

Tips and tricks for Koopman analysis

Jean-Christophe Loiseau

$$\ddot{x} = x - x^3$$

$$= -\nabla U(x)$$

$$m\ddot{x} = \underbrace{F}_{\text{ma}}$$

$$\text{where } U(x) = \frac{x^4}{4!} - \frac{x^2}{2}$$

$$\dot{x} = v$$

$$\dot{v} = x - x^3$$



Steve Brunton



Jean-Christophe Loiseau



Bernard Koopman (1900-1981)

Overview of Koopman theory

Poincaré point of view

$$\begin{aligned}\mathbf{x}_{i+1} &= \mathbf{F}(\mathbf{x}_i, \tau) \\ \mathbf{y}_{i+1} &= \mathbf{g}(\mathbf{x}_i)\end{aligned}$$

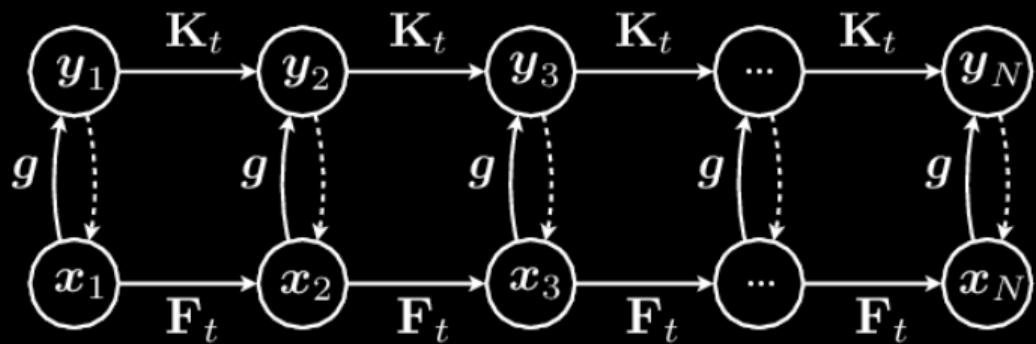
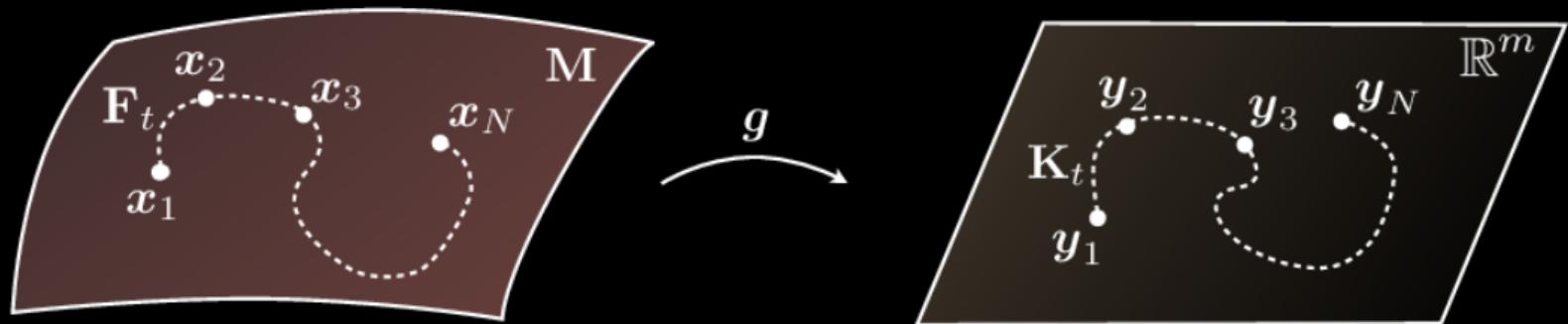
Koopman point of view

$$\begin{aligned}\mathcal{K}_\tau g &= g \circ \mathbf{F} \\ \mathcal{K}_\tau g(\mathbf{x}_i) &= g(\mathbf{x}_{i+1})\end{aligned}$$

$$\mathcal{K}_\tau(\alpha g_1 + \beta g_2) = (\alpha g_1 + \beta g_2) \circ \mathbf{F}$$

⇓

$$\alpha \mathcal{K}_\tau g_1 + \beta \mathcal{K}_\tau g_2 = \alpha g_1 \circ \mathbf{F} + \beta g_2 \circ \mathbf{F}$$



$\mathbf{F}_t: x_k \mapsto x_{k+1}$
$g: x_k \mapsto y_k$
$\mathbf{K}_t : y_k \mapsto y_{k+1}$

$$\left\| \hat{\mathcal{K}} - \mathcal{K} \right\|_{HS}^2 = \left\| \hat{\mathcal{K}} \right\|_{HS}^2 - 2\langle \hat{\mathcal{K}} | \mathcal{K} \rangle_{HS} + \left\| \mathcal{K} \right\|_{HS}^2$$

