

The Hitchhiker's Guide to the DMD Multiverse

Matthew Colbrook

University of Cambridge

23/05/2024

- 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.

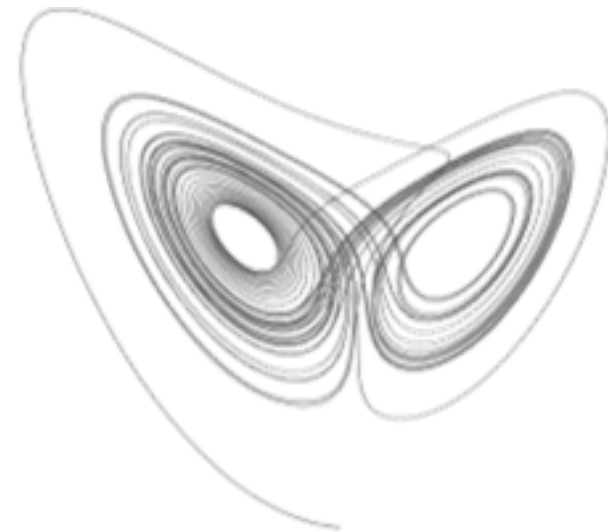
Data-driven dynamical systems

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

Unknown function $F: \Omega \rightarrow \Omega$ governs dynamics: $x_{n+1} = F(x_n)$.

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

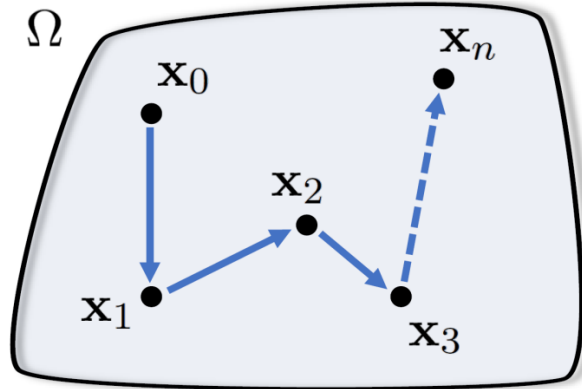
Applications: chemistry, climatology, control, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, etc.



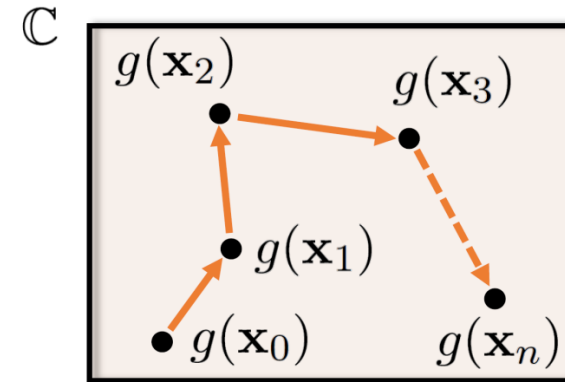
Surveys:

- 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.

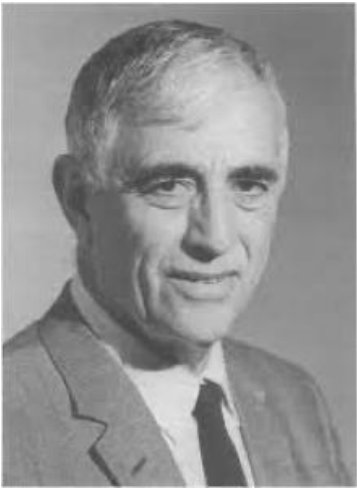
Koopman Operator \mathcal{K} : A global linearization



$g: \Omega \rightarrow \mathbb{C}$
 "observable"



