 \xi_i = L(L\xi_i) = L(\pi_i \xi_i) = \pi_i^2 \xi_i$$

the **normal modes coincide with the singular vectors $\xi_I = v_I$**. The **singular values** are

$$\sigma_i = \pi_i$$

Ex1 SVs & NMs: singular vectors and normal modes: $t \to \infty$

- **Leading singular vector ν_1 if L is not self-adjoint for long time intervals ($t \to \infty$).**

The (normalized) normal modes can be used as a basis onto which any vector can be expanded:

$$x(t) = \sum_i c_i \xi_i e^{\omega_i t}$$

The coefficients c_i are defined by considering the inner product of ***x(0)*** with the eigenvectors of the adjoint operator:

$$< \eta_k ; x(t=0) > = < \eta_k ; \sum_i c_i \xi_i >$$

Applying the relationship between the eigenvectors and the adjoint eigenvector, it follows that:

$$c_i = \frac{< \eta_i ; x_0 >}{< \eta_i ; \xi_i >} = \frac{< \eta_i ; x_0 >}{\cos(\alpha)}$$

Ex1 SVs & NMs: singular vectors and normal modes: t→∞

For $t \to \infty$:

$$x(t) = \sum_i c_i \xi_i e^{\omega_i t} \xrightarrow{t\to\infty} c_1 \xi_1 e^{\omega_1 t}$$

This equation indicates that to maximize the final-time norm the initial normalized (I.e. with unit norm) pattern ***x(0)*** must have the largest possible coefficient c_1. One possible choice would be to define ***x(0)*** as the initial-time leading normal mode:

$$x(0) = \xi_1$$

In this case

$$c_1 = \frac{< \eta_1 ; x_0 >}{< \eta_1 ; \xi_1 >} = \frac{< \eta_1 ; \xi_1 >}{< \eta_1 ; \xi_1 >} = 1$$

and the final-time norm would be:

$$\left\| x(t) \right\|^2 = e^{2\omega_1 t}$$

Ex1 SVs & NMs: singular vectors and normal modes: t→∞

Another possible choice would be to define ***x(0)*** as the initial-time (normalized) adjoint normal mode:

$$x(0) = \eta_1$$

In this case:

$$c_1 = \frac{<\eta_1; x_0>}{<\eta_1; \xi_1>} = \frac{<\eta_1; \eta_1>}{<\eta_1; \xi_1>} = \frac{1}{\cos(\alpha)} > 1$$

and the final-time norm would be:

$$\|x(t)\|^2 = (\frac{1}{\cos(\alpha)})^2 e^{2\omega_1 t} > e^{2\omega_1 t}$$

Ex1 SVs & NMs: singular vectors and normal modes: t→∞

Any other choice

$$x(0) = \sum_j \beta_j \eta_j$$

would yield (*β_j***<1** since the initial state has unit norm) :

$$c_1 = \frac{<\eta_1;x_0>}{<\eta_1;\xi_1>} = \beta_1 \frac{<\eta_1;\eta_1>}{<\eta_1;\xi_1>} = \frac{\beta_1}{\cos(\alpha)} < \frac{1}{\cos(\alpha)}$$

and the final-time norm would be:

$$\|x(t)\|^2 \xrightarrow{t\to\infty} (\frac{\beta_1}{\cos(\alpha)})^2 e^{2\omega_1 t} < (\frac{1}{\cos(\alpha)})^2 e^{2\omega_1 t}$$

Ex1 SVs & NMs: singular vectors and normal modes: t→∞

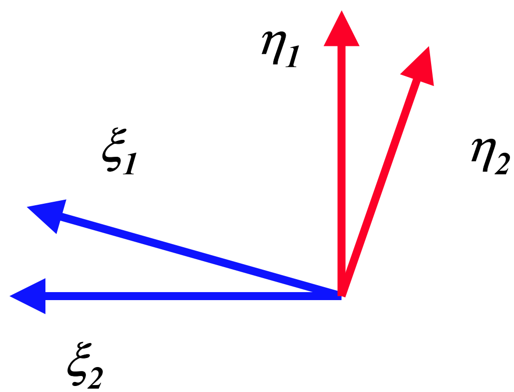
Thus, for t → ∞ the leading singular vector at final time t asymptote to the leading normal mode and at initial time is determined by the first adjoint normal mode

