







Solves the problem of computing spectra of general Koopman operators on  $L^2$  spaces and controlling projection error of inf dim  $\rightarrow$  fin dim. (EDMD does **not** converge in general)

Matthew Colbrook University of Cambridge

20/05/2024

- 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.









Unitary version of EDMD which converges (spectra, measures, KMD) for any measure-preserving system (EDMD does **not** converge in general)

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Computes spectral measures and generalized eigenfunctions of measure-preserving systems. Matthew Colbrook University of Cambridge 20/05/2024

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#### Matthew Colbrook

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Recent review of DMD methods from a spectral computations point of view.

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### The setup

State  $x \in \Omega \subseteq \mathbb{R}^d$ . ( $\Omega$  does not need to be an attractor)

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

**Koopman operator:**  $\mathcal{K}$  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  $\omega$ , inner product  $\langle \cdot, \cdot \rangle$ .

**Goal:** Learn spectral properties from snapshot data  $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^{M}$ .

**NB:** No assumptions yet on snapshots or  $\Omega$  or F or  $\omega$ . (Other than F non-singular w.r.t.  $\omega$ ,  $\mathcal{K}$  a closed operator (can be unbounded).) Warmup on  $\ell^2(\mathbb{Z})$  - \*\*\*\* happens... even for measure-preserving systems



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

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

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

Dangers when we truncate/discretize  $\mathcal{K} \to \mathbb{K} \in \mathbb{C}^{N \times N}$ 

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Caution

$$Sp(\mathcal{K}) = \{\lambda \in \mathbb{C} : \mathcal{K} - \lambda I \text{ is not invertible}\}$$

- Too much: Spurious eigenvalues  $\lambda \in Sp(\mathbb{K})$  far from  $Sp(\mathcal{K})$
- Too little:  $Sp(\mathbb{K})$  misses parts of  $Sp(\mathcal{K})$
- Continuous spectra (Sp( $\mathcal{K}$ ) not just eigenvalues!)
- Verification (e.g., subspace)
- Instability (non-normal  $\mathcal{K}$ , non-normal discretizations of normal  $\mathcal{K}$ )

#### Methods like EDMD do not avoid these dangers as $N \rightarrow \infty$ !

C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," Commun. Pure Appl. Math., 2024.

## Outline

#### • <u>General</u> systems:

- Residual Dynamic Mode Decomposition.
- <u>Measure-preserving</u> systems:
  - Rigged Dynamic Mode Decomposition
  - Measure-Preserving Extended Dynamic Mode Decomposition.
- The Solvability Complexity Index classification of problems and optimality of algorithms.
- Where are we? Open questions and future research.



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Functions  $\psi_j: \Omega \to \mathbb{C}, j = 1, ..., N$ 

 $\left\{x^{(m)}, y^{(m)} = F(x^{(m)})\right\}_{m=1}^{M}$ 

- Schmid, "Dynamic mode decomposition of numerical and experimental data," J. Fluid Mech., 2010.
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$$\begin{aligned} \text{Functions } \psi_{j} \colon \Omega \to \mathbb{C}, j = 1, \dots, N \\ \text{quadrature points} \\ \langle \psi_{k}, \psi_{j} \rangle \approx \sum_{m=1}^{M} w_{m} \overline{\psi_{j}(x^{(m)})} \psi_{k}(x^{(m)}) = \begin{bmatrix} (\psi_{1}(x^{(1)}) \cdots \psi_{N}(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_{1}(x^{(M)}) \cdots & \psi_{N}(x^{(M)}) \end{bmatrix}^{*} \\ \text{quadrature weights} \\ \mathcal{K}\psi_{k}, \psi_{j} \rangle \approx \sum_{m=1}^{M} w_{m} \overline{\psi_{j}(x^{(m)})} \underbrace{\psi_{k}(y^{(m)})}_{[\mathcal{K}\psi_{k}](x^{(m)})} = \begin{bmatrix} (\psi_{1}(x^{(1)}) \cdots \psi_{N}(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_{1}(x^{(M)}) \cdots & \psi_{N}(x^{(M)}) \end{bmatrix}^{*} \\ \underbrace{\psi_{x}} \\ \psi_{x} \\ \hline \psi_{x$$

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**Residuals**: 
$$g = \sum_{j=1}^{N} \mathbf{g}_{j} \psi_{j}$$
,  $\|\mathcal{K}g - \lambda g\|^{2} = \langle \mathcal{K}g - \lambda g, \mathcal{K}g - \lambda g \rangle$ 

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## **ResDMD: Avoiding the dangers**

If quadrature rule converges (ask me later)

- **1 limit**  $\lim_{M\to\infty}$ : Avoid spurious eigenvalues.
- **2 limits**  $\lim_{N\to\infty} \lim_{M\to\infty}$ : Compute  $\operatorname{Sp}_{\varepsilon}(\mathcal{K}) = \bigcup_{\|\mathcal{B}\|\leq\varepsilon} \operatorname{Sp}(\mathcal{K}+\mathcal{B})$ .
- **3 limits**  $\lim_{\varepsilon \downarrow 0} \lim_{N \to \infty} \lim_{M \to \infty}$ : Compute Sp( $\mathcal{K}$ ).
- Verification: dictionaries, approximate eigenfunctions, coherency,...
- Error bounds of forecasts.

