

Data-Driven Spectral Measures and Generalized Eigenfunctions of Koopman Operators

Matthew Colbrook University of Cambridge 18/06/2024

- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems" Communications on Pure and Applied Mathematics, 2024.
- C., "The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems," SIAM Journal on Numerical Analysis, 2023.
- C., Drysdale, Horning, "Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators", arxiv preprint.
- C., "The Multiverse of Dynamic Mode Decomposition Algorithms," Handbook of Numerical Analysis, 2024.

Data-driven dynamical systems

State $x \in \Omega \subseteq \mathbb{R}^d$.

<u>**Unknown</u>** function $F: \Omega \to \Omega$ governs dynamics: $x_{n+1} = F(x_n)$.</u>

Goal: Learning from data $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^{M}$.

Applications: chemistry, climatology, control, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, etc.



Surveys:

- Brunton, Budišić, Kaiser, Kutz, "Modern Koopman theory for dynamical systems," SIAM Review, 2022.
- Budišić, Mohr, Mezić, "Applied Koopmanism," Chaos, 2012.
- C., "The Multiverse of Dynamic Mode Decomposition Algorithms," Handbook of Numerical Analysis, 2024.

Koopman Operator \mathcal{K} : A global linearization



Koopman von Neumann





- 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.

Koopman Operator \mathcal{K} : A global linearization



- \mathcal{K} acts on <u>functions</u> $g: \Omega \to \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- Function space: $L^2(\Omega, \omega)$, positive measure ω , inner product $\langle \cdot, \cdot \rangle$.

[•] 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.

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Koopman mode decomposition



Encodes: geometric features, invariant measures, transient behavior, long-time behavior, coherent structures, quasiperiodicity, etc.

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

[•] Mezić, "Spectral properties of dynamical systems, model reduction and decompositions," Nonlinear Dynamics, 2005.

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Setting: Measure-preserving systems

$$[\mathcal{K}g](x) = g(F(x)), \qquad g \in L^2(\Omega, \omega)$$

$$F \text{ preserves } \omega \iff \|\mathcal{K}g\| = \|g\| \text{ (isometry)}$$
$$\iff \mathcal{K}^*\mathcal{K} = I$$
$$\implies \operatorname{Sp}(\mathcal{K}) \subseteq \{z : |z| \le 1\}$$

(NB: unitary extensions of \mathcal{K} via Wold decomposition.)

Shift example (on $\ell^2(\mathbb{Z})$)

- Spectrum is unit circle.
- Spectrum is stable.
- Continuous spectra.
- Unitary evolution.

• Spectrum is {0}.

• Discrete spectra.

• Spectrum is unstable.

- Caution
- Nilpotent evolution.

Lots of Koopman operators are built up from operators like these!

How to fix a Jordan block

- Spectrum is {0}.
- Spectrum is unstable.
- Nilpotent evolution.

- Spectrum converges to unit circle as $N \rightarrow \infty$.
- Spectrum is stable.
- Unitary evolution.

Extended Dynamic Mode Decomposition (EDMD)

- 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.

$$G_{jk} = \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) \approx \langle \psi_k, \psi_j \rangle$$

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

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

$$G_{jk} = \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) \approx \langle \psi_k, \psi_j \rangle$$

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

The mpEDMD algorithm

Algorithm 4.1 The mpEDMD algorithm

Input: Snapshot data $\mathbf{X} \in \mathbb{C}^{d \times M}$ and $\mathbf{Y} \in \mathbb{C}^{d \times M}$, quadrature weights $\{w_m\}_{m=1}^M$, and a dictionary of functions $\{\psi_j\}_{j=1}^N$.