$$x(0) = \eta_1$$

$$x(t) \xrightarrow{t \to \infty} \frac{1}{\cos(\alpha)} \xi_1 e^{\omega_1 t}$$

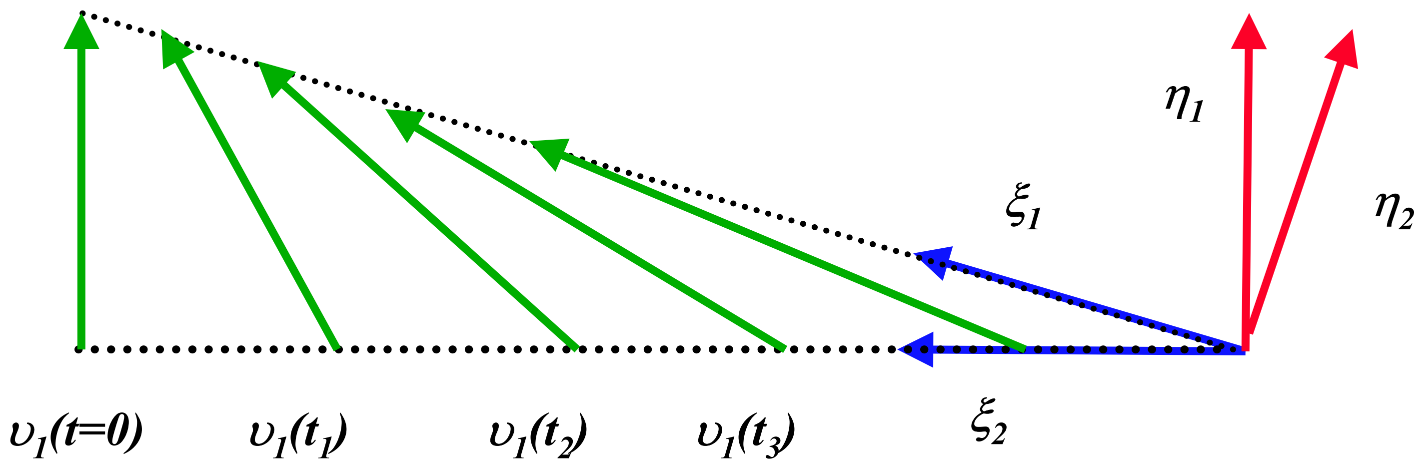
Example 2: SVs & NMs for a 2d system with decaying NMs

Example 2. Compare normal modes and singular vectors with growth measured using the Euclidean inner product for a 2-dimensional system with **two decaying (non-orthogonal) normal modes** ξ_1 and ξ_2 with eigenvalues $\mathbf{0>\omega_1>\omega_2}$. The two adjoint normal modes η_1 and η_2 are orthogonal, respectively, to ξ_2 and ξ_1 .



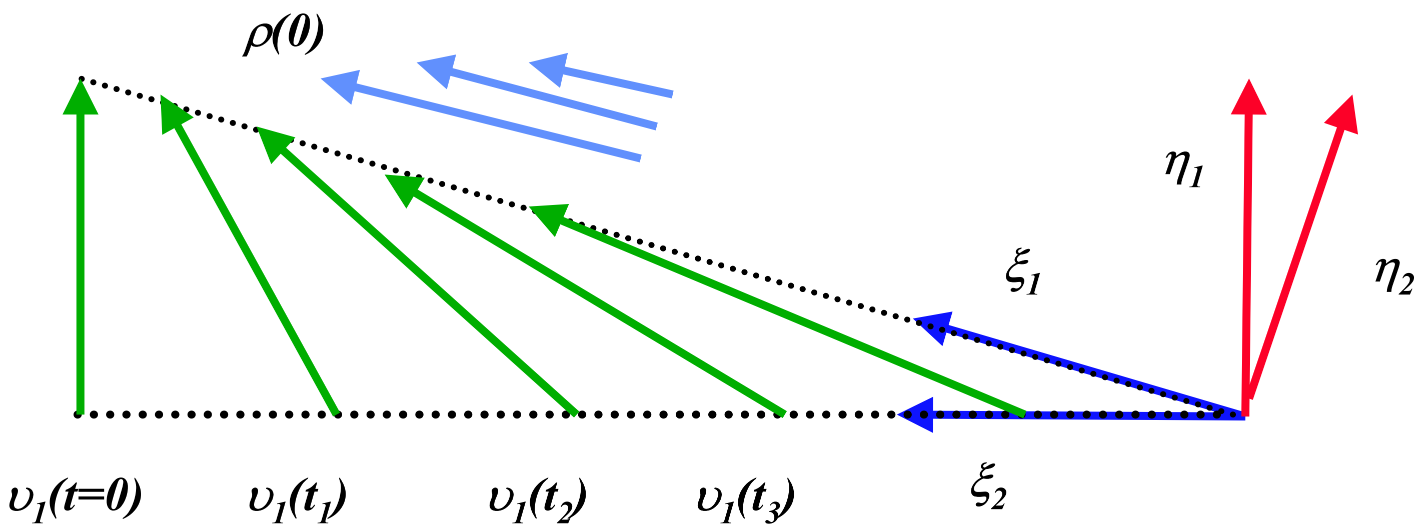
Ex2: SVs & NMs for a 2d system with decaying NMs

Consider a normalized initial vector $\upsilon_1(0)$ parallel to η_1. Its time evolution can be mapped along the ξ_1 and ξ_2 directions. Since the two normal modes are decaying, the components along the two directions shrink with time. As time progresses, the norm of $\upsilon_1(t)$ increases and the vector is aligning along the least-decaying normal mode ξ_1 .



