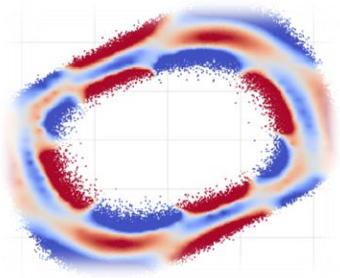

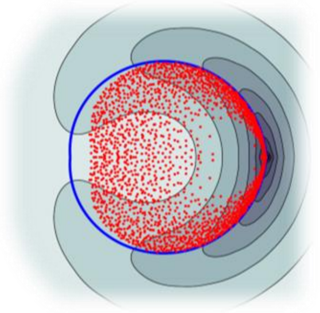

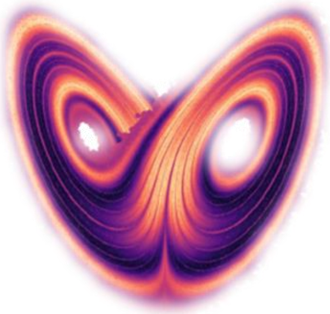

Data-driven computation of spectral properties of Koopman operators

Matthew Colbrook

University of Cambridge

19/08/2024

For papers, lectures, and talk slides/videos, visit:
http://www.damtp.cam.ac.uk/user/mjc249/home.html

Recap and notation

- Compact metric space $(\mathcal{X}, d_{\mathcal{X}})$ – the state space, $x \in \mathcal{X}$ – the state
- ***Unknown*** cts $S: \mathcal{X} \to \mathcal{X}$ – the dynamics: $x_{n+1} = S(x_n)$
- Borel measure ω on $\mathcal{X}$
- Function space $L^2 = L^2(\mathcal{X}, \omega)$ (elements g called "observables")
- Koopman operator $\mathcal{K} = \mathcal{K}_S: L^2 \to L^2$; $[\mathcal{K}_S g](x) = g(S(x))$
- ***Available*** Snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = S\left(x^{(m)}\right)\right) : m = 1, \dots, M\right\}$

NB: Pointwise definition of $\mathcal{K}_S$ needs $S\#\omega \ll \omega$ – this will hold throughout.
NB: $\mathcal{K}_S$ bounded equivalent to $\mathrm{d}S\#\omega/\mathrm{d}\omega \in L^\infty$ – this will hold throughout (can be dropped).

Recap and notation

- Compact metric space $(\mathcal{X}, d_{\mathcal{X}})$ – the state space, $x \in \mathcal{X}$ – the state
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GOAL: Data-driven approximation of $\mathcal{K}_S$ and its spectral properties.

Perils of discretization: Warmup on $\ell^2(\mathbb{Z})$

$$\begin{pmatrix} \ddots & \ddots & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & 0 & 1 & \\ & & & & 0 & \ddots \\ & & & & & \ddots \end{pmatrix} \longrightarrow \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{N \times N}$$

Two-way infinite

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

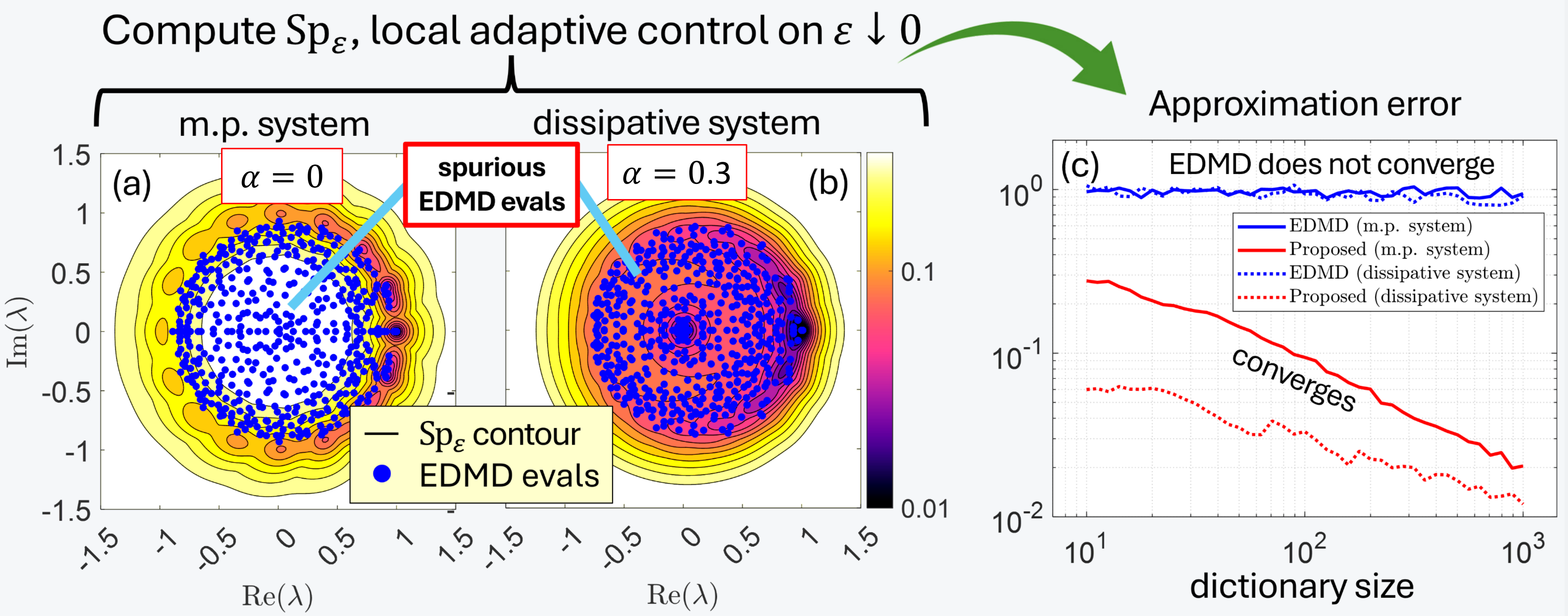
- Spectrum is $\{0\}$.
- Spectrum is unstable.
- Discrete spectra.
- Nilpotent evolution.

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

Example: EDMD does NOT converge

- Duffing oscillator: $\dot{x} = y, \dot{y} = -\alpha y + x(1 - x^2)$, sampled $\Delta t = 0.3$.
- Gaussian radial basis functions, Monte Carlo integration ($M = 50000$)

$$\mathrm{Sp}_\varepsilon(\mathcal{K}_S) = \{z \in \mathbb{C}: \|(\mathcal{K}_S - zI)^{-1}\|^{-1} \leq \varepsilon\}$$



Extended Dynamic Mode Decomposition (EDMD)

Functions $\psi_j : \mathcal{X} \to \mathbb{C},\, j = 1, \ldots, N$

$$\{x^{(m)}, y^{(m)} = S(x^{(m)})\}_{m=1}^{M}$$

- Schmid, "*Dynamic mode decomposition of numerical and experimental data,*" **J. Fluid Mech.**, 2010.
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quadrature points

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) = \Bigg[\underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix}^*}_{\Psi_X} \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_{W} \underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix}}_{\Psi_X} \Bigg]_{jk}$$

quadrature weights

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \Bigg[\underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix}^*}_{\Psi_X} \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_{W} \underbrace{\begin{pmatrix} \psi_1(y^{(1)}) & \cdots & \psi_N(y^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(y^{(M)}) & \cdots & \psi_N(y^{(M)}) \end{pmatrix}}_{\Psi_Y} \Bigg]_{jk}$$

