measure-preserving Extended Dynamic Mode Decomposition: Structure-preserving Koopmanism

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Data-driven dynamical systems

• State $x \in \Omega \subseteq \mathbb{R}^d$, *unknown* function $F: \Omega \to \Omega$ governs dynamics

$$x_{n+1} = F(x_n)$$

- Given: Trajectory data $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^{M}$
- Koopman operator \mathcal{K} acts on <u>functions</u> $g: \Omega \to \mathbb{C}$ $[\mathcal{K}g](x) = g(F(x))$
- \mathcal{K} is *linear* but acts on an *infinite-dimensional* space.
- Work in $L^2(\Omega, \omega)$ for positive measure ω , with inner product $\langle \cdot, \cdot \rangle$.

GOAL: Data-driven approximation of $\mathcal K$ and its spectral properties.

- Koopman, "Hamiltonian systems and transformation in Hilbert space," Proc. Natl. Acad. Sci. USA, 1931.
- Koopman, v. Neumann, "Dynamical systems of continuous spectra," Proc. Natl. Acad. Sci. USA, 1932.
- Mezić, "Spectral properties of dynamical systems, model reduction and decompositions," Nonlinear Dynam., 2005.

Setting

Typical approach: $\mathcal{K} \longrightarrow \mathbb{K} \in \mathbb{C}^{N \times N}$

Challenges:

- **1)** Spectral pollution: Approximate spurious modes $\lambda \notin \text{Spec}(\mathcal{K})$.
- **2)** Spectral invisibility: Miss parts of $Spec(\mathcal{K})$.
- 3) Continuous spectra.

Assume: System is measure-preserving

 $\Leftrightarrow \mathcal{K}^*\mathcal{K} = I \text{ (isometry)} \quad \text{(we consider unitary extensions)}$

 $\Rightarrow \operatorname{Spec}(\mathcal{K}) \subseteq \{z \colon |z| \le 1\}$

WANT: Method preserves measure (e.g., stability, long-time behavior etc.)...

Motivating example



- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension $(d) \approx 100,000$ (velocity at measurement points)

*Raw measurements provided by Máté Szőke (Virginia Tech)



• Baddoo, Herrmann, McKeon, Kutz, Brunton, "Physics-informed dynamic mode decomposition (piDMD)," preprint.

• Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending aynamic mode decomposition," J. Nonlinear Sci., 2015.

Extended Dynamic Mode Decomposition (EDMD)

$$\begin{array}{l} \text{Given dictionary } \{\psi_1, \dots, \psi_N\} \text{ of functions } \psi_j \colon \Omega \to \mathbb{C}, \\ \{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^M \\ \langle\psi_k, \psi_j\rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) = \left[\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix} \\ \hline \psi_X \\ \langle\mathcal{K}\psi_k, \psi_j\rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix} \\ \hline \psi_X \\$$

- Schmid, "Dynamic mode decomposition of numerical and experimental data," J. Fluid Mech., 2010.
- Rowley, Mezić, Bagheri, Schlatter, Henningson, "Spectral analysis of nonlinear flows," J. Fluid Mech., 2009.
- Kutz, Brunton, Brunton, Proctor, "Dynamic mode decomposition: data-driven modeling of complex systems," SIAM, 2016.
- Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," J. Nonlinear Sci., 2015.

Another interpretation

$$\Psi(x) = [\psi_1(x) \dots \psi_N(x)], \qquad g = \sum_{j=1}^N \mathbf{g}_j \psi_j = \Psi \mathbf{g}, \qquad \mathcal{K}g = \Psi \mathbb{K}\mathbf{g} + R(g, \cdot)$$

$$\min_{\mathbb{K}\in\mathbb{C}^{N\times N}} \left\{ \int_{\Omega} \max_{\|\mathbf{g}\|_{2}=1} |R(g,x)|^{2} d\omega(x) = \int_{\Omega} \|\Psi(F(x)) - \Psi(x)\mathbb{K}\|_{2}^{2} d\omega(x) \right\}$$

quadrature
$$\min_{\mathbb{K}\in\mathbb{C}^{N\times N}} \sum_{m=1}^{M} w_{m} \|\Psi(y^{(m)}) - \Psi(x^{(m)})\mathbb{K}\|_{2}^{2}$$