Let f_i , g_i and $\hat{\sigma}_i$ be the i^{th} singular triplet of $\hat{\mathcal{K}}$. We can then write

$$\|\hat{\mathcal{K}} - \mathcal{K}\|_{HS}^2 = \sum_{i=1}^r \hat{\sigma}_i^2 \langle f_i | f_i \rangle_{\rho_1} \langle g_i | g_i \rangle_{\rho_0} - 2 \sum_{i=1}^r \hat{\sigma}_i \langle f_i | \mathcal{K} g_i \rangle + \sum_{j=1}^{\infty} \sigma_j^2$$

Maximize this score based on data

$$\left\| \hat{\mathcal{K}} - \mathcal{K} \right\|_{HS}^2 = -\mathcal{R}_E(\hat{\sigma}, f, g) + \|\mathcal{K}\|_{HS}^2$$

Let $\chi_0 = [\chi_0^{(1)} \ \chi_0^{(2)} \ \chi_0^{(3)} \ \dots]^T$ be an arbitrary basis for the input space \mathcal{L}_0^2 , and let $\mathbf{g} = \mathbf{V}^T \chi_0$ be an orthonormal basis for this space. It must then satisfy

$$\langle g_i | g_j \rangle_{\rho_0} = \mathbf{v}_i^T \mathbf{C}_{00} \mathbf{v}_j = \delta_{ij}$$

with $\mathbf{C}_{00} = \mathbb{E} [\chi_0(\mathbf{x}_t) \chi_0(\mathbf{x}_t)^T]$. A similar expression applies for f with basis χ_1 and density ρ_1 .

After some algebraic manipulations, we arrive at

$$\underset{\mathbf{U}, \mathbf{V}}{\text{maximize}} \quad \text{Tr} (\mathbf{U}^T \mathbf{C}_{10} \mathbf{V})$$

$$\text{subject to} \quad \mathbf{U}^T \mathbf{C}_{11} \mathbf{U} = \mathbf{I}_r$$

$$\mathbf{V}^T \mathbf{C}_{00} \mathbf{V} = \mathbf{I}_r$$

with $\mathbf{C}_{10} = \mathbb{E} [\boldsymbol{\chi}_1(\mathbf{x}_t) \boldsymbol{\chi}_0(\mathbf{x}_{t+\tau})]$.

1. Compute the covariance matrices \mathbf{C}_{00} , \mathbf{C}_{11} , and \mathbf{C}_{10} .
2. Perform the truncated SVD

$$\mathbf{C}_{11}^{-\frac{1}{2}} \mathbf{C}_{10} \mathbf{C}_{00}^{-\frac{1}{2}} = \mathbf{U}' \mathbf{K} \mathbf{V}'^T$$

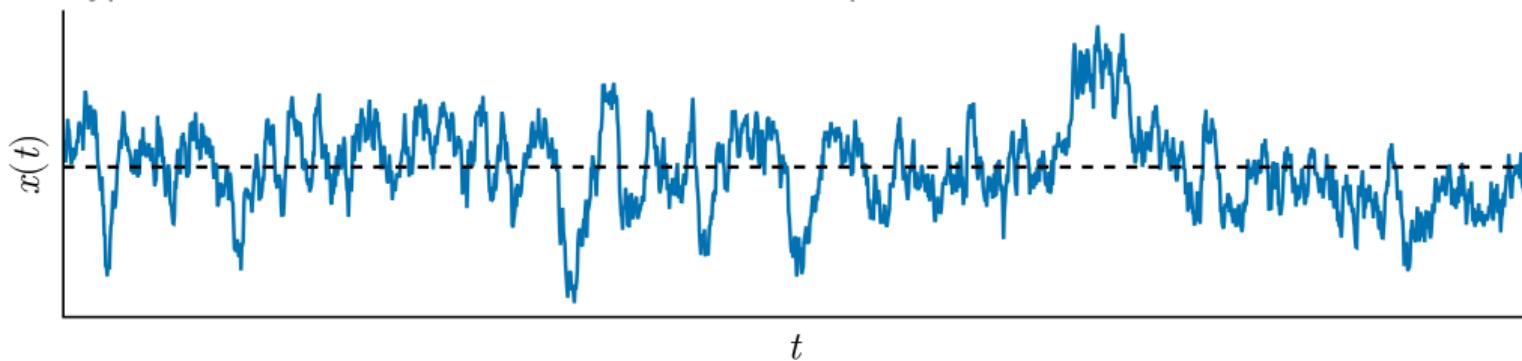
3. Compute $\mathbf{U} = \mathbf{C}_{11}^{-\frac{1}{2}} \mathbf{U}'$ and $\mathbf{V} = \mathbf{C}_{00}^{-\frac{1}{2}} \mathbf{V}'$.
4. Output the singular values K_{ii} and singular functions $f_i = \mathbf{u}_i^T \boldsymbol{\chi}_1$ and $g_i = \mathbf{v}_i^T \boldsymbol{\chi}_0$.

Orstein-Uhlenbeck process

$$d\mathbf{x}_t = \mathbf{A}\mathbf{x}_t dt + \mathbf{B} d\mathbf{w}_t$$

Orstein-Uhlenbeck process

Typical time-series of the Orstein-Uhlenbeck process with $a = -1$ and $b = 0.2$.