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Galerkin Approximation

$$\mathcal{K} \longrightarrow \mathbb{K} = (\Psi_X{}^* W \Psi_X)^{-1} \Psi_X{}^* W \Psi_Y = (\sqrt{W}\Psi_X)^{\dagger} \sqrt{W} \Psi_Y \in \mathbb{C}^{N \times N}$$

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Residual DMD (ResDMD)

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})}\, \psi_k\left(x^{(m)}\right) = \Big[\underbrace{\Psi_X{}^* W \Psi_X}_{G}\Big]_{jk}$$

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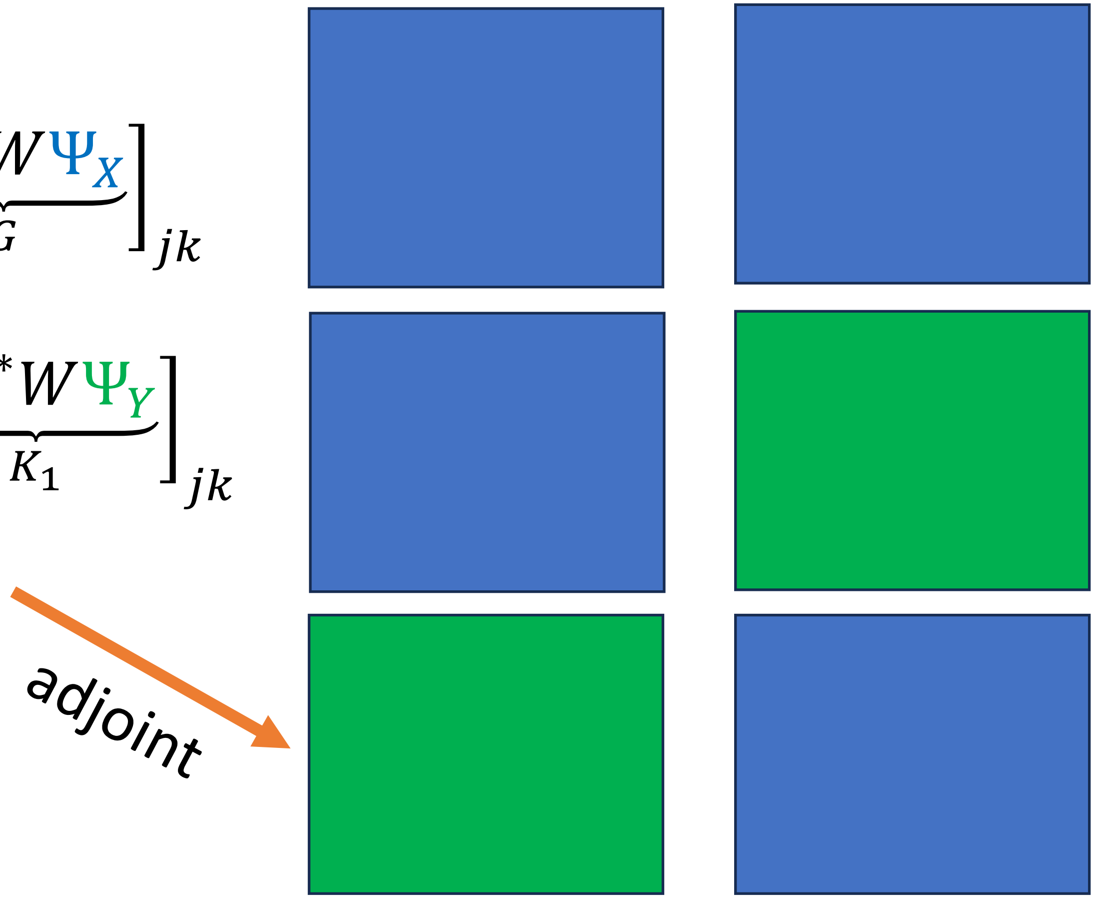

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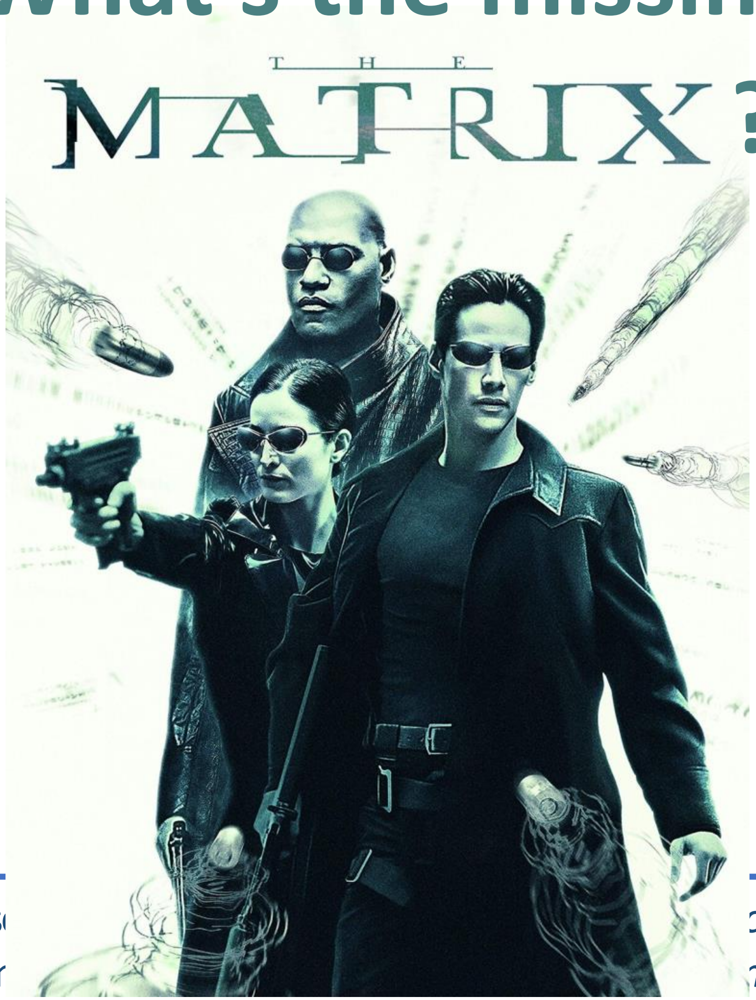
Residual DMD (ResDMD)

