Learning Koopman Invariant Subspaces for Dynamic Mode Decomposition

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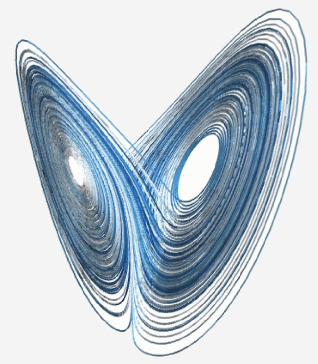
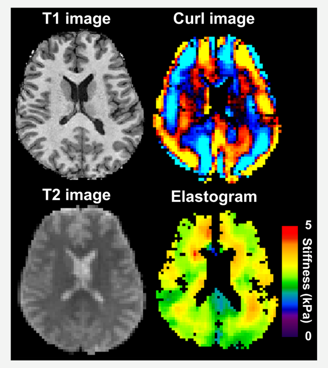
Motivation: Analysis of Nonlinear Dynamical Systems

- A variety of physical/biological phenomena are modeled using dynamical systems (differential/difference eqs).

$$\boldsymbol{x}_{t+1} = \boldsymbol{f}(\boldsymbol{x}_t), \quad \boldsymbol{x} \in \mathcal{M} \text{ (state space)}$$

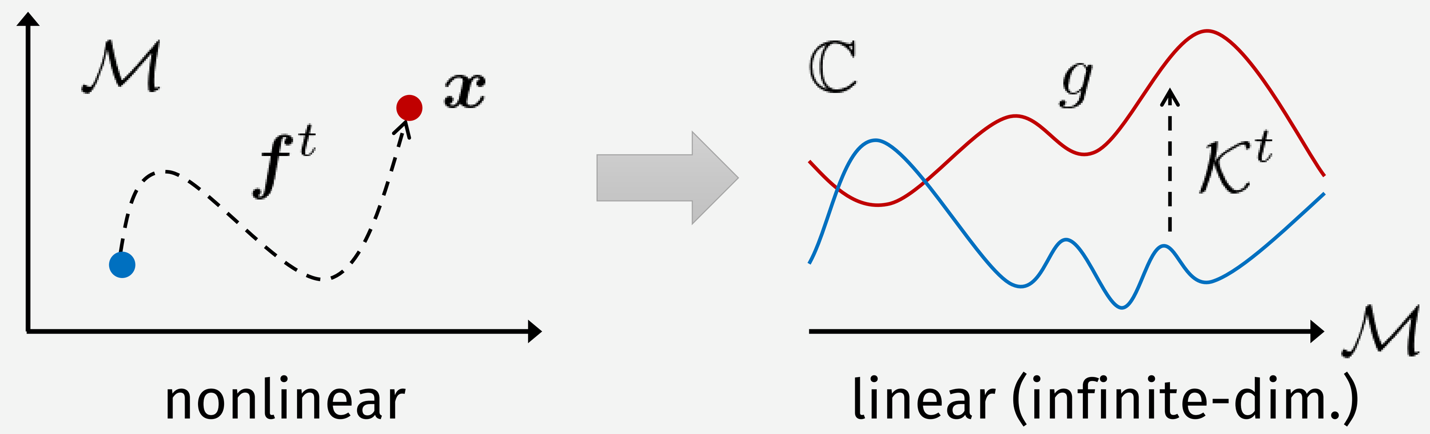
- When $\boldsymbol{f}$ is highly nonlinear, analyzing $\boldsymbol{f}$ is difficult.

Background: Operator-theoretic view of dynamical systems

- **Definition** (Koopman operator) [Koopman '31]
  - Koopman operator $\mathcal{K}$ is a linear operator that represents time-evolution of observables $g : \mathcal{M} \to \mathbb{C}$.

$$\mathcal{K}g(\boldsymbol{x}) = g(\boldsymbol{f}(\boldsymbol{x})), \quad g \in \mathcal{F} \text{ (function space)}$$

- $\mathcal{K}$ lifts nonlinear dynamics to a linear regime!
  - Can be utilized for modal decomposition, etc.