- 1: Compute the matrices Ψ_X and Ψ_Y and $\mathbf{W} = \text{diag}(w_1, \ldots, w_M)$.
- 2: Compute an economy QR decomposition $\mathbf{W}^{1/2}\Psi_X = \mathbf{QR}$, where $\mathbf{Q} \in \mathbb{C}^{M \times N}$, $\mathbf{R} \in \mathbb{C}^{N \times N}$.
- 3: Compute an SVD of $(\mathbf{R}^{-1})^* \Psi_Y^* \mathbf{W}^{1/2} \mathbf{Q} = \mathbf{U}_1 \Sigma \mathbf{U}_2^*$.
- 4: Compute the eigendecomposition $\mathbf{U}_2\mathbf{U}_1^* = \hat{\mathbf{V}}\Lambda\hat{\mathbf{V}}^*$ (via a Schur decomposition).
- 5: Compute $\mathbb{K} = \mathbf{R}^{-1}\mathbf{U}_2\mathbf{U}_1^*\mathbf{R}$ and $\mathbf{V} = \mathbf{R}^{-1}\hat{\mathbf{V}}$.

Output: Koopman matrix \mathbb{K} with eigenvectors \mathbf{V} and eigenvalues $\boldsymbol{\Lambda}$.

$$\begin{split} V_N &= \text{span} \left\{ \psi_1, \dots, \psi_N \right\} \\ \mathcal{P}_{V_N} \colon L^2(\Omega, \omega) \to V_N \\ \text{orthogonal projection} \end{split}$$

As $M \to \infty$, unitary part of polar decomposition of $\mathcal{P}_{V_N} \mathcal{KP}_{V_N}^*$.

- C., "The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems," SINUM, 2023.
- Code: <u>https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition</u>

Convergence properties (theorems in paper)

- Spectral measures.
- Functional calculus, L^2 forecasting etc.
- Koopman mode decomposition.
- Spectrum.
- Resolvent (see later!)

Key ingredient: **unitary** discretization.

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

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

"Solve"
$$(U - zI)u_z = 0$$

 $u_z = \sum_{j=-\infty}^{\infty} z^j e_j$

Generalised eigenfunctions u_z and generalised eigenvalues $\{z: |z| = 1\}$

Generalised eigenfunctions u_z and generalised eigenvalues $\{z: |z| = 1\}$ **RIGGED HILBERT SPACE**

Example: Nonlinear pendulum

$$\begin{aligned} \dot{x}_1 &= x_2, & \dot{x}_2 &= -\sin(x_1) \\ \Omega &= [-\pi,\pi]_{\text{per}} \times \mathbb{R}, \\ \Delta_t &= 1, \end{aligned}$$

 ω = Lebesgue measure

Considered a challenge in Koopman theory!

nature

ARTICLE

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Deep learning for universal linear embeddings of nonlinear dynamics

Bethany Lusch D^{1,2}, J. Nathan Kutz¹ & Steven L. Brunton^{1,2}

Identifying coordinate transformations that make strongly nonlinear dynamics approximately linear has the potential to enable nonlinear prediction, estimation, and control using linear theory. The Koopman operator is a leading data-driven embedding, and its eigenfunctions provide intrinsic coordinates that globally linearize the dynamics. However, identifying and representing these eigenfunctions has proven challenging. This work leverages deep learning to discover representations of Koopman eigenfunctions from data. Our network is parsimonious and interpretable by construction, embedding the dynamics on a low-dimensional manifold. We identify applicate coordinates an which the dynamics are clobally linear using a

 χ_1

Explicit diagonalization using Radon transform!

• Action-angle coordinates (*n* degrees of freedom):

$$\dot{\mathbf{I}} = \mathbf{0}, \qquad \dot{\mathbf{\Theta}} = \mathbf{I}, \qquad \Omega = \mathbb{R}^n \times [-\pi, \pi]_{\text{per}}^n$$

Explicit diagonalization using Radon transform!