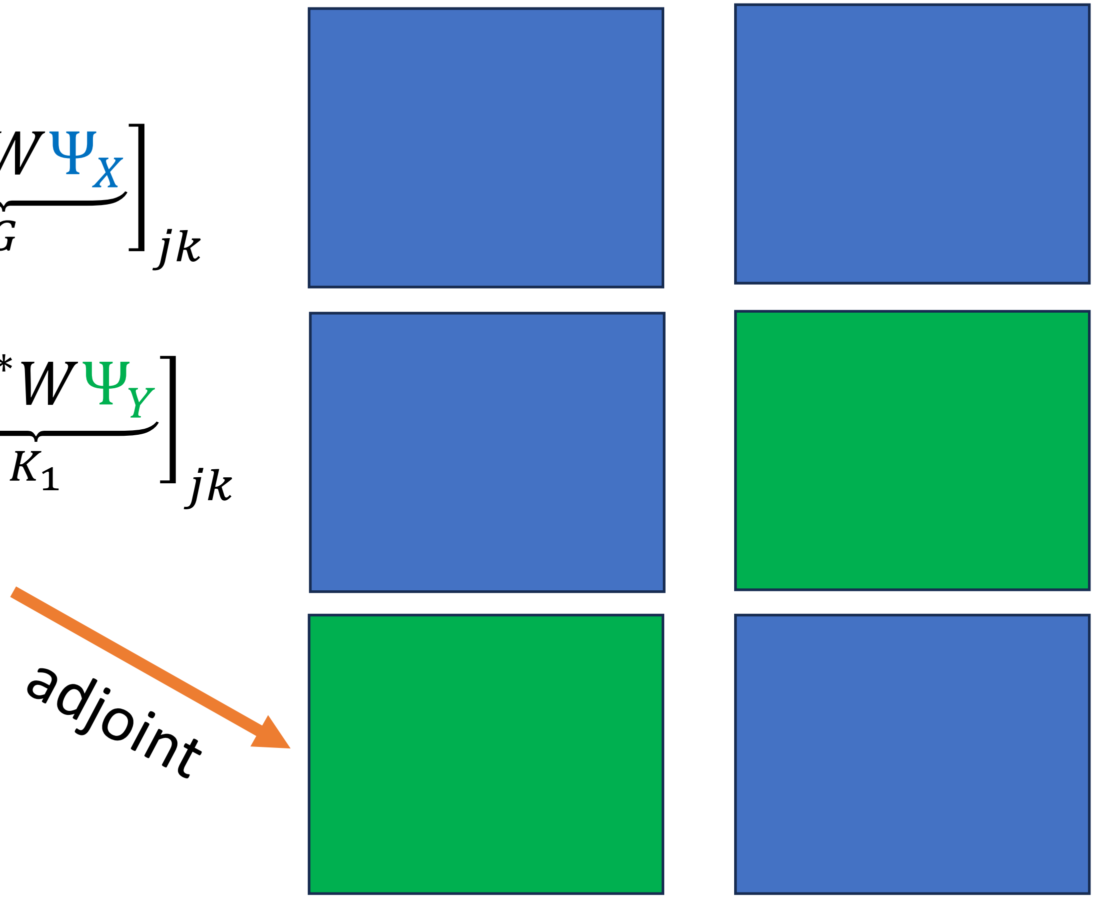
What’s the missing



?

$$= \Big[\underbrace{{\Psi_X}^* W \Psi_X}_{G}\Big]_{jk}$$

$$) \quad = \Big[\underbrace{{\Psi_X}^* W \Psi_Y}_{K_1}\Big]_{jk}$$



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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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Bound projection errors!

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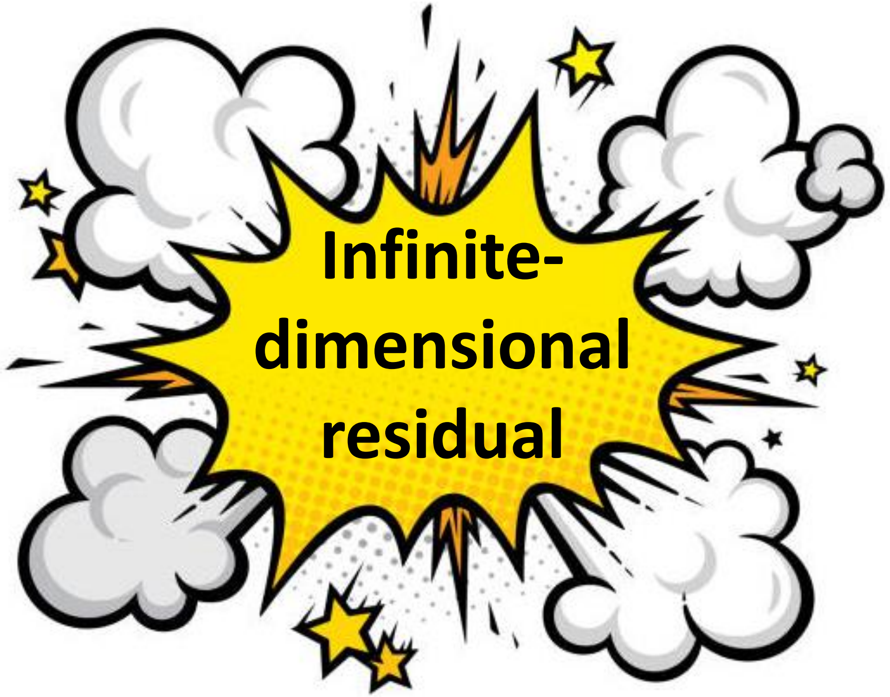

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ResDMD: Avoiding the dangers

If quadrature rule converges

Convergent methods for general $\mathcal{K}$

- $\lim_{M\to\infty}$: Avoid spurious eigenvalues.
- $\lim_{N\to\infty}\lim_{M\to\infty}$: Compute $\mathrm{Sp}_\varepsilon(\mathcal{K}) = \cup_{\|\mathcal{B}\|\leq\varepsilon} \mathrm{Sp}(\mathcal{K}+\mathcal{B})$.
- $\lim_{\varepsilon\downarrow 0}\lim_{N\to\infty}\lim_{M\to\infty}$: Compute $\mathrm{Sp}(\mathcal{K})$.
- Verification: dictionaries, approximate eigenfunctions, coherency,…
- Error bounds of forecasts.

M = number of snapshots
N = number of basis functions

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- Extends to kernel methods and $M < N$ (dual residual).

- C., *"Another look at Residual Dynamic Mode Decomposition in the regime of fewer Snapshots than Dictionary Size,"* **Physica D,** to appear.

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- Verification: dictionaries, approximate eigenfunctions, coherency,…
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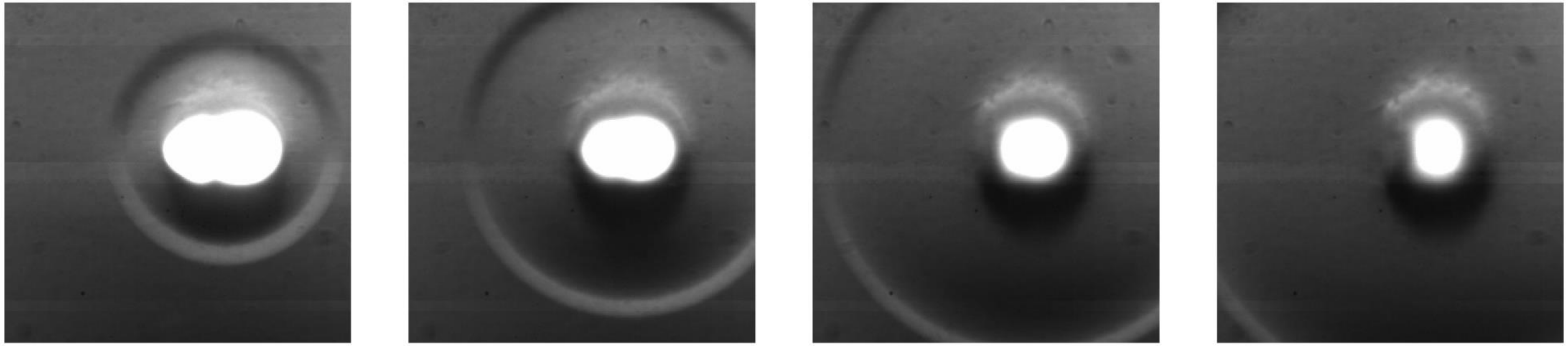
- Extends to kernel methods and $M < N$ (dual residual).
- Extends to stochastic systems (+ variance through Koopman).