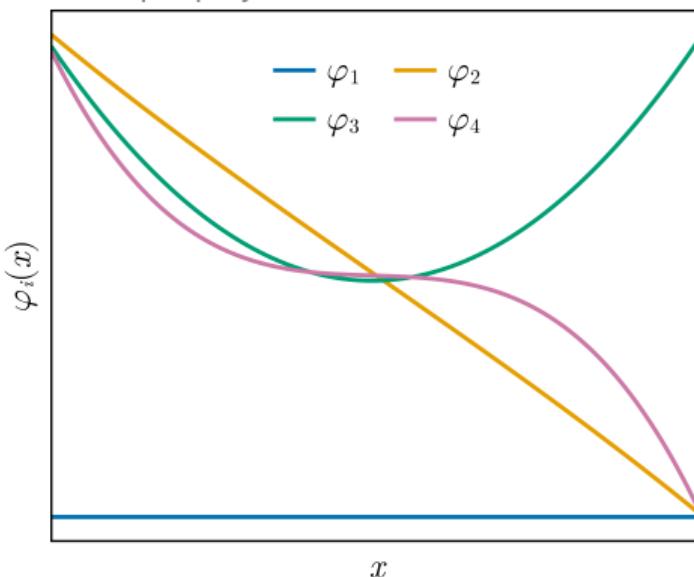
Given an ergodic time-series, use

$$\chi_0 = \chi_1 = [1 \quad x \quad x^2 \quad x^3 \quad \dots]^T$$

to approximate the Koopman singular functions.

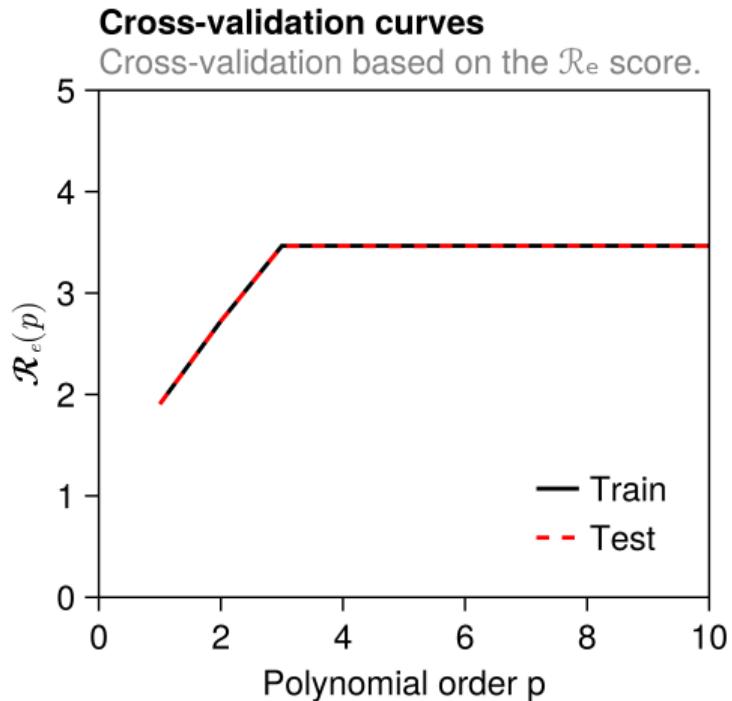
Orstein-Uhlenbeck process

Leading Koopman eigenfunctions consist in simple polynomials in x .



Use the VAMP-E score $\mathcal{R}_e(p)$ for cross-validation purposes.

For the OU process, setting $p > 3$ is unnecessary.

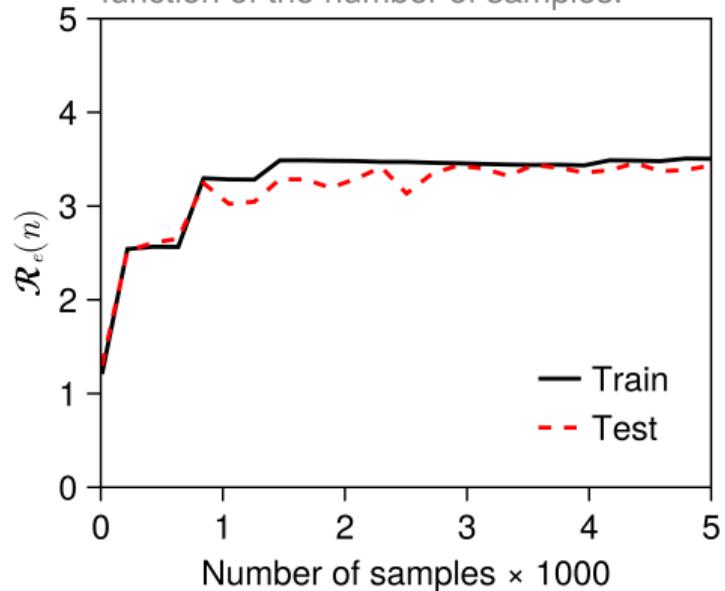


\mathcal{R}_e can also be used to check convergence w.r.t the size of the dataset.