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• g in Schwartz space,

$$g(\mathbf{I}, \mathbf{\theta}) = \sum_{\mathbf{k} \in \mathbb{Z}^n} \hat{g}_{\mathbf{k}}(\mathbf{I}) e^{i\mathbf{k} \cdot \mathbf{\theta}}, \qquad \hat{g}_{\mathbf{k}}(\mathbf{I}) = \frac{1}{(2\pi)^n} \int_{[-\pi, \pi]_{\text{per}}^n} g(\mathbf{I}, \mathbf{\theta}) e^{-i\mathbf{k} \cdot \mathbf{\theta}} d\mathbf{\theta}$$

Explicit diagonalization using Radon transform!

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Gelfand's theorem \rightarrow diagonalisation

• Finite matrix: $B \in \mathbb{C}^{n \times n}$, $B^*B = BB^*$, orthonormal basis of e-vectors $\{v_j\}_{j=1}^n$

$$v = \sum_{j=1}^{n} (v_j^* v) v_j, \qquad Bv = \sum_{j=1}^{n} \lambda_j (v_j^* v) v_j \qquad \forall v \in \mathbb{C}^n$$

• Infinite dimensions: Unitary \mathcal{K} . Typically, no basis of eigenfunctions! Some technical assumptions (can always be realized):

Carathéodory function:

$$F_g(z) = (\mathcal{K} + zI)(\mathcal{K} - zI)^{-1}g = \int_{[-\pi,\pi]_{\text{per}}} \frac{e^{i\theta} + z}{e^{i\theta} - z} \langle g_{\theta}^* | g \rangle g_{\theta} d\nu(\theta)$$

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Let $r = 1 + \varepsilon > 1, \theta_{0} \in [-\pi,\pi]_{\text{per}}$,

$$\frac{1}{4\pi} \left[F_g(r^{-1}e^{i\theta_0}) - F_g(re^{i\theta_0}) \right]$$

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$$\frac{1}{4\pi} \left[F_g(r^{-1}e^{i\theta_0}) - F_g(re^{i\theta_0}) \right]$$
$$= \frac{1}{2\pi} \int_{[-\pi,\pi]_{\text{per}}} \frac{r^2 - 1}{1 + r^2 - 2r\cos(\theta_0 - \theta)} \langle g_{\theta}^* | g \rangle g_{\theta} d\nu(\theta)$$

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Smoothed generalized eigenfunction

Smoothed generalized eigenfunction

 F_g requires $(\mathcal{K} - zI)^{-1}$

EDMD diverges:

$$F_q$$
 requires $(\mathcal{K} - zI)^{-1}$

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Rigged DMD converges:

- For general \mathcal{K} : $\left(\mathbb{K}_{mpEDMD} - zI\right)^{-1} \mathbf{g}$ converges to $(\mathcal{K} - zI)^{-1}g$ as $\lim_{N \to \infty M \to \infty}$
- Hence, Rigged DMD converges as $\lim_{\epsilon \downarrow 0} \lim_{N \to \infty} \lim_{M \to \infty} \lim$
- ResDMD allows us to select $\varepsilon = \varepsilon(N)$ adaptively (convergence in **2 limits**)

Better smoothing kernels as $\varepsilon \downarrow 0$

- Poisson kernel: **slow** convergence $\mathcal{O}(\varepsilon \log(1/\varepsilon))$.
- Construct high-order *rational* kernels using $F_a(z)$.

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Smaller ε

Better smoothing kernels as $\varepsilon \downarrow 0$

- Poisson kernel: slow convergence $\mathcal{O}(\varepsilon \log(1/\varepsilon))$.
- Construct high-order *rational* kernels using $F_q(z)$.

Theorem: Suppose quadrature rule converges & $\lim_{N\to\infty} \operatorname{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega, \omega)$. Choosing $N = N(\varepsilon)$, fast $\mathcal{O}(\varepsilon^m \log(1/\varepsilon))$ convergence for: • Generalized eigenfunctions (topology of \mathcal{S}^*).

- Spectral measures (gen. efun. projections): pointwise, L^p, weak,...
- Forecasting (i.e., iterating Koopman mode decomposition), coherency etc.

Smaller ε

Rigged DMD

• C., Drysdale, Horning, "Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators", arxiv preprint.

