Data-Driven Methods for Dynamical Systems

Yuanchao Xu

University of Alberta

October 23, 2024

Outline

1. Introduction
2. Koopman Operator Theory
3. Koopman Operator Computation for Deterministic Systems
4. Koopman Operator Computation for Stochastic Systems
5. Conclusion

Introduction

- Complex dynamical systems challenge:
  - Understanding and predicting long-term behavior
  - Traditional models often inadequate for complex systems
- Data-driven methods advantages:
  - Extract insights directly from experimental/simulation data
  - Reduce dependence on explicit mathematical models
  - Capture hidden dynamics not easily modeled analytically
- Koopman operator theory benefits:
  - Transforms nonlinear dynamics into linear representations
  - Enables powerful spectral analysis tools for nonlinear systems
  - Bridges data-driven approaches with dynamical systems theory

Koopman Operator Theory - Overview

- Introduced by B.O. Koopman in 1931
- Core idea: Lift nonlinear dynamics to linear but infinite-dimensional space
- Consider a dynamical system $(\mathcal{M}, \mu)$:

$$\dot{x} = f(x)$$

  where $x \in \mathcal{M} \subseteq \mathbb{R}^d$ and μ is a probability measure.
- Koopman operator $\mathcal{K} : L^2(\Omega, \mu) \to L^2(\Omega, \mu)$ acts on observable $g : \mathcal{M} \to \mathbb{C}$:

$$(\mathcal{K}g)(x) = g(f(x))$$

- Key properties:
  - Linear: $\mathcal{K}(\alpha g_1 + \beta g_2) = \alpha \mathcal{K} g_1 + \beta \mathcal{K} g_2$
  - Infinite-dimensional: Operates on function space
  - Preserves nonlinear dynamics information

Koopman Operator Theory: Methods and Applications

- Data-driven approximation methods:
  - Extended Dynamic Mode Decomposition (EDMD)
  - Residual Dynamic Mode Decomposition (ResDMD)
  - Generator Extended Dynamic Mode Decomposition (gEDMD)
- Key applications:
  - Model reduction for complex systems
  - Identification of coherent structures in fluid dynamics
  - Stability analysis
  - Nonlinear control problems

Extended Dynamic Mode Decomposition

- Collect Data: Gather i.i.d. data points $\{x_1, \ldots, x_m\}$ and their corresponding next states $\{y_1, \ldots, y_m\}$.
- Construct the Data Matrices: Define the data matrices X and Y:

$$X = \begin{bmatrix} | & & | \\ x_1 & \cdots & x_m \\ | & & | \end{bmatrix}, \; Y = \begin{bmatrix} | & & | \\ y_1 & \cdots & y_m \\ | & & | \end{bmatrix}$$

  Evaluate the dictionary $\Psi = \{\psi_1, \ldots, \psi_N\}$ on these data to form matrices:

$$\Psi_X = \begin{bmatrix} \psi_1(x_1) & \cdots & \psi_N(x_1) \\ \vdots & \ddots & \vdots \\ \psi_1(x_m) & \cdots & \psi_N(x_m) \end{bmatrix}, \; \Psi_Y = \begin{bmatrix} \psi_1(y_1) & \cdots & \psi_N(y_1) \\ \vdots & \ddots & \vdots \\ \psi_1(y_m) & \cdots & \psi_N(y_m) \end{bmatrix}$$

Extended Dynamic Mode Decomposition

- Solve the Linear System: Solve the least-squares problem to find $\mathbf{K}$:

$$\mathbf{K} = \Psi_X^{\dagger} \Psi_Y = \widehat{G}^{\dagger} \widehat{A}$$

  where $\widehat{G} := \frac{1}{m} \Psi_X^* \Psi_X$, $\widehat{A} := \frac{1}{m} \Psi_X^* \Psi_Y$, $\dagger$ is the pseudoinverse.
- Koopman Modes and Eigenvalues: Once $\mathbf{K}$ is computed, solve the eigenvalue problem:

$$\mathbf{K}\mathbf{v} = \lambda \mathbf{v}$$

  where λ are the Koopman eigenvalues, and $\mathbf{v}$ are the (right) eigenvectors.

Extended Dynamic Mode Decomposition

- Eigenvalues λ_j: frequencies or growth rates of the system's dynamics
- Eigenfunctions ϕ_j: Functions satisfying $\mathcal{K}\phi_j = \lambda_j\phi_j$
  - Computed as: $\phi_j(\mathbf{x}) = \sum_{k=1}^{N} \mathbf{v}_{jk}\psi_k(\mathbf{x})$ where $\mathbf{v}_j = [v_{j1}, \ldots, v_{jN}]^T$ is the j-th right eigenvector of $\mathbf{K}$
  - Capture fundamental patterns in the nonlinear dynamics
- Koopman Modes $\boldsymbol{\xi}_j$: Spatial patterns associated with eigenfunction ϕ_j
  - For observable $\mathbf{g} = [g_1(x), g_2(x), \ldots, g_n(x)]^T$:

$$\boldsymbol{\xi}_j = \left[\frac{\langle g_1, \phi_j\rangle_\mu}{\langle \phi_j, \phi_j\rangle_\mu}, \frac{\langle g_2, \phi_j\rangle_\mu}{\langle \phi_j, \phi_j\rangle_\mu}, \ldots, \frac{\langle g_n, \phi_j\rangle_\mu}{\langle \phi_j, \phi_j\rangle_\mu}\right]^T$$