For the OU process, a few thousands samples are sufficient.

Learning curves

Evolution of the VAMP-E \mathcal{R}_e score as a function of the number of samples.



Lorenz system

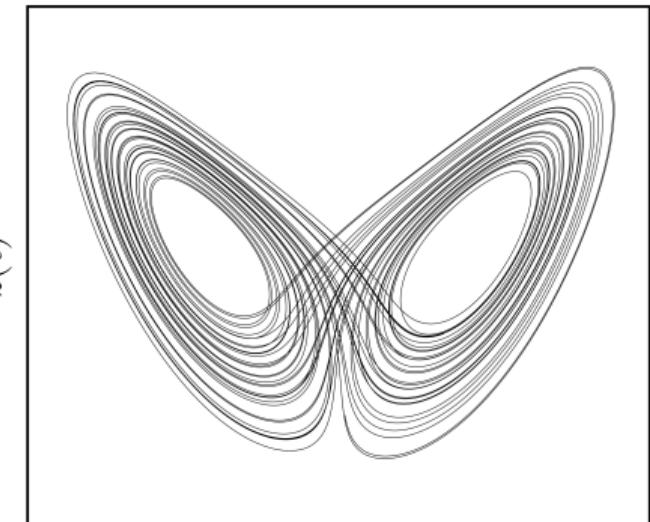
$$\dot{x} = \sigma(y - x)$$

$$\dot{y} = x(\rho - z) - y$$

$$\dot{z} = xy - \beta z$$

Lorenz attractor

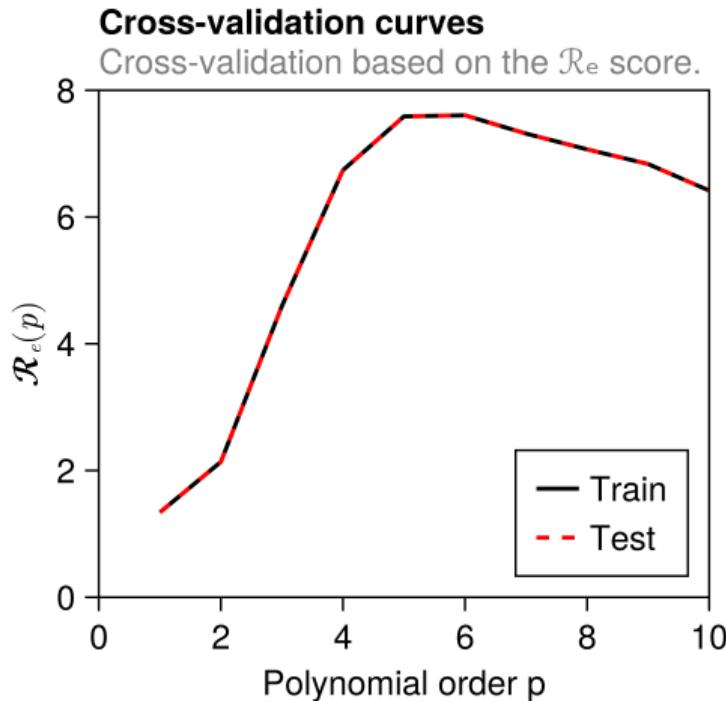
The poster child of chaos theory



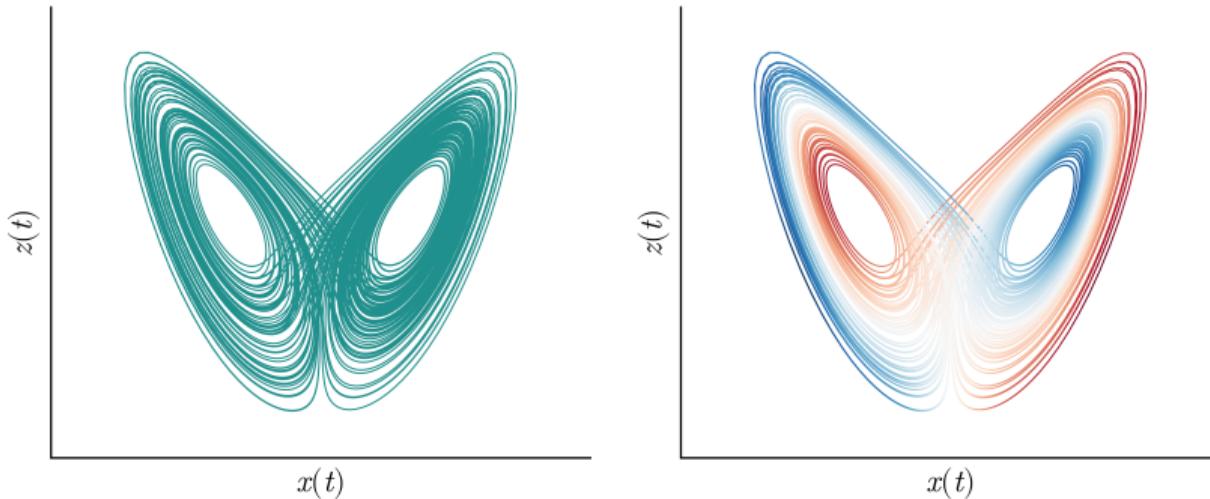
Given an ergodic time-series, use

$$\chi = [x \ y \ z \ x^2 \ xy \ xz \ y^2 \ \dots]^T$$

to approximate the Koopman singular functions.