- Assume $\mathcal{K}$ has only discrete spectra (eigenvalues).
- **Definition** (Koopman mode decomposition) [Mezić '05, Budišić+ '12]
  - eigenvalues λ and eigenfunctions φ:

$$\mathcal{K}\varphi_i(\boldsymbol{x}) = \lambda_i \varphi_i(\boldsymbol{x}) \quad \text{for} \quad i = 1, 2, \dots$$

  - g's projection to $\mathrm{span}\{\varphi_1, \varphi_2, \dots\}$: Koopman modes v

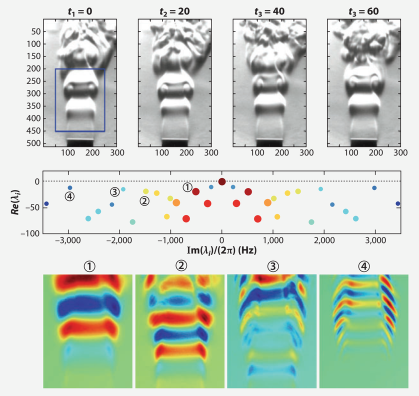
$$g(\boldsymbol{x}) = \sum_{i=1}^{\infty} \varphi_i(\boldsymbol{x}) v_i$$

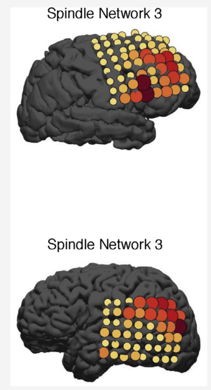
  - Then, $g(\boldsymbol{x}_t)$ is decomposed into multiple modes:

$$g(\boldsymbol{x}_t) = \sum_{i=1}^{\infty} \lambda_i^t \underbrace{\varphi_i(\boldsymbol{x}_0) v_i}_{w_i}, \quad \begin{cases} |\lambda_i| = \text{decay rate of } w_i \\ \angle\lambda_i = \text{frequency of } w_i. \end{cases}$$

Background: Dynamic Mode Decomposition (DMD)

- **Algorithm** (DMD) [Rowley+ '09, Schmid '10, Tu+ '14]
  1. Compute eigenvalues λ_i and right-/left-eigenvectors $\boldsymbol{w}_i, \boldsymbol{z}_i^{\mathsf{H}}$ of $\boldsymbol{A}$, where $\boldsymbol{y}_{t+1} \approx \boldsymbol{A}\boldsymbol{y}_t$.
  2. Normalize eigenvectors so that $\boldsymbol{w}_{i'}^{\mathsf{H}} \boldsymbol{z}_i = \delta_{i'i}$.
  3. Compute $\varphi_{i,t} = \boldsymbol{z}_i^{\mathsf{H}} \boldsymbol{y}_t$.


[Schmid+ '11]



[Brunton+ '16]


[Takeishi+ '17]

- DMD approximates Koopman modes if dataset is generated from appropriate nonlinear observables.
- **Assumption** (Data from $\mathcal{K}$-invariant subspace)
  - Dataset is generated by $\boldsymbol{y}_t = \left[g_1(\boldsymbol{x}_t), \cdots, g_n(\boldsymbol{x}_t)\right]^{\mathsf{T}}$, and $\{g_1, \dots, g_n\}$ spans $\mathcal{K}$-invariant subspace, i.e.,

$$\exists G \subset \mathcal{G} \text{ s.t. } \forall g \in G, \ \mathcal{K}g \in G \ \text{ and } \ \mathrm{span}\{g_1, \dots, g_n\} = G$$

- Previous approaches:
  - transform data by nonlinear basis functions [Williams+ '15]
  - define Koopman mode decomposition in RKHS [Kawahara '16]