Convergent methods for general  $\mathcal K$ 

M = number of snapshots N = number of basis functions

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- Extends to stochastic systems (+ variance through Koopman).

Convergent methods for general  ${\mathcal K}$ 

22

M = number of snapshots N = number of basis functions

C., Li, Raut, Townsend, "Beyond expectations: Residual Dynamic Mode Decomposition and Variance for Stochastic Dynamical Systems," Nonlinear Dynamics, 2024.

#### Example: Verified spectra and modes



acoustic vibrations

### **Example: Verified dictionary**



0.8

0.6

0.4

0.2

#### **Example: Verified KMD and compression**



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#### 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.)



**Problem:** Often  $\mathcal{K}$  doesn't have basis of eigenfunctions (i.e., continuous spectra)

### 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**:

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

#### **Carathéodory function**:

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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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Smoothed generalized eigenfunction



Smoothed generalized eigenfunction

# Better smoothing kernels as $\varepsilon \downarrow 0$

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

Smaller  $\varepsilon$ requires more data



• **Theorems:** fast  $\mathcal{O}(\varepsilon^m \log(1/\varepsilon))$  convergence for

- Generalized eigenfunctions (topology of  $\mathcal{S}^*$ ).
- Spectral measures (traces of generalized eigenfunctions): pointwise, L<sup>p</sup>, weak,...
- Forecasting (i.e., iterating Koopman mode decomposition), coherency etc.

# Final ingredient: $F_g$ requires $(\mathcal{K} - zI)^{-1}$

#### **EDMD diverges:**







#### **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

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# Example: Noisy cavity flow (spectral measures)

Experimental Details
Single trajectory
M = 10000, N varies
Basis: POD modes
20% Gaussian noise





# Example: Noisy cavity flow (generalized Koopman modes)

Re=30000 Deep in the continuous spectrum!!!





## Outline

#### • <u>General</u> systems:

- Residual Dynamic Mode Decomposition.
- <u>Measure-preserving</u> systems:
  - Rigged Dynamic Mode Decomposition
  - Measure-Preserving Extended Dynamic Mode Decomposition.
- The Solvability Complexity Index classification of problems and optimality of algorithms.
- Where are we? Open questions and future research.



- ResDMD: convergence as  $\lim_{N\to\infty} \lim_{M\to\infty}$
- Rigged DMD: convergence ( $\varepsilon = \varepsilon(N)$ ) as  $\lim_{N \to \infty} \lim_{M \to \infty} \lim_{M \to \infty} \lim_{N \to \infty} \lim_{M \to \infty} \lim_$

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Convergence in multiple successive limits

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Convergence in multiple successive limits

• FACT: Unless you have very strong assumptions (e.g., uniform ergodicity, finite-dimensional invariant subspace etc.), <u>EVERY</u> convergent Koopman algorithm to date needs multiple limits. These limits can be different things.

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- Solvability Complexity Index (SCI): smallest number k for which we can solve problem with  $\lim_{n_k \to \infty} \dots \lim_{n_1 \to \infty}$  via an algorithm  $(n_1, \dots, n_k \text{ can be } anything)$ .

- C., Hansen, "The foundations of spectral computations via the solvability complexity index hierarchy," J. Eur. Math. Soc., 2022.
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 $\Rightarrow$  Classification of problems, optimality of algorithms.

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**Zoo of problems:** spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete spectra, essential spectra, eigenspaces + multiplicity, spectral radii, essential numerical ranges, geometric features of spectrum (e.g., capacity), spectral gap problem, resonances ...



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# Coming soon... SCI for Koopman (with Mezić)

- General systems (computing spectrum).
- Measure-preserving systems (spectrum, spectral type etc.)

Bottom line:

• Many problems are impossible in one limit, even with perfect and unlimited snapshots, probabilistic algorithms, nice smooth F on compact manifolds.

E.g., computing spectrum (as a set) of smooth measure-preserving systems on unit disc.

• Problems can be tackled in multiple limits under very general conditions.

 $\Rightarrow$  New program on foundations and classification for Koopman.

• A complete picture has emerged on  $L^2(\Omega, \omega)$ 

**Practical + theoretical guarantees** 

- General systems: Compute spectral properties with error control. CONTROL INFINITE-DIMENSIONAL RESIDUALS
- Measure-preserving systems: Continuous spectra (and generalized eigenfunctions) SMOOTHING KERNELS and the RESOLVENT.



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- What about other function spaces?
- What further classifications can we prove? Only starting to scratch the surface!
- Beyond spectra: Applications such as control.



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Buzz was right!

**Practical + theoretical guarantees** 

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