See Weds talk!

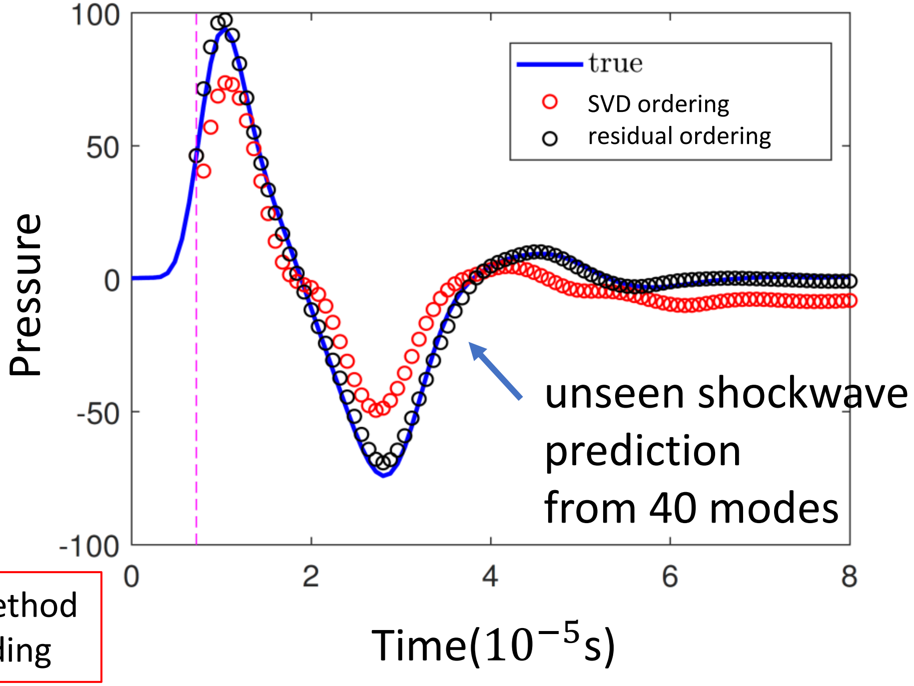
- C., "*Another look at Residual Dynamic Mode Decomposition in the regime of fewer Snapshots than Dictionary Size,*" **Physica D,** to appear.
- C., Li, Raut, Townsend, *"Beyond expectations: Residual Dynamic Mode Decomposition and Variance for Stochastic Dynamical Systems,"* **Nonlinear Dynamics**, 2024.

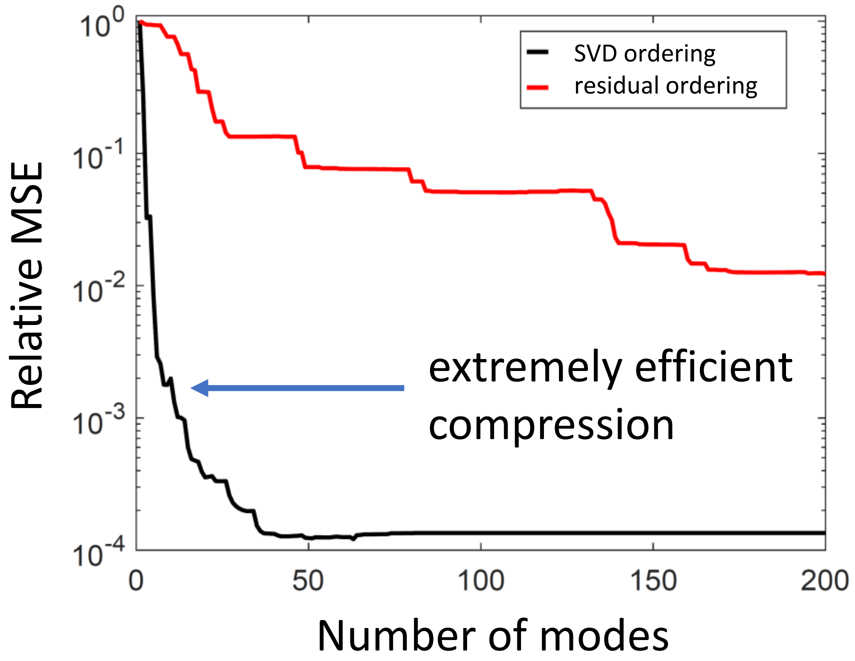
Example: Verified KMD and compression



a) $t = 5\ \mu s$ b) $t = 10\ \mu s$ c) $t = 15\ \mu s$ d) $t = 20\ \mu s$

Matt Szőke's laser cannon!





Use a kernel method
+ delay embedding

Measure-preserving systems

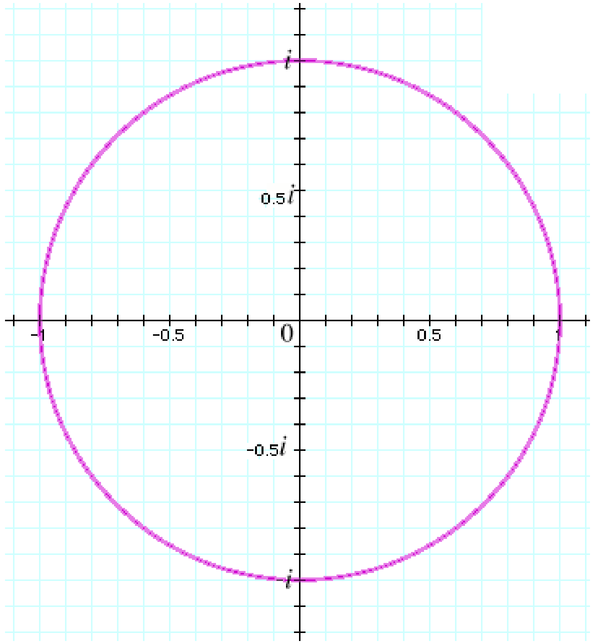
$$[\mathcal{K}g](x) = g\big(S(x)\big), \qquad g \in L^2(\mathcal{X}, \omega)$$

S preserves ω $\Leftrightarrow \|\mathcal{K}g\| = \|g\|$ (isometry)

$\Leftrightarrow \mathcal{K}^*\mathcal{K} = I$

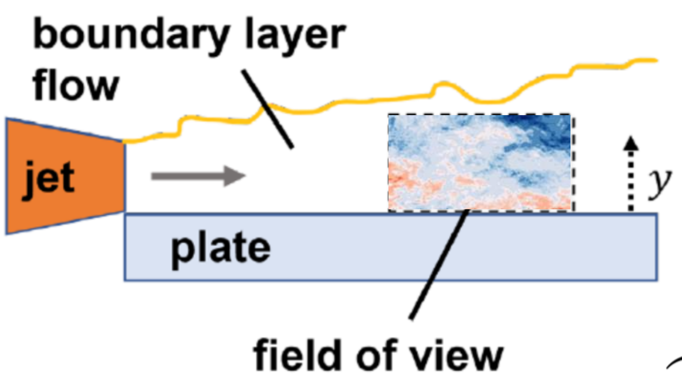
$\Longrightarrow \mathrm{Sp}(\mathcal{K}) \subseteq \{z : |z| \leq 1\}$