A simple idea

$$G = \Psi_X^* W \Psi_X, \qquad G_{jk} \approx \langle \psi_k, \psi_j \rangle$$

Measure-preserving: $\|\Psi \mathbf{g}\| = \|\Psi \mathbb{K} \mathbf{g}\|, \|\Psi \mathbf{g}\|^2 \approx g^* G g, \|\Psi \mathbb{K} \mathbf{g}\|^2 \approx g^* \mathbb{K}^* G \mathbb{K} g$

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Enforce: $G = \mathbb{K}^* G \mathbb{K}$

A simple idea

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Measure-preserving: $\|\Psi \mathbf{g}\| = \|\Psi \mathbb{K} \mathbf{g}\|, \|\Psi \mathbf{g}\|^2 \approx g^* G g, \|\Psi \mathbb{K} \mathbf{g}\|^2 \approx g^* \mathbb{K}^* G \mathbb{K} g$



The mpEDMD algorithm

Algorithm: mpEDMD for approximating spectral properties of \mathcal{K} .

Input: Snapshot data $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)} = F(\boldsymbol{x}^{(m)})\}_{m=1}^{M}$, quadrature weights $\{w_m\}_{m=1}^{M}$, and a dictionary of functions $\{\psi_j\}_{j=1}^{N}$.

- 1: Compute $G = \Psi_X^* W \Psi_X$ and $A = \Psi_X^* W \Psi_Y$
- 2: Compute an SVD of $G^{-1/2}A^*G^{-1/2} = U_1\Sigma U_2^*$
- 3: Compute the eigendecomposition $U_2 U_1^* = \hat{V} \Lambda \hat{V}^*$
- 4: Compute $\mathbb{K} = G^{-1/2}U_2U_1^*G^{1/2}$ and $V = G^{-1/2}\hat{V}$

Output: Koopman matrix \mathbb{K} , with eigenvectors V and eigenvalues Λ .

In a nutshell: Galerkin meets polar decomposition.

(This also allows us to prove <u>numerical stability</u>.)

Relation to previous approaches

• **Physics-informed DMD:** Similar approach but doesn't use nonlinear observables or matrix *G*. Hence in general, not measure-preserving.

Baddoo, Herrmann, McKeon, Kutz, Brunton, "Physics-informed dynamic mode decomposition (piDMD)," preprint.

• Periodic approximations via partitioning of state-space (e.g., on tori): Can be considered a particular case of mpEDMD, related to Ulam's method.

Govindarajan, Mohr, Chandrasekaran, Mezić, "On the approximation of Koopman spectra for measure preserving transformations," SIAM J. Appl. Dyn. Syst., 2019.

• Compact regularizations of the skew-adjoint generator: Measurepreserving method in continuous time through RKHS.

Das, Giannakis, Slawinska, "Reproducing kernel Hilbert space compactification of unitary evolution groups," Appl. Comput. Harm. Anal., 2021.

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Spectral measures \rightarrow diagonalisation

• Fin.-dim.: $B \in \mathbb{C}^{n \times n}$, $B^*B = BB^*$, o.n. basis of e-vectors $\{v_j\}_{i=1}^n$

$$v = \left[\sum_{j=1}^{n} v_{j} v_{j}^{*}\right] v, \qquad Bv = \left[\sum_{j=1}^{n} \lambda_{j} v_{j} v_{j}^{*}\right] v, \qquad \forall v \in \mathbb{C}^{n}$$

• Inf.-dim.: Operator $\mathcal{L}: \mathcal{D}(\mathcal{L}) \to \mathcal{H}$. Typically, no basis of e-vectors! Spectral theorem: (projection-valued) spectral measure \mathcal{E}

$$g = \left[\int_{\operatorname{Spec}(\mathcal{L})} 1 \, \mathrm{d}\mathcal{E}(\lambda) \right] g, \qquad \mathcal{L}g = \left[\int_{\operatorname{Spec}(\mathcal{L})} \lambda \, \mathrm{d}\mathcal{E}(\lambda) \right] g, \qquad \forall g \in \mathcal{H}$$

• Spectral measures: $\mu_g(U) = \langle \mathcal{E}(U)g, g \rangle (||g|| = 1)$ prob. measure.