Ex2: SVs & NMs for a 2d system with decaying NMs

By contrast, the norm of an initial normalized vector $\rho(0)$ parallel to ξ_1 would decrease as time progresses. Thus, despite the fact that the normal modes are decaying, an initial perturbation aligned along the adjoint of the leading normal mode can amplify as time progresses.



Example 3: SVs & NMs for a 2d system

Example 3. Consider a 2-dimensional linear system defined by the real matrix:

$$\frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = A\begin{pmatrix} x \\ y \end{pmatrix} \qquad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

Problem: compare the normal modes and the singular vectors with growth measured using the Euclidean inner product. Suppose that the eigenvalue problem $\boldsymbol{Ax=\lambda x}$ that defines the normal modes as two distinct solutions:

$$\omega_{1,2} = \frac{a+d\pm\sqrt{\Delta}}{2} \qquad \Delta = (a+d)^2 - 4(ad-bc)$$

with corresponding eigenvectors ξ_1 and ξ_2. The two normal modes are $\xi_i e^{\omega_i t}$.

Ex3: SVs & NMs for a 2d system

- ***Δ>0***. In this case there are two distinct real eigenvalues and corresponding real eigenvectors.

A generic vector ***x(t)*** can be written in terms of the normal modes as:

$$x(t) = \alpha_1 \xi_1 e^{\omega_1 t} + \alpha_2 \xi_2 e^{\omega_2 t}$$

and the norm would be:

$$\|x(t)\|^2 = \alpha_1^2 e^{2\omega_1 t} + \alpha_2^2 e^{2\omega_2 t} + 2\alpha_1 \alpha_2 < \xi_1 ; \xi_2 > e^{(\omega_1 + \omega_2) t}$$

Ex3: SVs & NMs for a 2d system

- ***Δ<0***. In this case the two eigenvalues are complex conjugate:

$$\omega_{1,2} = \omega_r \pm i\omega_i$$

where ω_r and ω_i are the two real numbers, and the eigenvectors are also complex, with:

$$\xi_2 = \xi_1^{cc}$$

A generic vector ***x(t)*** can be written in terms of the normal modes as:

$$x(t) = \alpha\xi_1 e^{(\omega_r + i\omega_i)t} + c.c. = 2[\mathrm{Re}(\alpha\xi_1)\cos(\omega_i t) - \mathrm{Im}(\alpha\xi_1)\sin(\omega_i t)]e^{\omega_r t}$$

and the norm would be:

$$\|x(t)\|^2 = 4[\|\mathrm{Re}(\alpha\xi_1)\|^2(\cos(\omega_i t))^2 + \|\mathrm{Im}(\alpha\xi_1)\|^2(\sin(\omega_i t))^2$$
$$- < \mathrm{Re}(\alpha\xi_1); \mathrm{Im}(\alpha\xi_1) > \sin(2\omega_i t)]e^{\omega_r t}$$

Ex3: SVs & NMs for a 2d system

Consider the case of a neutral or damped system (i.e. $\omega_r \leq 0$ $\omega_i \leq 0$ when $\Delta > 0$ or $\omega_r \leq 0$ when $\Delta < 0$). In both cases the contribution to the time-t norm that depends from the inner product between the two normal modes can increase the norm between the initial and final time:

$$\Delta \geq 0 \qquad \|x(t)\|^2 = \alpha_1^2 e^{2\omega_1 t} + \alpha_2^2 e^{2\omega_2 t} + 2\alpha_1\alpha_2 < \xi_1;\xi_2 > e^{(\omega_1+\omega_2)t}$$

$$\Delta < 0 \qquad \|x(t)\|^2 = 4[\|\mathrm{Re}(\alpha\xi_1)\|^2 (\cos(\omega_i t))^2 + \|\mathrm{Im}(\alpha\xi_1)\|^2 (\sin(\omega_i t))^2 - < \mathrm{Re}(\alpha\xi_1);\mathrm{Im}(\alpha\xi_1) > \sin(2\omega_i t)]e^{\omega_r t}$$

Thus **if the two normal modes are not orthogonal** there could be finite-time growth even if the normal modes are neutral or damped.