Code: <u>https://github.com/MColbrook/Rigged-Dynamic-Mode-Decomposition</u>

Example: Arnold's cat map

 $F(x,y) = (2x + y, x + y) \mod 2\pi$ $\Omega = [-\pi,\pi]_{per}^2, \quad \omega = Lebesgue measure$

Arnold's "Ergodic Problems of Classical Mechanics"

Example: Arnold's cat map

 $F(x, y) = (2x + y, x + y) \mod 2\pi$

 $\Omega = [-\pi, \pi]_{per}^2$, $\omega = Lebesgue measure$

Experimental details Length-one trajectories, $M = 50 \times 50, N = 500$ $g(x, y) = \sin(x) + \frac{1}{2}\sin(2x + y) + \frac{i}{4}\sin(5x + 3y)$ Krylov subspace: $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$

Explicit formula: g_{θ} become more oscillatory as $\epsilon \downarrow 0$ (non-decaying Fourier series)

Higher kernel order (accuracy)

Higher resolution ($\varepsilon \downarrow 0$)

Example: Nonlinear pendulum

Experimental Details
Length-one trajectories over grid

$$M = 500 \times 500, N = 300$$

 $g(x_1, x_2) = \exp(ix_1) / \cosh(x_2)$
Krylov subspace: $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$

 $\dot{x}_1 = x_2, \ \dot{x}_2 = -\sin(x_1), \qquad \Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R}, \qquad \Delta_t = 1, \qquad \omega = \text{ Lebesgue measure}$

Explicit formula: g_{θ} become plane waves concentrated on unions of lines of constant energy as $\epsilon \downarrow 0$.

S constructed from Krylov subspace

- If \mathcal{K} is represented by an infinite matrix with finitely many non-zero entries in each column, can build \mathcal{S} using weighted sequence spaces.
- Always possible using time-delay embedding:

{Unions (different g) of spaces span{ $g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g, \dots$ } } $\subset S$

• Generalises shift example: in coefficient space w.r.t. Krylov subspaces.

$\boldsymbol{\mathcal{S}}$ constructed from Krylov subspace

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• Generalises shift example: in coefficient space w.r.t. Krylov subspaces.

Let's do this for Lorenz...

Example: Lorenz system

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No formula for

generalized eigenfunctions!!

Experimental Details

M = 10000, N = 1000

 $g(x_1, x_2, x_3) = \tanh\left(\frac{x_1x_2 - 5x_3}{10}\right) - c$

 $\dot{x}_1 = 10(x_2 - x_1), \ \dot{x}_2 = x_1(28 - x_3) - x_2, \ \dot{x}_3 = x_1x_2 - 8/3x_3, \ \Delta_t = 0.05, \ \Omega = \text{attractor}, \ \omega = \text{SRB}$ measure

Example: Lorenz system

 $\dot{x}_1 = 10(x_2 - x_1), \ \dot{x}_2 = x_1(28 - x_3) - x_2, \ \dot{x}_3 = x_1x_2 - 8/3x_3, \ \Delta_t = 0.05, \ \Omega = \text{attractor}, \ \omega = \text{SRB}$ measure

Example: Noisy cavity flow (spectral measures)

Example: Noisy cavity flow (generalized Koopman modes)

Re=30000 Deep in the continuous spectrum!!!

Summary

Interest in Koopman boils down to a data-driven inf-dim spectral problem.

mpEDMD

- EDMD + enforcing measure-preserving (polar decomposition of Galerkin)
- Convergence of spectral measures, spectra, Koopman mode decomposition.
- Long-time stability, improved qualitative behavior, increased stability to noise.

Rigged DMD

Futur

- Continuous spectra and generalized eigenfunctions.
- Smoothing kernels + resolvent (using mpEDMD).
- High-order convergence.
 - Use in control.
 - work • Other function spaces? E.g., RKHS

[General (non-measure-preserving) systems: ResDMD]

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