Convergence of projection-valued measure

$$d\mathcal{E}_{N,M}(\lambda) = \sum_{j=1}^{N} v_j v_j^* G\delta(\lambda - \lambda_j) d\lambda$$
This assumption
cannot be dropped
in general!

Theorem: Suppose that the quadrature rule converges, \mathcal{K} is unitary, $\lim_{N \to \infty} \operatorname{dist}(h, V_N) = 0 \text{ for any } h \in L^2(\Omega, \omega). \text{ Then for any Lipschitz test}$ function $\xi, g \in L^2(\Omega, \omega)$ and $\boldsymbol{g}_N \in \mathbb{C}^N$ with $\lim_{N \to \infty} \|g - \Psi \boldsymbol{g}_N\| = 0$, $\lim_{N \to \infty} \limsup_{M \to \infty} \left\| \int_{\mathbb{T}} \xi(\lambda) d\mathcal{E}(\lambda) g - \Psi \int_{\mathbb{T}} \xi(\lambda) d\mathcal{E}_{N,M}(\lambda) \boldsymbol{g}_N \right\| = 0$

Key ingredients:

- Strong convergence of Galerkin approximation.
- Discretization by normal operators.

K: mpEDMD matrix λ_j : eigenvalues of K v_j : eigenvectors of K $V_N = \text{span} \{\psi_1, \dots, \psi_N\}$

Convergence of scalar-valued measure

$$\mu_{\boldsymbol{g}}^{(N,M)}(U) = \boldsymbol{g}^* G \mathcal{E}_{N,M}(U) \boldsymbol{g} = \sum_{\lambda_j \in U} \left| v_j^* G \boldsymbol{g} \right|^2$$
$$W_1(\mu,\nu) = \sup \left\{ \int_{\mathbb{T}} \xi(\lambda) d(\mu-\nu)(\lambda) : \xi \text{ Lipschitz 1} \right\}$$

Theorem: Suppose quad. rule converges, $\lim_{N \to \infty} \operatorname{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega, \omega)$. Then for $g \in L^2(\Omega, \omega)$ and $g_N \in \mathbb{C}^N$ with $\lim_{N \to \infty} ||g - \Psi g_N|| = 0$, $\lim_{N \to \infty} \limsup_{M \to \infty} W_1\left(\mu_g, \mu_g^{(N,M)}\right) = 0$. If $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$ and $g = \Psi g$, then Matching autocorrelations! $\lim_{M \to \infty} W_1\left(\mu_g, \mu_g^{(N,M)}\right) \lesssim \frac{\log(N)}{N}$. \mathbb{K} : mpEDMD matrix λ_j : eigenvalues of \mathbb{K} v_j : eigenvectors of \mathbb{K} v_j : eigenvectors of \mathbb{K} $V_N = \operatorname{span} \{\psi_1, \dots, \psi_N\}$

Avoid spectral invisibility!

$$\operatorname{Spec}_{\operatorname{ap}}(\mathcal{K}) = \left\{ \lambda : \exists u_n, \|u_n\| = 1, \lim_{n \to \infty} \|(\mathcal{K} - \lambda)u_n\| = 0 \right\} = \operatorname{Spec}(\mathcal{K}) \cap \mathbb{T}$$

Theorem: Suppose quad. rule converges, $\lim_{N \to \infty} \operatorname{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega, \omega)$. Then $\lim_{N \to \infty} \limsup_{M \to \infty} \sup_{\lambda \in \operatorname{Spec}_{\operatorname{ap}}(\mathcal{K})} \operatorname{dist}(\lambda, \operatorname{Spec}(\mathbb{K})) = 0.$

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What about spectral pollution?