Main Idea: Learning $\mathcal{K}$-invariant Subspace from Data

- **Theorem** ($\mathcal{K}$-invariant subspace)
  - $\{g_1, \dots, g_n\}$ spans a $\mathcal{K}$-invariant subspace if and only if $\boldsymbol{g} = [g_1 \ \cdots \ g_n]^{\mathsf{T}}$ and $\boldsymbol{g} \circ \boldsymbol{f}$ are linearly dependent.
- Minimize residual sum of squares of linear least-squares regression between $\boldsymbol{g}$ and $\boldsymbol{g} \circ \boldsymbol{f}$:

$$\mathcal{L}_{\mathrm{RSS}}(\boldsymbol{g}; \boldsymbol{x}_{0:m}) = \|\mathbf{Y}_1 - (\mathbf{Y}_1 \mathbf{Y}_0^{\dagger})\mathbf{Y}_0\|_{\mathrm{F}}^2,$$
$$\mathbf{Y}_0 = [\boldsymbol{g}(\boldsymbol{x}_0) \ \cdots \ \boldsymbol{g}(\boldsymbol{x}_{m-1})],$$
$$\mathbf{Y}_1 = [\boldsymbol{g}(\boldsymbol{x}_1) \ \cdots \ \boldsymbol{g}(\boldsymbol{x}_m)]$$

- Modifications to loss function:
  - Estimate $\boldsymbol{x}$ using delay-coordinate embedding [Takens '81]:

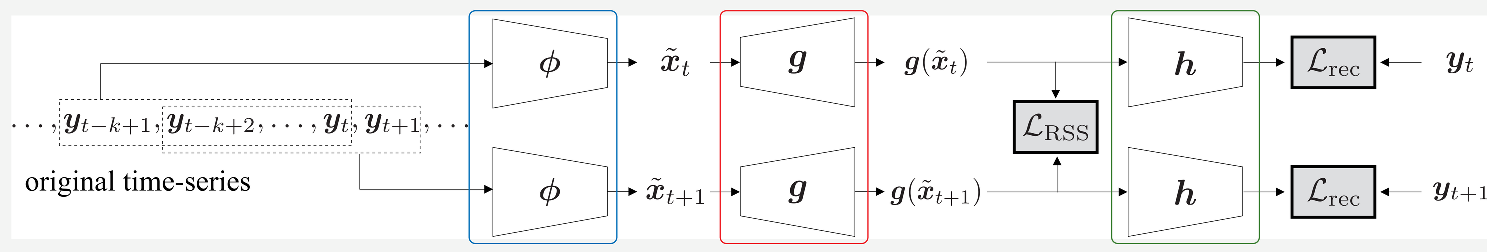
$$\boldsymbol{x}_t \approx \tilde{\boldsymbol{x}}_t = \boldsymbol{\phi}(\boldsymbol{y}_{t-k+1:t}) = \boldsymbol{W}[\boldsymbol{y}_{t-k+1}^{\mathsf{T}} \ \cdots \ \boldsymbol{y}_t^{\mathsf{T}}]^{\mathsf{T}}$$

  - Prevent trivial $\boldsymbol{g}$ by reconstructing $\boldsymbol{y}$ from $\boldsymbol{g}$'s values:

$$\boldsymbol{h}(\boldsymbol{g}(\tilde{\boldsymbol{x}}_t)) \approx \boldsymbol{y}_t \quad \to \quad \min \ \mathcal{L}_{\mathrm{rec}} = \sum \|\boldsymbol{h}(\boldsymbol{g}_t) - \boldsymbol{y}_t\|_2^2$$

→ Total loss: $\mathcal{L} = \tilde{\mathcal{L}}_{\mathrm{RSS}}(\boldsymbol{g}, \boldsymbol{W}; \boldsymbol{y}) + \alpha \mathcal{L}_{\mathrm{rec}}(\boldsymbol{g}, \boldsymbol{h}; \boldsymbol{y})$.