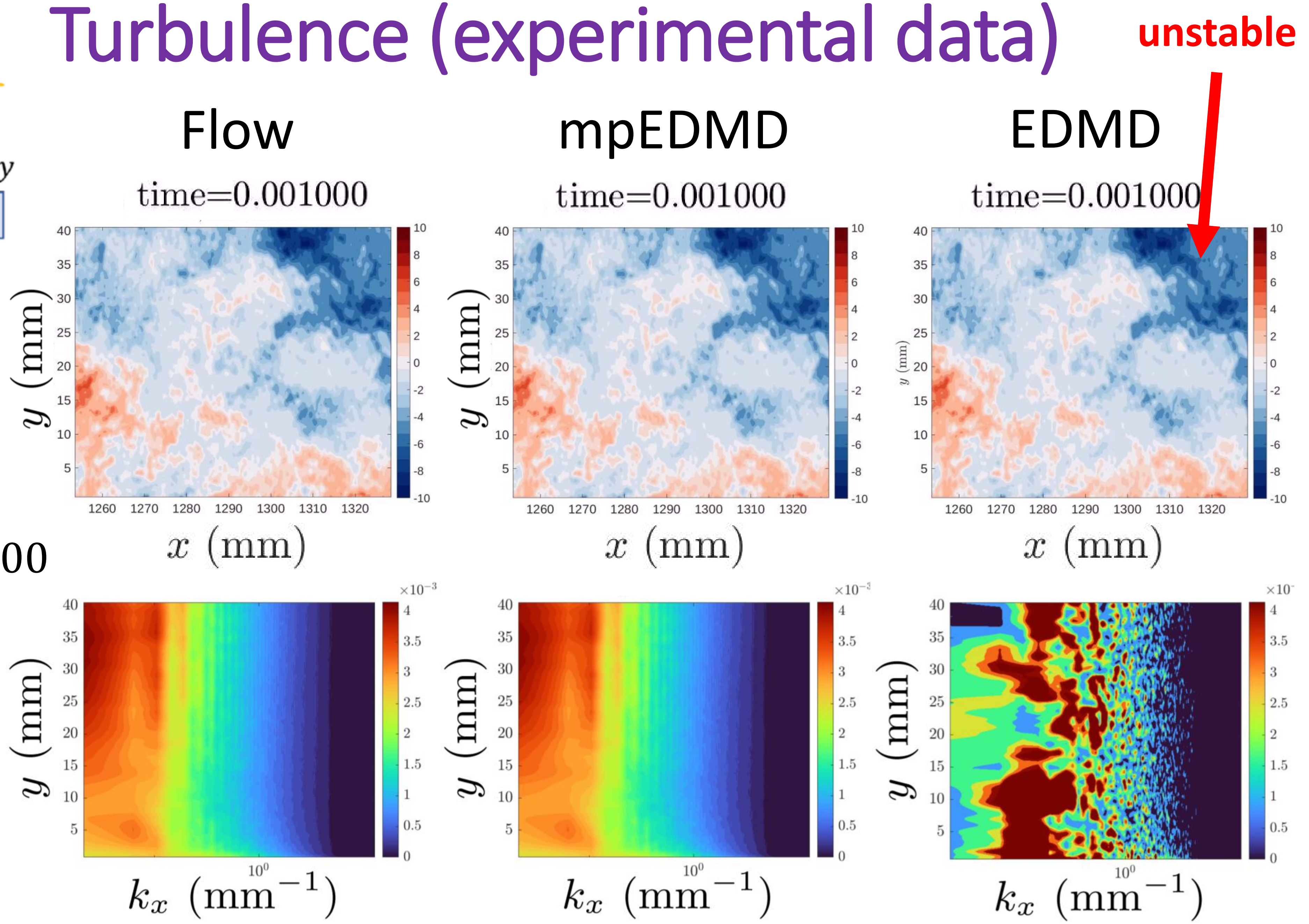
(NB: unitary extensions of $\mathcal{K}$ via Wold decomposition.)



Turbulence (experimental data)

Experimental setup





- Re $\approx 6.4 \times 10^4$
- Ambient dim $\approx$ 100,000 (velocity)

*PIV data provided by Máté Szőke (Virginia Tech)

Preserving measure can be crucial!!

Spectral measures → diagonalisation

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

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

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- **Infinite dimensions:** Unitary $\mathcal{K}$. Typically, no basis of e-vectors!
  Spectral theorem: (projection-valued) spectral measure $\mathcal{E}$

$$g = \left[\int_{\mathrm{Sp}(\mathcal{K})} 1 \, \mathrm{d}\mathcal{E}(\lambda)\right] g, \qquad \mathcal{K}g = \left[\int_{\mathrm{Sp}(\mathcal{K})} \lambda \, \mathrm{d}\mathcal{E}(\lambda)\right] g, \qquad \forall g \in L^2(\mathcal{X}, \omega)$$

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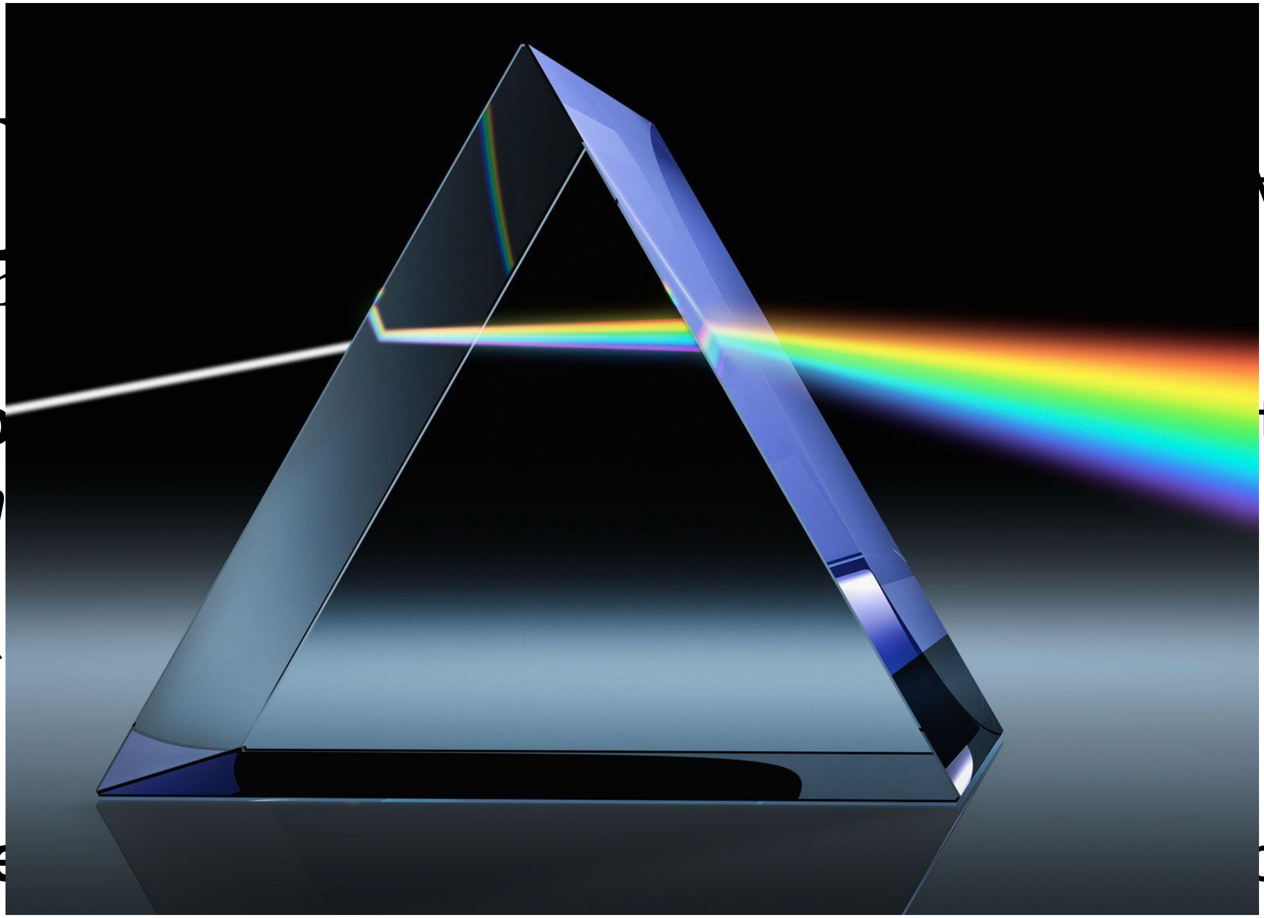
- **Spectral measures:** $\mu_g(U) = \langle \mathcal{E}(U)g, g\rangle$ ($\|g\| = 1$) probability measure.