K: mpEDMD matrix λ_j : eigenvalues of K v_j : eigenvectors of K $V_N = \text{span} \{\psi_1, \dots, \psi_N\}$

Residuals \Rightarrow avoid spectral pollution!

$$G = \Psi_X^* W \Psi_X, A = \Psi_X^* W \Psi_Y$$

$$\|(\mathcal{K} - \lambda)\Psi \boldsymbol{g}\|^{2} = \langle (\mathcal{K} - \lambda)\Psi \boldsymbol{g}, (\mathcal{K} - \lambda)\Psi \boldsymbol{g} \rangle$$
$$= \lim_{M \to \infty} \boldsymbol{g}^{*} [(1 + |\lambda|^{2})G - \bar{\lambda}A - \lambda A^{*}] \boldsymbol{g}$$

Suitable conditions $\Rightarrow \lim_{N \to \infty} \min_{g \in V_N} ||(\mathcal{K} - \lambda) \Psi g|| / ||g|| = \operatorname{dist}(\lambda, \operatorname{Spec}_{\operatorname{ap}}(\mathcal{K}))$

Two methods:

- Clean up procedure for tolerance ε .
- Local minimization algorithm converges to $\operatorname{Spec}_{\operatorname{ap}}(\mathcal{K})$.

• C., T., "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," preprint.

• C., Ayton, Szőke, "Residual Dynamic Mode Decomposition," J. Fluid Mech., 2023.

Residuals \Rightarrow avoid spectral pollution!

Executive summary of **ResDMD**: (considers <u>inf-dim</u> residuals)

- Rigorous convergence for spectra and pseudospectra of general Koopman operators from snapshot data.
- Error bounds ⇒ aposteri verification of spectral quantities,
 Koopman mode decompositions, and learned dictionaries.
- Deals with spectral measures of general measure-preserving systems with explicit high-order convergence.

Two methods:

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Lorenz system: scalar-valued spec meas

$$\dot{x}_1 = 10(x_2 - x_1), \quad \dot{x}_2 = x_1(28 - x_3) - x_2, \quad \dot{x}_3 = x_1x_2 - 8/3x_3, \quad \Delta_t = 0.1$$

$$g_j = c_j[x]_j, \quad V_N = \operatorname{span}\{g_j, \mathcal{K}g_j, \dots, \mathcal{K}^{N-1}g_j\}$$



Lorenz system: projection-valued spec meas



Lorenz system: projection-valued spec meas

$$V_N = \operatorname{span}\{g_1, g_2, g_3, \mathcal{K}g_1, \mathcal{K}g_2, \mathcal{K}g_3, \dots, \mathcal{K}^{q-1}g_1, \mathcal{K}^{q-1}g_2, \mathcal{K}^{q-1}g_3\}$$

$$\phi(\lambda) = (1-\lambda)^2 \log(1-\lambda)$$



Nonlinear pendulum

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$$\dot{x}_1 = x_2, \quad \dot{x}_2 = -\sin(x_1), \quad \Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R}, \quad \Delta_t = 0.5$$

 $g(x) = \exp(ix_1) x_2 \exp(-x_2^2/2), \quad V_N = \operatorname{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{99}g\}$



Robustness to noise: Gauss. noise for Ψ_X , Ψ_Y





Summary: Structure-preserving Koopmanism for arbitrary measure-preserving systems.

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- Convergence of spectral measures, spectra, Koopman mode decomposition.
- Long-time stability, improved qualitative behavior.
- Increased stability to noise.
- Simple, flexible: easy to combine with any DMD-type method!