- Implementation using multilayer perceptrons:

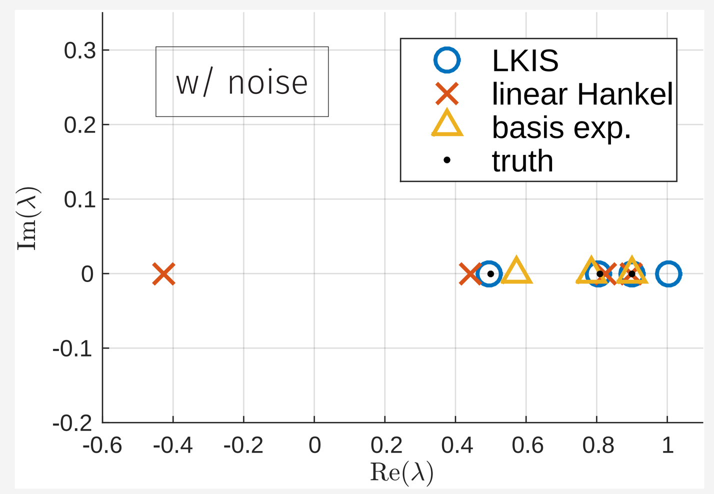


Numerical Examples and Application

Toy system

$$\boldsymbol{x}_{t+1} = \boldsymbol{f}(\boldsymbol{x}) = \begin{cases} \lambda x_{1,t}, \\ \mu x_{2,t} + (\lambda^2 - \mu) x_{1,t}^2 \end{cases}$$

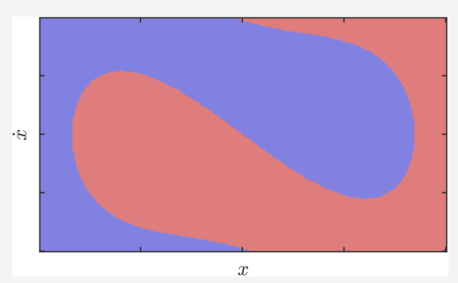
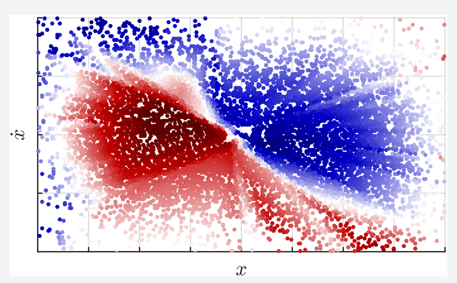
- True $\mathcal{K}$-inv. subspace: $\mathrm{span}\{x_1, x_2, x_1^2\}$.
- Proposed method can identify correct eigenvalues even w/ noise.



Unforced Duffing equation

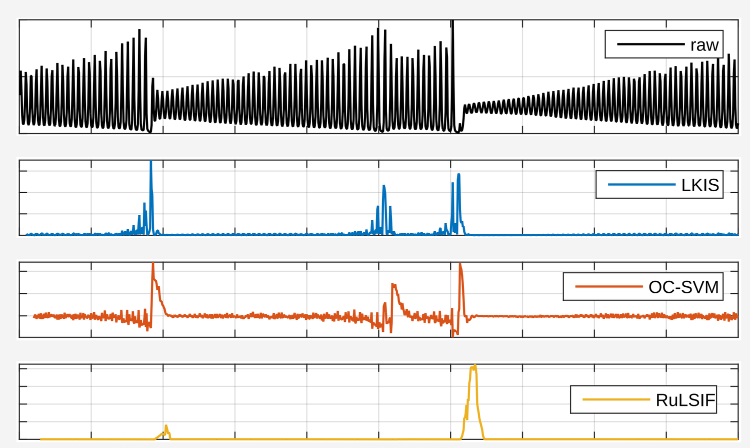
$$\ddot{x} = -\delta\dot{x} - x(\beta + \alpha x^2)$$

- In general, the level sets of Koopman eigenfunction with eigenvalue $\lambda = 1$ correspond to the basins of attraction. (*left*): True basins of attraction. (*right*): Computed eigenfunction.

Unstable phenomena detection

- A mode with a small eigenvalue corresponds to rapidly decaying (unstable) component of data.
- Apply proposed method to time-series of laser pulsation.
- Proposed method detects rapid changes of amplitude.



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