- Observable decomposition and prediction:
  - At time 0: $\mathbf{g}(\mathbf{x}_0) \approx \sum_{j=1}^{N} \phi_j(\mathbf{x}_0)\boldsymbol{\xi}_j$
  - After applying $\mathcal{K}$ for n times: $\mathbf{g}(\mathbf{x}_n) = \mathcal{K}^n\mathbf{g}(\mathbf{x}_0) \approx \sum_{j=1}^{N} \lambda_j^n \phi_j(\mathbf{x}_0)\boldsymbol{\xi}_j$

Convergence in large data limit

For finite m data points, the ij-th element of $\widehat{G}$ and $\widehat{A}$ are:

$$[\widehat{G}]_{ij} = \frac{1}{m}\sum_{i=1}^{m} \overline{\psi}_i(x_i)\psi_j(x_i)$$

$$[\widehat{A}]_{ij} = \frac{1}{m}\sum_{i=1}^{m} \overline{\psi}_i(x_i)\psi_j(y_i)$$

In the large data limit, EDMD converges to a Galerkin projection, i.e., as $m \to \infty$, by SLLN we have

$$\lim_{m\to\infty}[\widehat{G}]_{ij} \to \langle \psi_i, \psi_j \rangle_\mu$$

$$\lim_{m\to\infty}[\widehat{A}]_{ij} \to \langle \psi_i, \mathcal{K}\psi_j \rangle_\mu$$

Residual Dynamic Mode Decomposition (ResDMD) (1/3)

- Addresses spectral pollution in EDMD
- Considers both $\mathcal{K}$ and $\mathcal{K}^*\mathcal{K}$
- Computes squared relative residual:

$$\mathrm{res}(\lambda, g)^2 := \frac{\int_\Omega |\mathcal{K}g(x) - \lambda g(x)|^2 d\mu(x)}{\int_\Omega |g(x)|^2 d\mu(x)}$$

Residual Dynamic Mode Decomposition (ResDMD) (2/3)

- For normalized eigenfunction g, this becomes:

$$\begin{aligned}\operatorname{res}(\lambda, g)^2 = \sum_{i,j=1}^{N_K} \overline{v}_i \big(& \langle \mathcal{K}\psi_i, \mathcal{K}\psi_j \rangle_\mu - \lambda \langle \psi_i, \mathcal{K}\psi_j \rangle_\mu \\ & - \overline{\lambda} \langle \mathcal{K}\psi_i, \psi_j \rangle_\mu + |\lambda|^2 \langle \psi_i, \psi_j \rangle_\mu \big) v_j\end{aligned}$$

- Where $g = \mathbf{\Psi} v$ for some $v \in \mathbb{C}^N$

Residual Dynamic Mode Decomposition (ResDMD) (3/3)

- Practical computation of residual using Ψ_X and Ψ_Y:

$$\widehat{\mathrm{res}}(\lambda, g)^2 := \frac{1}{m} v^* \left(\Psi_Y^* \Psi_Y - \lambda (\Psi_X^* \Psi_Y)^* - \overline{\lambda} \Psi_X^* \Psi_Y + |\lambda|^2 \Psi_X^* \Psi_X\right) v$$

- Provides more accurate spectral approximation
- Allows detection and discarding of spurious eigenvalues

Neural Network ResDMD (NN-ResDMD)

- Uses neural network to learn dictionary functions
- Adaptive to complex systems
- Loss function: $J_K = \frac{1}{\sqrt{m}} \|\Psi_Y - \Psi_X K V\|_F^2$
- Iterative process:
  - Update $K = (G + \sigma I)^\dagger A$
  - Adjust network parameters using gradient descent

EDMD for Koopman Generator (gEDMD)

- Approximates generator A for continuous-time stochastic systems
- SDE: $dX_t = b(X_t)dt + \sigma(X_t)dW_t$
- Generator: $Ag(x) = b(x) \cdot \nabla g(x) + \frac{1}{2}\sum_{i,j} a_{ij}(x)\frac{\partial^2 g(x)}{\partial x_i \partial x_j}$
- Approximation: $A \approx \Psi_X^{\dagger}\dot{\Psi}_X$

Stochastic Extended DMD (S-EDMD)

- Addresses unboundedness of generator in stochastic systems
- Constructs sequence of bounded operators A_n
- $A_n := \frac{K_n(\frac{1}{n}) - I}{\frac{1}{n}}$
- Uses Trotter-Kato Approximation theorem for convergence
- Ensures numerical stability and accuracy

Conclusion

- Addressed limitations of existing Koopman operator approximation methods
- Proposed NN-ResDMD for complex deterministic systems
- Introduced S-EDMD for stochastic systems
- Future work:
  - Implementation and testing
  - Performance evaluation across various dynamical systems

Thank You

Thank you for your attention!

Any questions?