Example 4: examples of SVs/NMs for a 2d system

Example 4. Consider a 2-dimensional linear system defined by the real matrix:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad \frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}$$

and suppose for simplicity that the time integration is done with a simple forward method:

$$\frac{dx}{dt} = \frac{x(t+dt) - x(t)}{dt}$$

Thus the differential equation becomes:

$$\begin{pmatrix} x(t+dt) \\ y(t+dt) \end{pmatrix} = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} + dt\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} x(t) \\ y(t) \end{pmatrix}$$

Ex 4: examples of SVs/NMs for a 2d system

The linear propagator is:

$$L(t,0) = \prod_{n=1,N} (\mathrm{I} + dt \cdot A) = \prod_{n=1,N} \begin{pmatrix} 1 + dt \cdot a & b \\ c & 1 + dt \cdot d \end{pmatrix}$$

Suppose for simplicity that dt=1, N=1, and that: $A = \begin{pmatrix} -5 & 1 \\ 2 & -3 \end{pmatrix}$

Then:

$$L = \begin{pmatrix} -4 & 1 \\ 2 & -2 \end{pmatrix} \qquad L^* = \begin{pmatrix} -4 & 2 \\ 1 & -2 \end{pmatrix} \qquad L^* L = \begin{pmatrix} 20 & -8 \\ -8 & 5 \end{pmatrix}$$

Ex 4: examples of SVs/NMs for a 2d system

The normal modes are:

$$\xi_1 = \begin{pmatrix} 0.80 \\ -0.59 \end{pmatrix} \qquad \omega_1 = -5.7$$

$$\xi_2 = \begin{pmatrix} 0.34 \\ 0.93 \end{pmatrix} \qquad \omega_2 = -2.2 \qquad <\xi_1;\xi_2> = -0.27$$

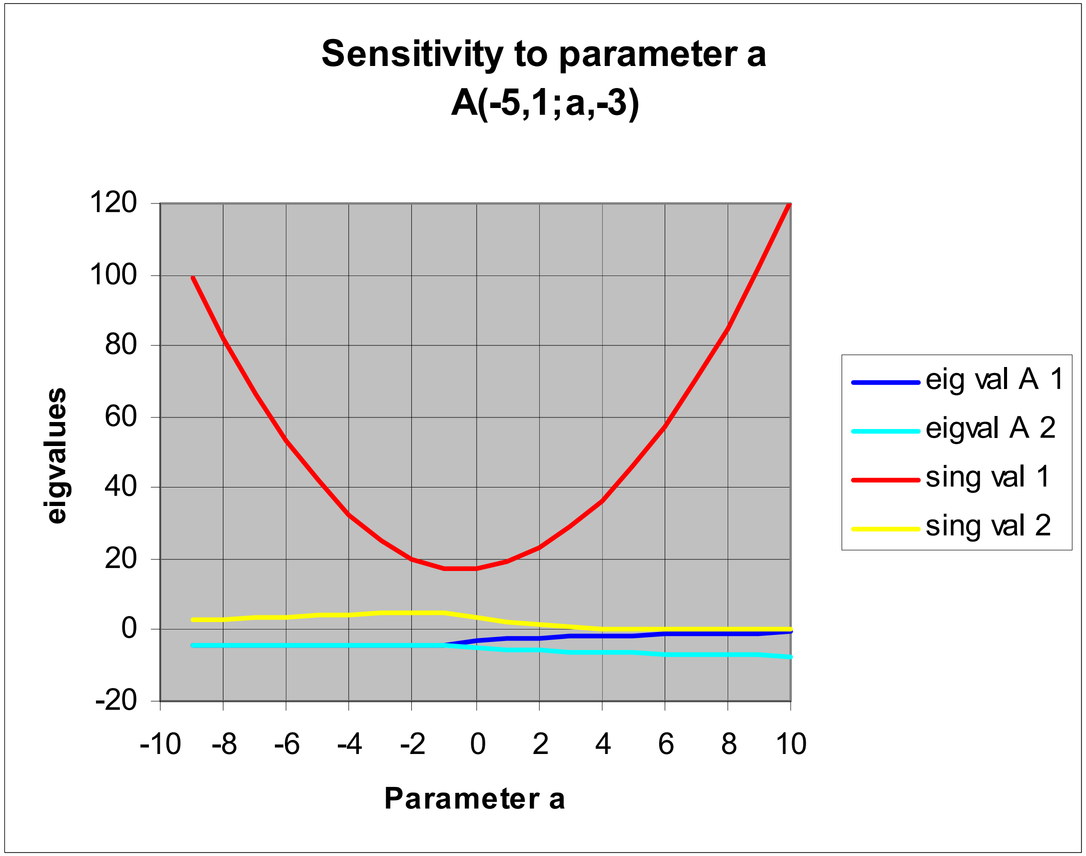
The singular vectors are:

$$v_1 = \begin{pmatrix} 0.91 \\ -0.39 \end{pmatrix} \qquad \sigma_1 = 4.84$$

$$v_2 = \begin{pmatrix} 0.39 \\ 0.91 \end{pmatrix} \qquad \sigma_2 = 1.23$$

Ex 4: examples of SVs/NMs for a 2d system

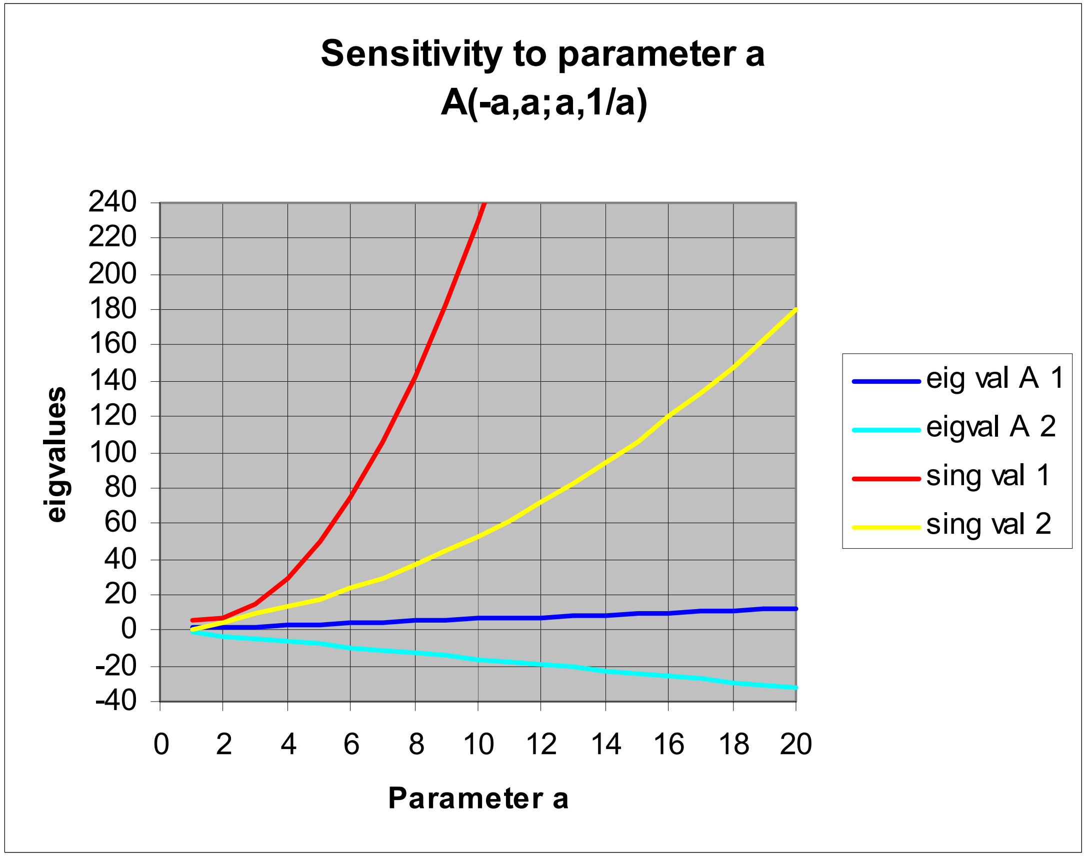
$$A = \begin{pmatrix} -5 & 1 \\ a & -3 \end{pmatrix}$$



This figure shows the eigenvalues ω_1 and ω_2 and the singular values σ_1 and σ_2 as a function of the parameter a for N=1 time units (dt=1).

Ex 4: examples of SVs/NMs for a 2d system

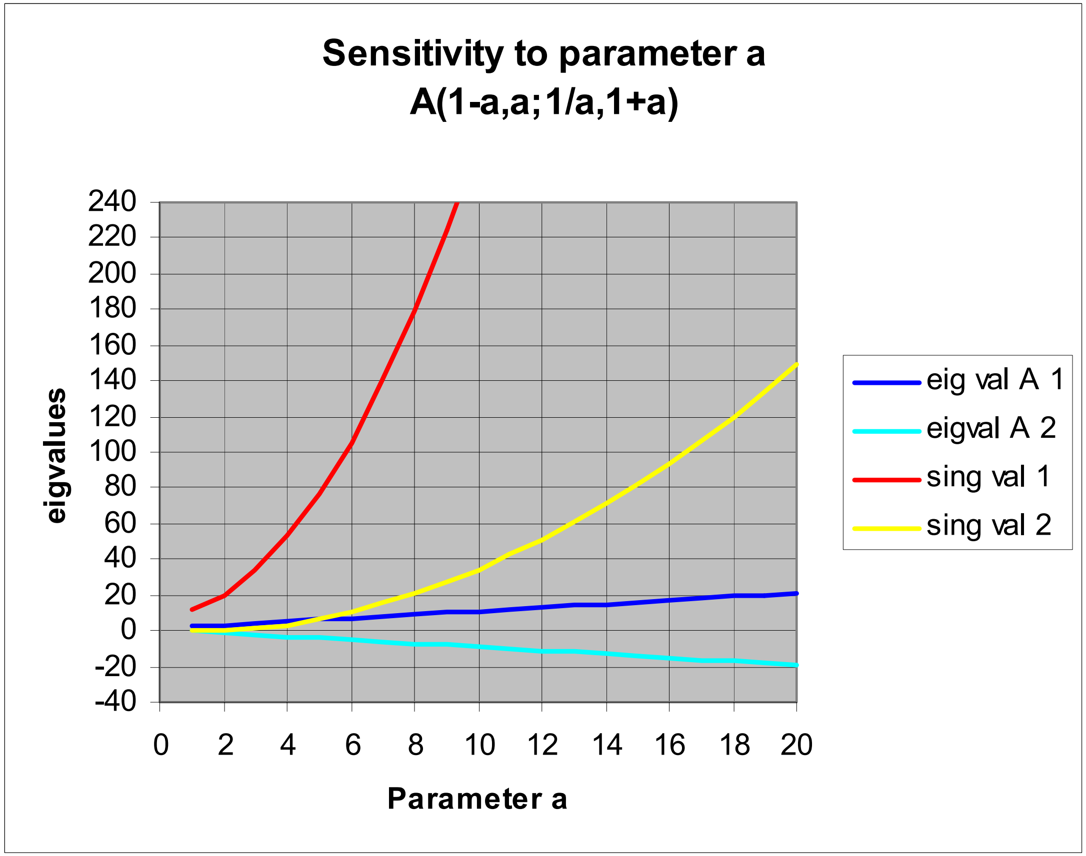
$$A = \begin{pmatrix} -a & a \\ a & 1/a \end{pmatrix}$$