Spectral measures → diagonalisation

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

$$v = \left[\sum_{j=1} \right. \quad \forall v \in \mathbb{C}^n$$



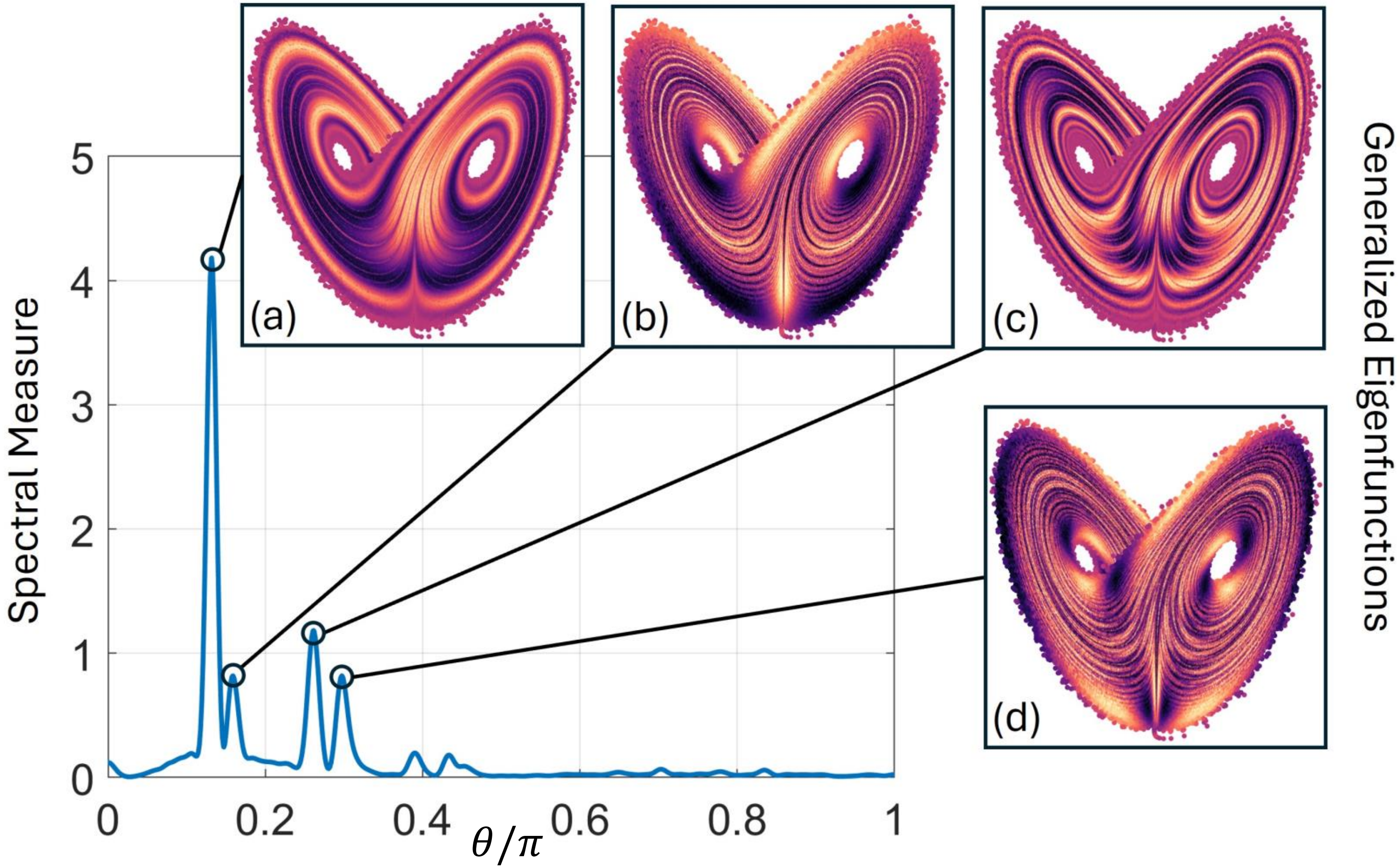
- **Infinite dimensio** tors!
  Spectral theorem

$$g = \left[\int_{\mathrm{Sp}(\mathcal{K})} 1\, \mathrm{d}\mathcal{E} \right. \quad \forall g \in L^2(\mathcal{X},\omega)$$

- **Spectral measure** bility measure.

Example: Seeing cts. spectrum of Lorenz system

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



No formula for generalized eigenfunctions!!

Experimental Details

Single trajectory (ergodic system)

$$M = 10000, N = 1000$$

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

Krylov subspace: $V_N = \{g, \mathcal{K}g, \ldots, \mathcal{K}^{N-1}g\}$

- C., Drysdale, Horning, "*Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators*" **SIADS**, to appear.

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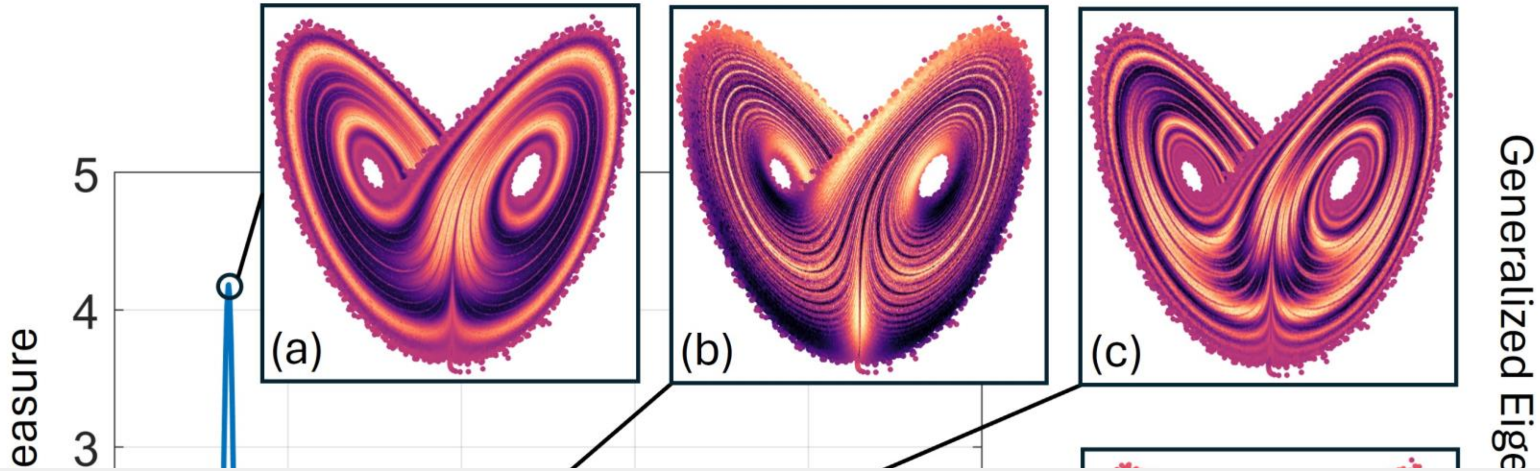