Summary

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Volume 56/ Issue 1 January/February 2023

Optimization and Learning with Zeroth-order Stochastic Oracles

Stefan M. Wild	sequence is that material properties are	An optimization solver specifies a particular composition of solvents and bases an oper-	through an inline nuclear magnetic reso
A athematical optimization is a foun- dational technology for machine ming and the solution of design, deci-	characterization. In the context of optimiza- tion, this scenario is called a "zeroth-order oracle" — our knowledge about a particular	ating temperature, and reaction times; this combination is then run through a continu- ous flow reactor. The material that exits the	of the synthesized materials. These sto chastic, zeroth-order oracle outputs return to the solver in a closed-loop setting that
n, and control problems. In most optimi-	system or property is data driven and limited by the black-box nature of measurement	reactor is then automatically characterized	See Optimization on page .
n is the availability of at least the	procurement. An additional challenge is		

Read more about these breakthroughs in SIAM News!



Summary

- Convergence of spectral measures, spectra, Koopman mode decomposition.
- Long-time stability, improved qualitative behavior.
- Increased stability to noise.
- Simple, flexible: easy to combine with any DMD-type method!

Short video summaries available on YouTube:

(Thank you Steve Brunton for letting me use your channel!)



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Optimization and Learning with Zeroth-order Stochastic Oracles

Figure 1-doing so is impossible Figure 1 displays an instantiation of

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ge. In order to create viable new materi-

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Extended Dynamic

Mode Decomposition

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Resilient Data-driven Dynamical Systems Residual Dynamic with Koopman: An Infinite-dimensional **Numerical Analysis Perspective** Mode Decomposition By Steven L. Brunton on the local analysis of fixed points, per odic orbits, stable or unstable manifold and Matthew J. Colbrook and so forth. Although Poincaré's framework has revolutionized our understandin D ynamical systems, which describe the evolution of systems in time, are ubiqof dynamical systems, this approach has a least two challenges in many modern appl uitous in modern science and engineerin cations: (i) Obtaining a global understand They find use in a wide variety of applia ing of the nonlinear dynamics and (ii) han any from mechanics and circuits to eli dling systems that are either too compleology, neuroscience, and epidemiolog onsider a discrete-time dynamical sys about the evolution (i.e., unknown, high with state x in a state space $\Omega \subset \mathbb{R}^d$ that ensional, and highly nonlinear F). governed by an unknown and typicall Koopman operator theory, which ori nated with Bernard Koonman and John von Neumann [6, 7], provides a powerfu $\mathbf{x}_{n} = \mathbf{F}(\mathbf{x}_{n}), \quad n \ge 0.$ The classical, geometric way to analyz uch systems-which dates back to th seminal work of Henri Poincaré-is based Measure-preserving

We lift the nonlinear system (1) into an infi nite-dimensional space of observable func tions $g: \Omega \rightarrow \mathbb{C}$ via a Koopman operator \mathcal{K} $\mathcal{K}q(\mathbf{x}) = q(\mathbf{x})$ The evolution dynamics thus become lin

ear, allowing us to utilize generic solution techniques that are based on spec yze or offer incomplete informati Koonman operators have captivated researchers because of emerging data-driv and numerical implementations that

alternative to the classical geometric view of dynamical systems because it addresse underlies the aforementioned challenge



oincide with the rise of machine learning nd high-performance computing [2]. One major goal of modern Koonm operator theory is to find a coordinat mation with which a linear syster nay approximate even strongly nonlinea mics: this coordinate system relates t spectrum of the Koopman operator. 2005 Jean Mezić introduced the Koonmar tode decomposition [8], which provided heoretical basis for connecting the dynam mode decomposition (DMD) with the opman operator [9, 10]. DMD quickl secame the workhorse algorithm for com putational approximations of the Koopman erator due to its simple and highly exte sible formulation in terms of linear algebra and the fact that it applies equally well data-driven modeling when no go rning equations are available. However esearchers soon realized that simply buil ng linear models in terms of the primitive neasured variables cannot sufficiently car ure nonlinear dynamics beyond period and quasi-periodic phenomena, A majo

> functions of the Koopman operator [11] See Dynamical Systems on

https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition

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