This figure shows the eigenvalues ω_1 and ω_2 and the singular values σ_1 and σ_2 as a function of the parameter a for N=1 time units (dt=1).

Ex 4: examples of SVs/NMs for a 2d system

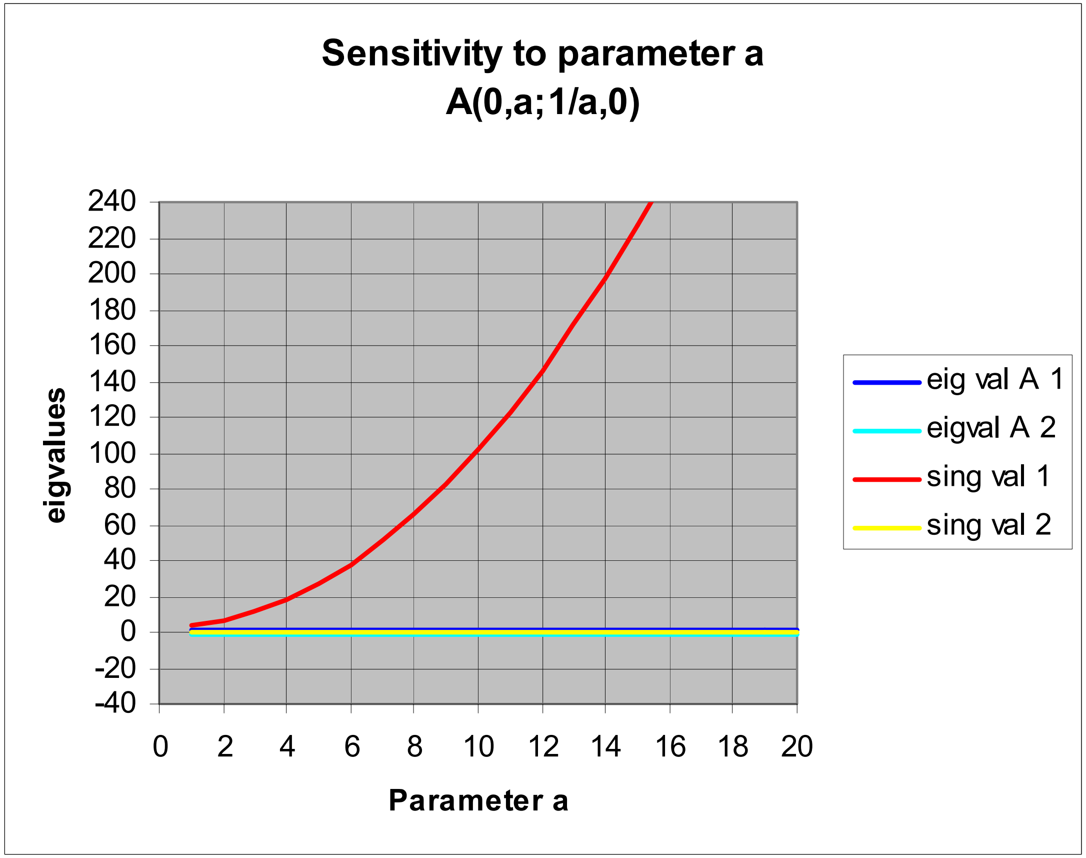
$$A = \begin{pmatrix} 1-a & a \\ 1/a & 1+a \end{pmatrix}$$



This figure shows the eigenvalues ω_1 and ω_2 and the singular values σ_1 and σ_2 as a function of the parameter a for N=1 time units (dt=1).