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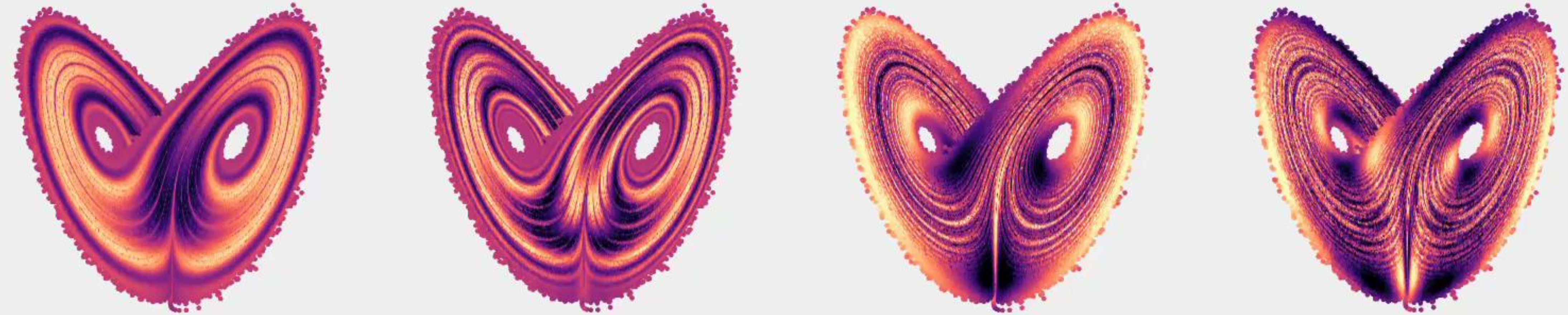
Experimental Details



Overview of methods

- Methods that directly preserve the measure ω (special Galerkin methods):
  - Measure-preserving EDMD (mpEDMD)
  - Periodic approximations (closely related to Ulam's method)
- Methods that involve smoothing:
  - Rigged DMD (computes measures and generalized eigenfunctions)
  - Christoffel-Darboux kernel
  - Compactification methods (for continuous time systems)

- C., *"The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems,"* **SINUM**, 2023.
- Govindarajan, Mohr, Chandrasekaran, Mezić, *"On the approximation of Koopman spectra for measure preserving transformations,"* **SIADS**, 2019.
- C., Drysdale, Horning, "*Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators*" **SIADS**, to appear.
- Korda, Putinar, Mezic, "Data-driven spectral analysis of the Koopman operator," **Appl. Comput. Harmon. Anal.**, 2020.
- Das, Giannakis, Slawinska, *"Reproducing kernel Hilbert space compactification of unitary evolution groups,"* **Appl. Comput. Harm. Anal.**, 2021.

What is actually possible?

- Almost every convergence result involves multiple successive limits,

e.g., first take $M \to \infty$ (large data limit) and then $N \to \infty$ (large dictionary limit)

- One can prove rigorous lower bounds on how many limits are needed.

What is actually possible?

- Almost every convergence result involves multiple successive limits,

e.g., first take $M \to \infty$ (large data limit) and then $N \to \infty$ (large dictionary limit)

- One can prove rigorous lower bounds on how many limits are needed.

Example:

$$\Omega_{\mathbb{D}} = \{S: \mathbb{D} \to \mathbb{D} \mid S \text{ cts, measure preserving, invertible}\}.$$

Input data: $\mathcal{T}_S = \{(x, y_m): x \in \mathbb{D}, \|S(x) - y_m\| \leq 2^{-m}\}$.

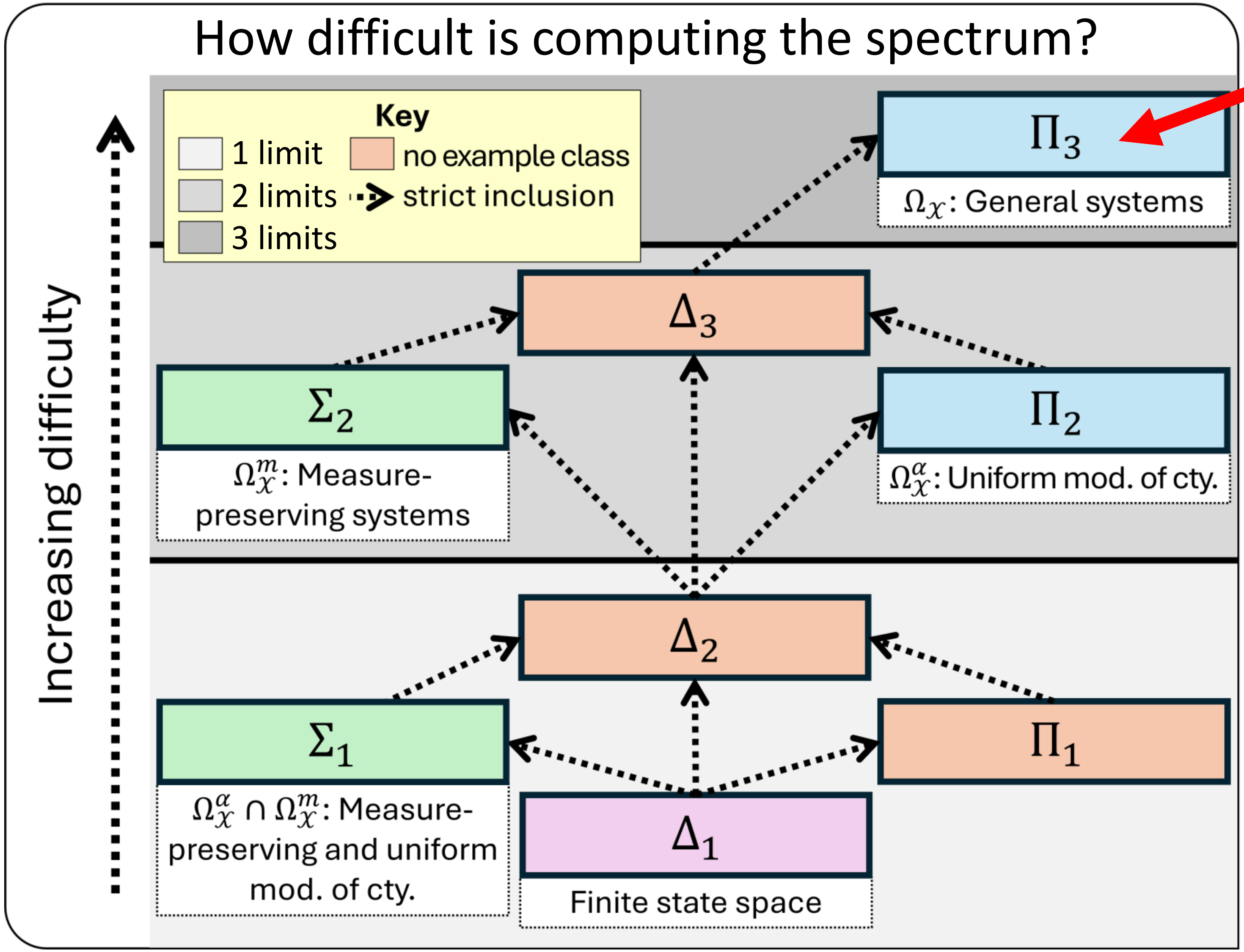
Theorem: There **does not exist** any single-limit sequence of deterministic algorithms $\{\Gamma_n\}$ using $\mathcal{T}_S$ such that $\lim_{n\to\infty} \Gamma_n(S) = \mathrm{Sp}(\mathcal{K}_S)\ \ \forall S \in \Omega_{\mathbb{D}}$.