Leading Koopman singular functions of the Lorenz system

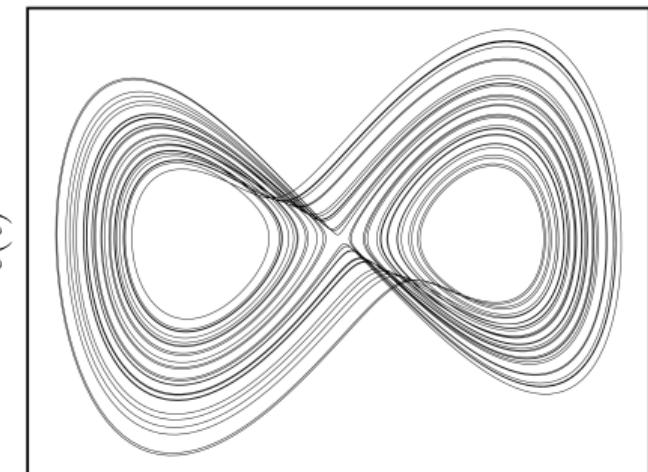


The leading non-trivial Koopman singular function partitions the state space into metastable (almost-invariants) sets.

If a single time-series is available, use Takens theorem and time-delay embedding to reconstruct the attractor.

Lorenz attractor

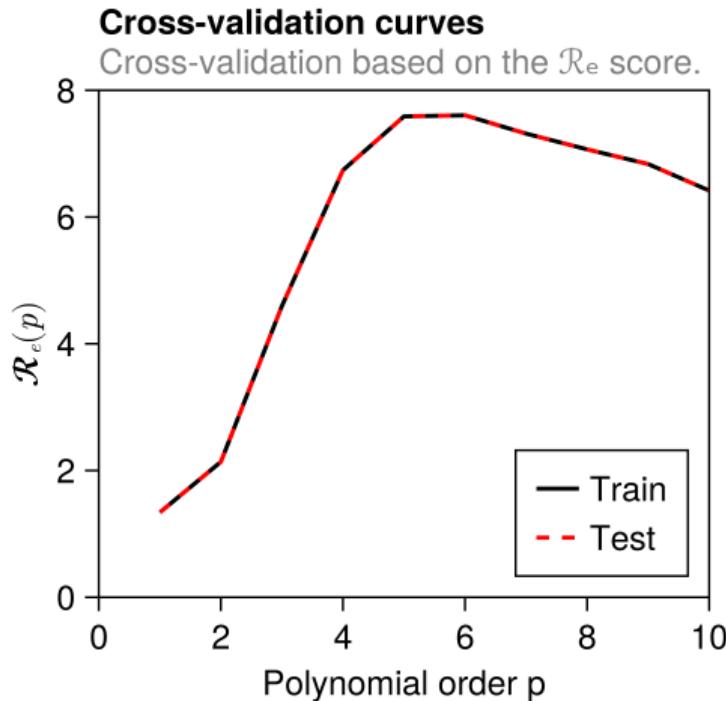
Broomhead-King reconstruction
of the attractor from $x(t)$.



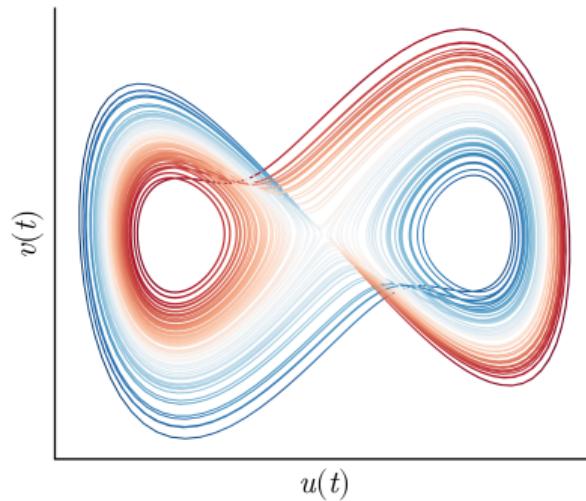
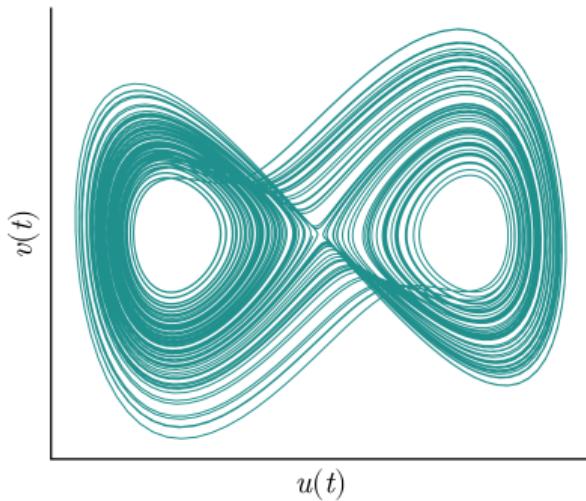
Given the reconstructed attractor, use

$$\chi = [u \ v \ w \ u^2 \ uv \ uw \ v^2 \ \dots]$$

to approximate the Koopman singular functions.