Ex 4: examples of SVs/NMs for a 2d system

$$A = \begin{pmatrix} 0 & a \\ 1/a & 0 \end{pmatrix}$$



This figure shows the eigenvalues ω_1 and ω_2 and the singular values σ_1 and σ_2 as a function of the parameter *c* for N=1 time units (dt=1).

Linear algebra: the singular value decomposition

Singular vectors derive from one of the most important decompositions in matrix computation: the singular value decomposition.

SVD theorem. If $A \in R^{mxn}$ then there exist orthogonal matrices

$$U = [u_1,..,u_m] \in R^{mxm} \qquad V = [v_1,..,v_n] \in R^{nxn}$$

such that

$$U^T AV = diag(\sigma_1,..,\sigma_p) \qquad p = \min\{m,n\} \qquad \sigma_1 \geq \sigma_2 \geq .. \geq \sigma_p \geq 0$$

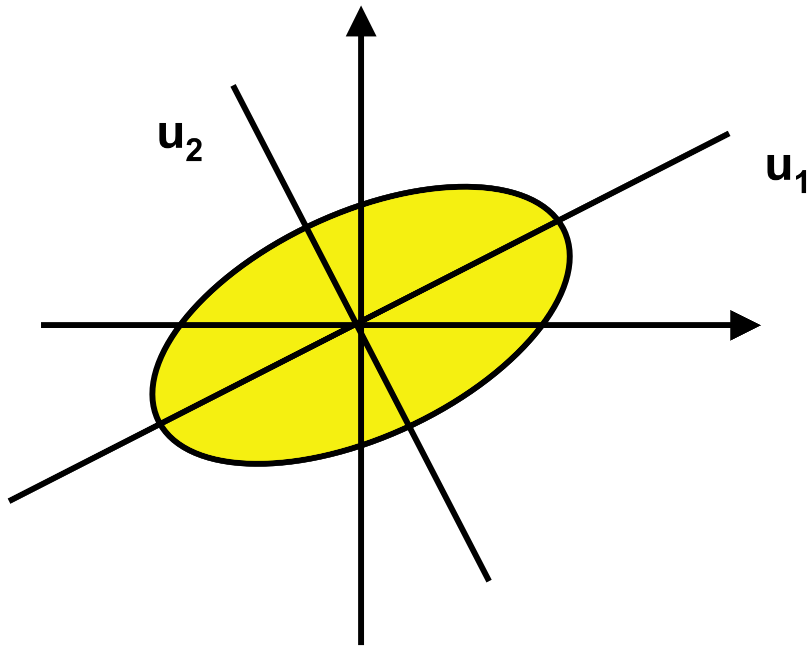
The σ_i are the **singular values**, the vectors u_i and v_i the **left** and **right singular vectors.** The singular vectors satisfy:

$$Av_i = \sigma_i u_i \qquad A^T u_i = \sigma_i v_i$$

Linear algebra: SVD

The singular values are the lengths of the semi-axes of the hyper-ellipsoid E defined by:

$$E = \{ y \mid y = Ax, \|x\|_2 = 1 \}$$



In fact, given a generic $x = au_1 + (1-a)u_2$:

$$Ax = a\sigma_1 u_1 + (1-a)\sigma_2 u_2$$

The length of the vector x is:

$$\|Ax\| = \sqrt{a^2\sigma_1^2 + (1-a)^2\sigma_2^2}$$

Since $\sigma_1 \geq \sigma_2$, this length is maximum for a=1.

Linear algebra: SVD properties

Define the following norms:

- **Frobenius norm:** $$\|A\|_F = \sqrt{\sum_{i=1,m}\sum_{j=1,n}|a_{i,j}|^2}$$

- **p-norms:** $$\|A\|_p = \sup_{x\neq 0}\frac{\|Ax\|_p}{\|x\|_p}$$

Given the SVD of A: $$U^T A V = \Sigma$$

then: $$\|A\|_F = \sqrt{\sum_{j=1,p}\sigma_j^2}$$

$$\|A\|_2 = \sigma_1^2$$

Linear algebra: SVD example

The SVD reveals a great deal about the structure of a matrix.

Consider for example:

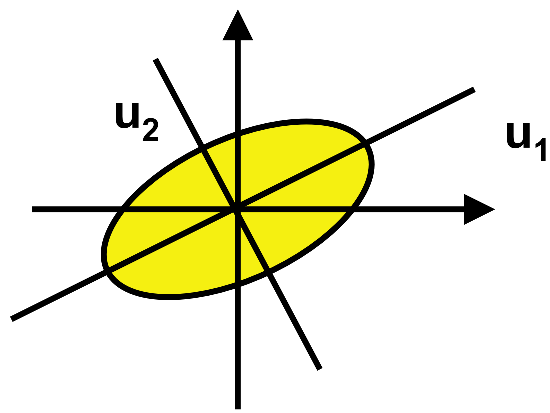
$$A = USV^T = \begin{pmatrix} 2.11 & -0.74 \\ 1.74 & 2.23 \end{pmatrix}$$

where:

$$U = \begin{pmatrix} 1/\sqrt{5} & 2/\sqrt{5} \\ 2/\sqrt{5} & -1/\sqrt{5} \end{pmatrix} \qquad V = \begin{pmatrix} 3/\sqrt{13} & 2/\sqrt{13} \\ 2/\sqrt{13} & -3/\sqrt{13} \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$$