NB: Impossibility extends to random algorithms converging with probability $> 1/2$.

- C., Mezić, Stepanenko, "*Limits and Powers of Koopman Learning,*" **preprint**, 2024.

Classifications

3 limits needed in general!



Different classes:

$\Omega_{\mathcal{X}} = \{S: \mathcal{X} \to \mathcal{X} \text{ s.t. } S \text{ cts}\}$

$\Omega_{\mathcal{X}}^{m} = \{S: \mathcal{X} \to \mathcal{X} \text{ s.t. } S \text{ cts, m.p.}\}$

$\Omega_{\mathcal{X}}^{\alpha} = \{S: \mathcal{X} \to \mathcal{X} \text{ s.t. } S \text{ mod. cty. } \alpha\}$

$[d_{\mathcal{X}}(S(x), S(y)) \leq \alpha(d_{\mathcal{X}}(x,y))]$

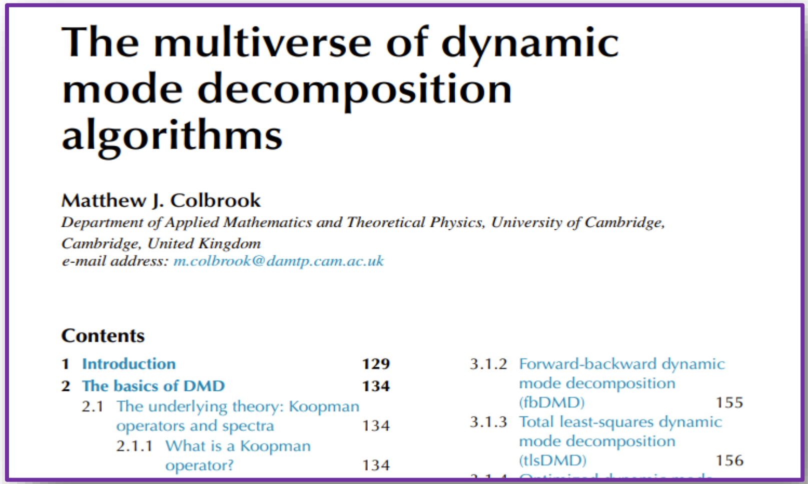
Optimal algorithms and classifications of dynamical systems.

- C., Mezić, Stepanenko, *"Limits and Powers of Koopman Learning,"* **preprint**, 2024.

Conclusion

- **WARNING:** EDMD does not converge to spectral properties of $\mathcal{K}$.
- **GOOD NEWS:** There are now tools that fix this, including:
  - Computing spectra with error bounds
  - Dealing with continuous spectra
  - Dealing with instability
- Most convergent methods necessarily require multiple limits $\Longrightarrow$ Classifiction

Review of the vast array of DMD methods:



The multiverse of dynamic mode decomposition algorithms

Matthew J. Colbrook

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Contents

This is an exciting time to develop methods that address the infinite-dimensional nature of Koopman operators. I encourage others to join the fray!

- C., "The Multiverse of Dynamic Mode Decomposition Algorithms," **Handbook of Numerical Analysis**, 2024.

References

[1] Colbrook, Matthew J., and Alex Townsend. "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems." Communications on Pure and Applied Mathematics 77.1 (2024): 221-283.

[2] Colbrook, Matthew J., Lorna J. Ayton, and Máté Szőke. "Residual dynamic mode decomposition: robust and verified Koopmanism." Journal of Fluid Mechanics 955 (2023): A21.

[3] Colbrook, M. J., Li, Q., Raut, R. V., & Townsend, A. "Beyond expectations: residual dynamic mode decomposition and variance for stochastic dynamical systems." Nonlinear Dynamics 112.3 (2024): 2037-2061.

[4] Colbrook, Matthew J. "The Multiverse of Dynamic Mode Decomposition Algorithms." arXiv preprint arXiv:2312.00137 (2023).

[5] Colbrook, Matthew J. "The mpEDMD algorithm for data-driven computations of measure-preserving dynamical systems." SIAM Journal on Numerical Analysis 61.3 (2023): 1585-1608.

[6] Colbrook, Matthew J., Catherine Drysdale, and Andrew Horning. "Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators." arXiv preprint arXiv:2405.00782 (2024).

[7] Boullé, Nicolas, and Matthew J. Colbrook. "Multiplicative Dynamic Mode Decomposition." arXiv preprint arXiv:2405.05334 (2024).

[8] Colbrook, Matthew J. "Another look at Residual Dynamic Mode Decomposition in the regime of fewer Snapshots than Dictionary Size." arXiv preprint arXiv:2403.05891 (2024).

[9] Colbrook, Matthew. "The foundations of infinite-dimensional spectral computations." Diss. University of Cambridge, 2020.

[10] Ben-Artzi, J., Colbrook, M. J., Hansen, A. C., Nevanlinna, O., & Seidel, M. (2020). "Computing Spectra--On the Solvability Complexity Index Hierarchy and Towers of Algorithms." arXiv preprint arXiv:1508.03280.

[11] Colbrook, Matthew J., Vegard Antun, and Anders C. Hansen. "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem." Proceedings of the National Academy of Sciences 119.12 (2022): e2107151119.

[12] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Computing spectral measures of self-adjoint operators." SIAM review 63.3 (2021): 489-524.

[13] Colbrook, Matthew J., Bogdan Roman, and Anders C. Hansen. "How to compute spectra with error control." Physical Review Letters 122.25 (2019): 250201.

[14] Colbrook, Matthew J., and Anders C. Hansen. "The foundations of spectral computations via the solvability complexity index hierarchy." Journal of the European Mathematical Society (2022).

[15] Colbrook, Matthew J. "Computing spectral measures and spectral types." Communications in Mathematical Physics 384 (2021): 433-501.

[16] Colbrook, Matthew J., and Anders C. Hansen. "On the infinite-dimensional QR algorithm." Numerische Mathematik 143 (2019): 17-83.

[17] Colbrook, Matthew J. "On the computation of geometric features of spectra of linear operators on Hilbert spaces." Foundations of Computational Mathematics (2022): 1-82.

[18] Brunton, Steven L., and Matthew J. Colbrook. "Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective."

[19] Colbrook, Matthew J., Igor Mezić, and Alexei Stepanenko. "Limits and Powers of Koopman Learning." arXiv preprint arxiv:2407.06312 (2024).