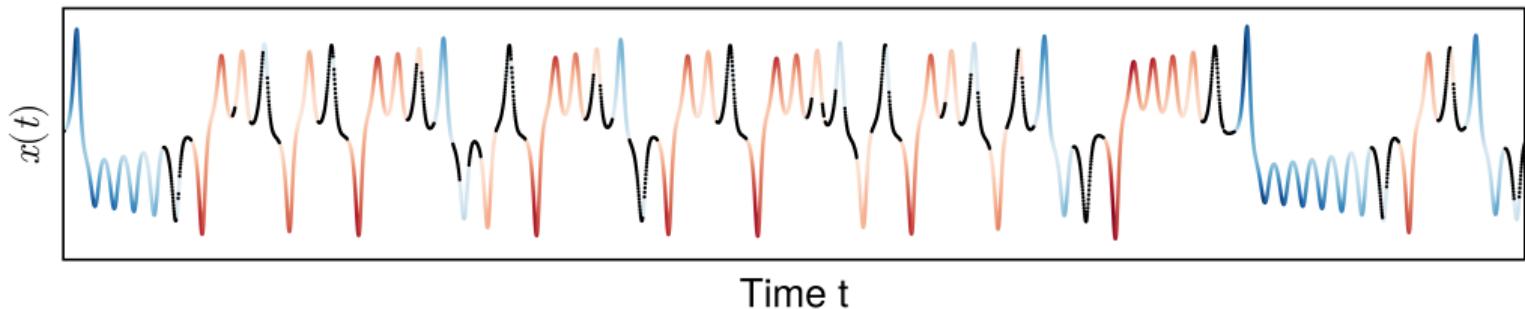


Leading Koopman singular functions of the Lorenz system with time-delay coordinates

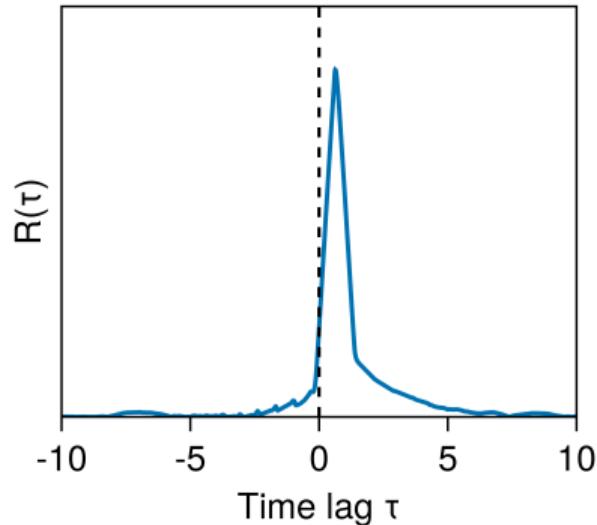


Koopman leading singular function evaluated along a trajectory

Points in black correspond to $|\varphi(x)| < \varepsilon$, highlighting that this Koopman function can be used as a predictor of incoming switching event.



Cross-correlation function



Let $f(t) = \text{sign}(x_t)$ and $g(t) = \text{sign}(\varphi_1(x_t))$. On average, $g(t)$ predicts a switching event **a whole period** before it occurs.

Application to a flow example



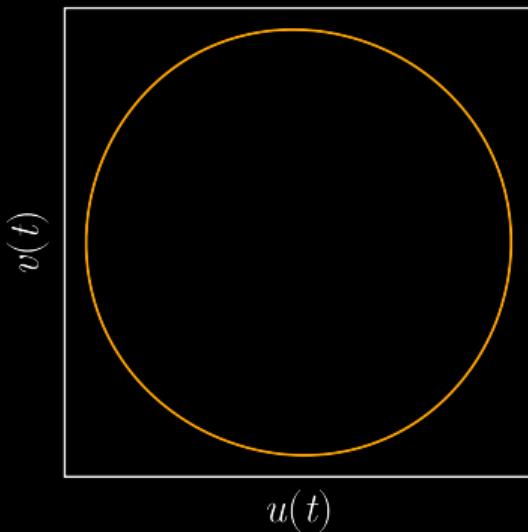
Low-Re cylinder flow : Canonical fluid example of a self-sustained weakly nonlinear oscillator.

In the rest, we'll assume that we only have access to the instantaneous lift and drag coefficients.

The dynamics being periodic, the attractor is a simple limit cycle.