Then:

$$\|A\|_F = \sqrt{13} \qquad \|A\|_2 = 3$$



Redefinition of SVs using the SVD theorem

Given the linear propagator L(t,0), denote by

$$U = [u_1, .., u_m] \in R^{mxm} \qquad V = [v_1, .., v_n] \in R^{nxn}$$

the two orthogonal matrices that define the SVD of L:

$$U^T L V = \Sigma \qquad L = U \Sigma V^T$$

From:

$$L v_i = \sigma_i u_i \qquad L^T u_i = \sigma_i v_i$$

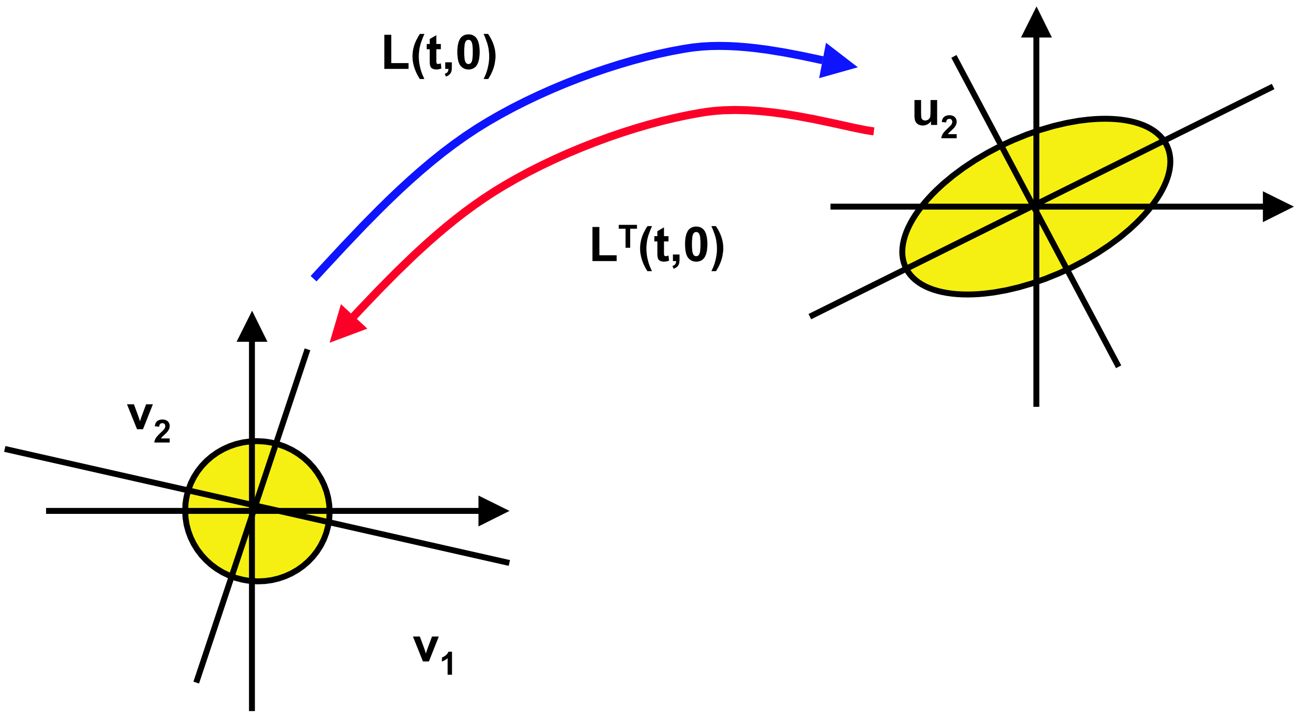
it follows that:

$$L^T L v_i = L^T \sigma_i u_i = \sigma_i^2 v_i \qquad L L^T u_i = L \sigma_i v_i = \sigma_i^2 u_i$$

The singular values σ_i are the length of the semi-axes of the hyper-ellipsoid E defined by $L^T L$ that coincide with the left singular vectors u_i.

Redefinition of SVs from SVD theorem

The right singular vectors v_i define the vectors that evolve into the left singular vectors.



Conclusions

- Singular vectors have been defined. They identify phase-space directions characterized by maximum growth (as measured by a matrix E) during a finite time interval (called the optimisation time interval).
- The singular vector and the normal mode approaches to stability analysis have been compared. Some simple 2-dim examples have been discussed.
- The SVD matrix decomposition theorem has been introduced.

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