Low-Re Cylinder flow

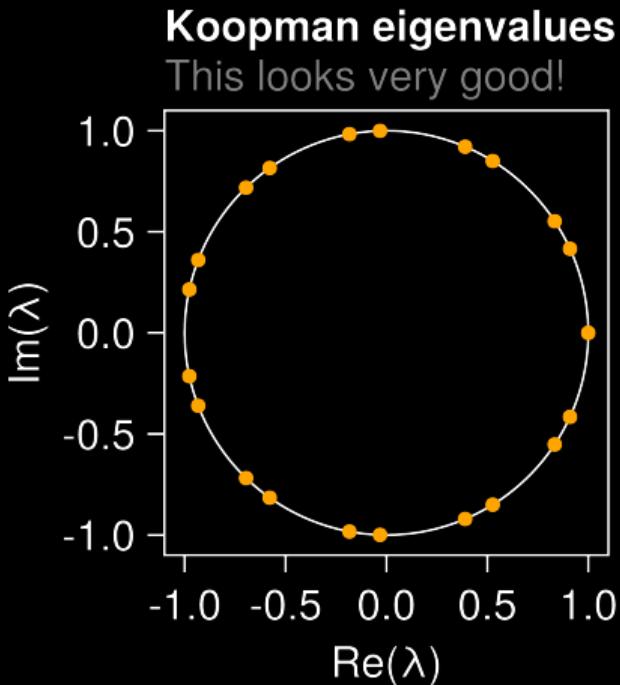
Reconstruction of the attractor from lift and drag.



Given \mathbf{U} , \mathbf{K} , and \mathbf{V} , compute the approximate Koopman eigenvalues

$$\lambda = \text{eig}(\mathbf{KV}^T \mathbf{U})$$

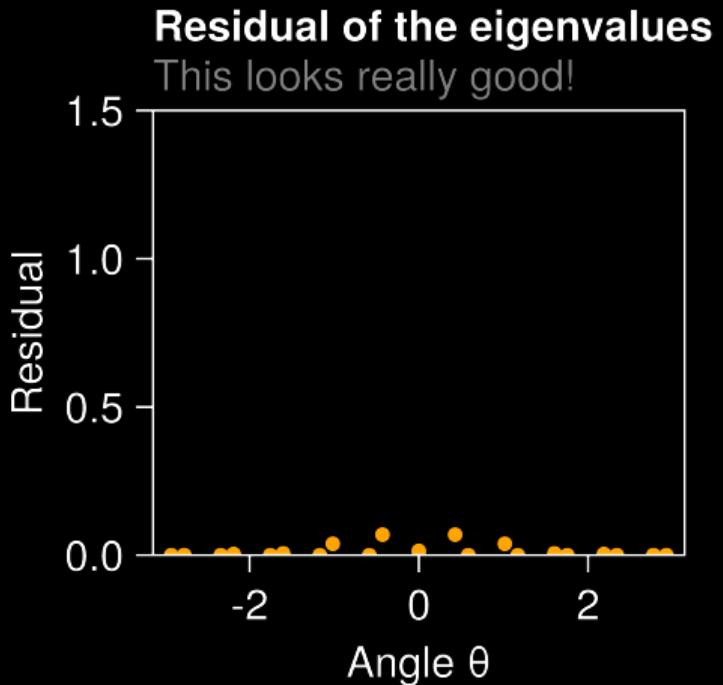
and corresponding residual.

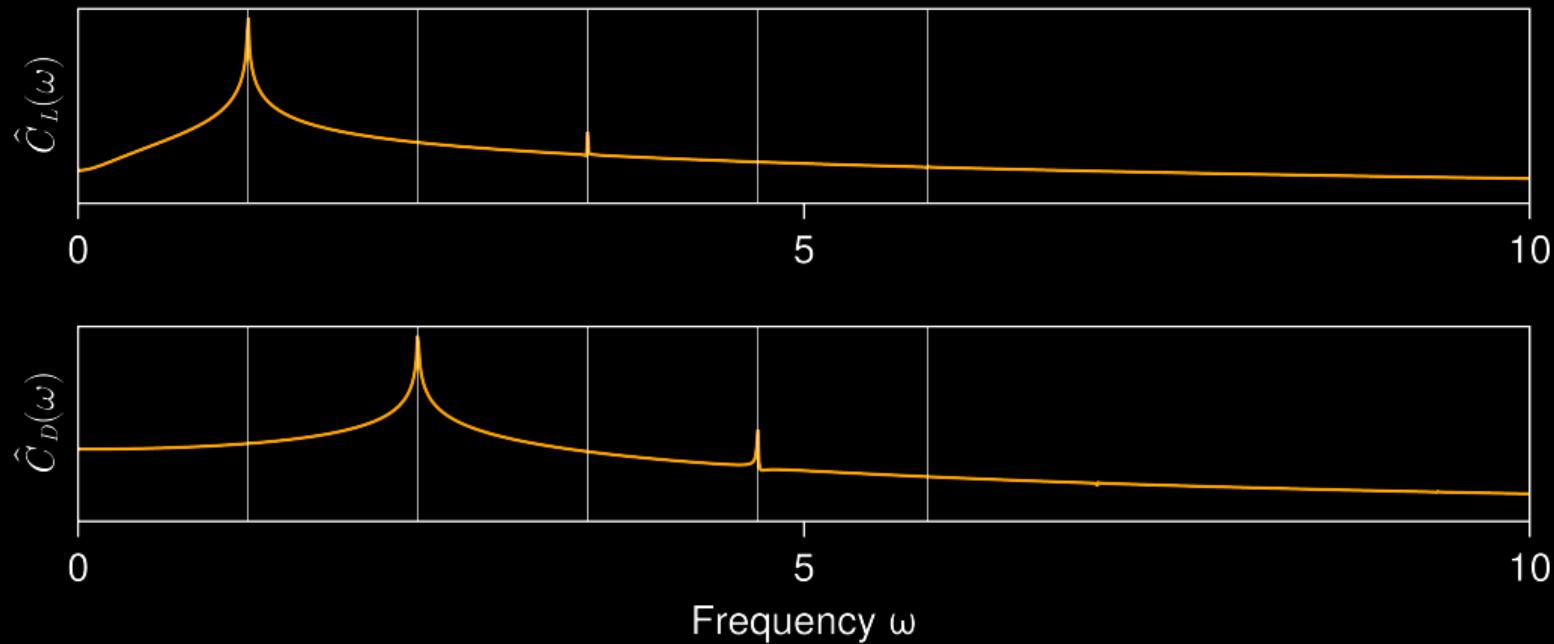


Given \mathbf{U} , \mathbf{K} , and \mathbf{V} , compute the approximate Koopman eigenvalues

$$\lambda = \text{eig}(\mathbf{KV}^T \mathbf{U})$$

and corresponding residual.





Shear-driven cavity flow : Canonical fluid example
for reduced-order modelling and flow control.

In the rest, we'll assume that we only have access to
the fluctuation's kinetic energy.

The dynamics being quasi-periodic,
the attractor is a T_2 -torus.

Given \mathbf{U} , \mathbf{K} , and \mathbf{V} , compute the approximate Koopman eigenvalues

$$\lambda = \text{eig}(\mathbf{KV}^T \mathbf{U})$$

and corresponding residual.

Given \mathbf{U} , \mathbf{K} , and \mathbf{V} , compute the approximate Koopman eigenvalues

$$\lambda = \text{eig}(\mathbf{KV}^T \mathbf{U})$$

and corresponding residual.

Thermosyphon : Example of chaotic thermal convection with Lorenz-like dynamics.

In the rest, we'll assume that we only have access to the instantaneous flow rate.

The dynamics being chaotic, it evolves on a strange attractor.

Given \mathbf{U} , \mathbf{K} , and \mathbf{V} , compute the approximate Koopman eigenvalues

$$\lambda = \text{eig}(\mathbf{KV}^T \mathbf{U})$$

and corresponding residual.

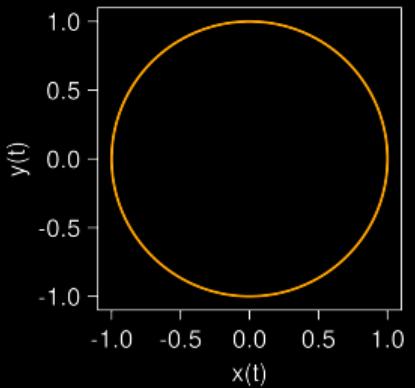
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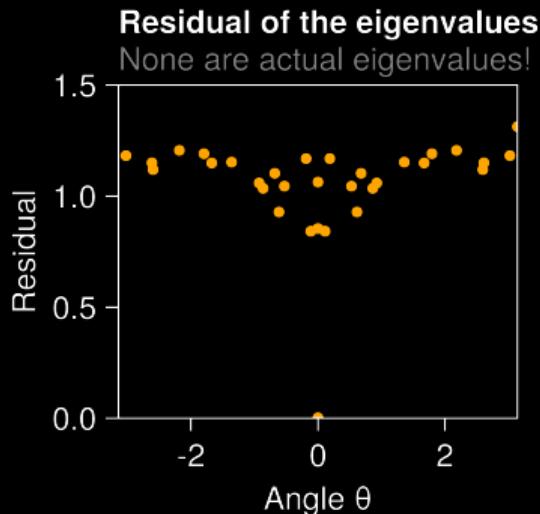
$$\lambda = \text{eig}(\mathbf{KV}^T \mathbf{U})$$

and corresponding residual.

Additional tips and tricks and conclusion

If the dynamics are periodic/quasi-periodic, the Koopman operator has a point spectrum. Use **FFT** to compute them more efficiently !





It is not because you can compute eigenvalues of your approximation that they necessarily are eigenvalues of the true Koopman operator !

Stay up-to-date with the current literature! A lot has been done since the pioneering work of Peter on DMD.





<https://loiseaujc.github.io/>



<https://loiseau-jc.medium.com/>



@loiseau_jc

Thank you for your attention!

Any question?