Koopman

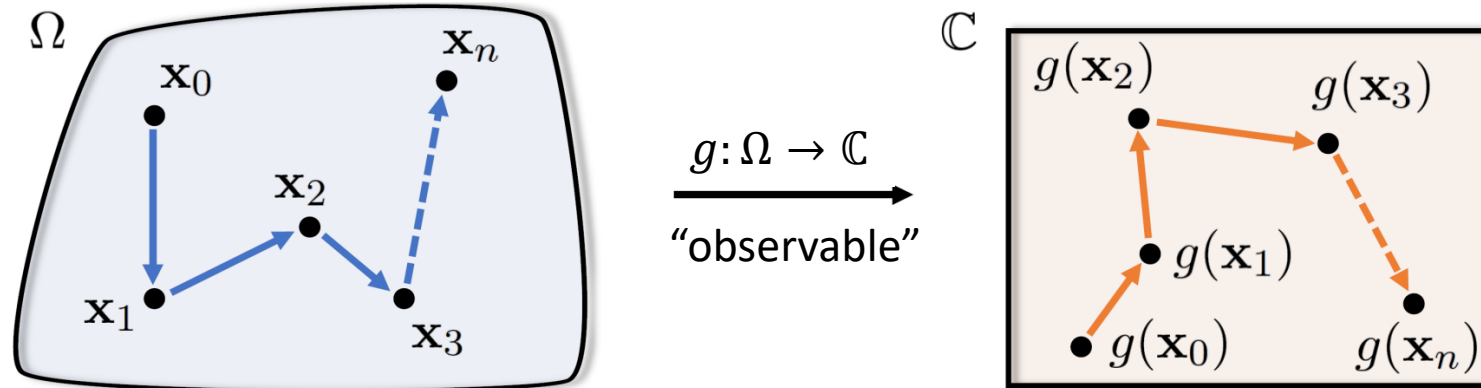


von Neumann



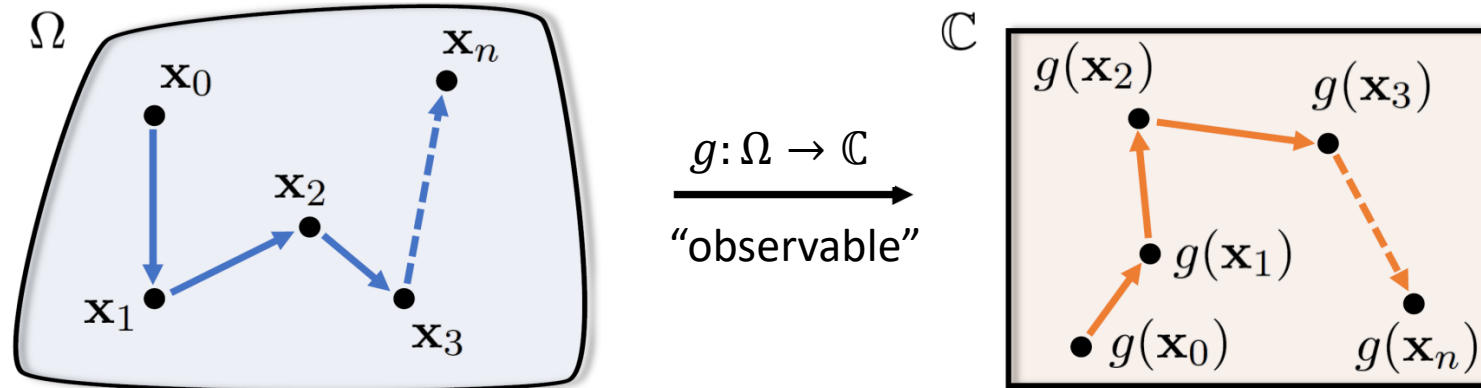
- Koopman, "Hamiltonian systems and transformation in Hilbert space," *Proc. Natl. Acad. Sci. USA*, 1931.
- Koopman, v. Neumann, "Dynamical systems of continuous spectra," *Proc. Natl. Acad. Sci. USA*, 1932.

Koopman Operator \mathcal{K} : A global linearization

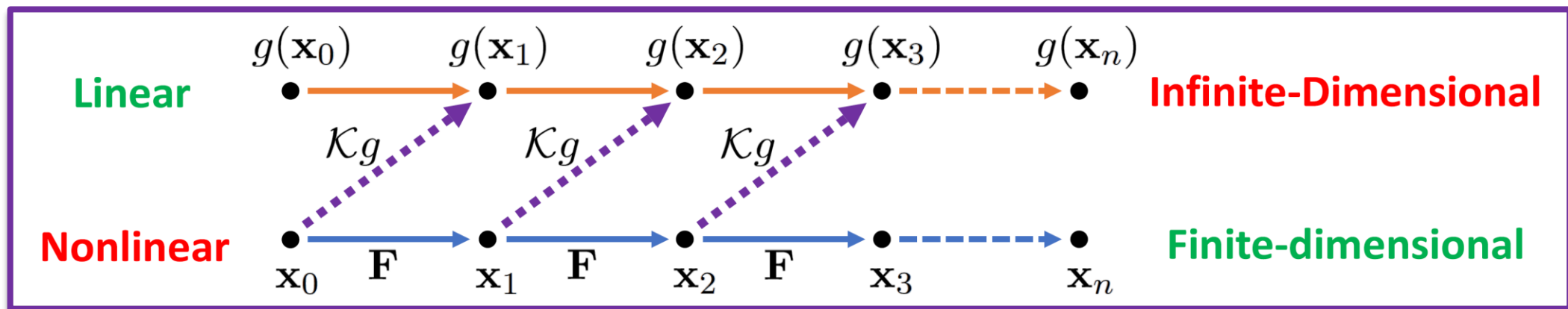


- \mathcal{K} acts on functions $g: \Omega \rightarrow \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- **Function space:** $L^2(\Omega, \omega)$, positive measure ω , inner product $\langle \cdot, \cdot \rangle$.

Koopman Operator \mathcal{K} : A global linearization



- \mathcal{K} acts on functions $g: \Omega \rightarrow \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- **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.

Koopman mode decomposition

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

$$[\mathcal{K}g](x) = g(F(x))$$

$$g(x) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \underbrace{\varphi_{\lambda_j}(x)}_{\text{eigenfunction of } \mathcal{K}} + \int_{-\pi}^{\pi} \underbrace{\phi_{\theta,g}(x)}_{\text{continuous spectrum}} d\theta$$

$$g(x_n) = [\mathcal{K}^n g](x_0) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \lambda_j^n \varphi_{\lambda_j}(x_0) + \int_{-\pi}^{\pi} e^{in\theta} \phi_{\theta,g}(x_0) d\theta$$

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.

Koopman mode decomposition

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

$$[\mathcal{K}g](x) = g(F(x))$$

$$g(x) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \varphi_{\lambda_j}(x) + \int_{-\pi}^{\pi} \phi_{\theta,g}(x) d\theta$$

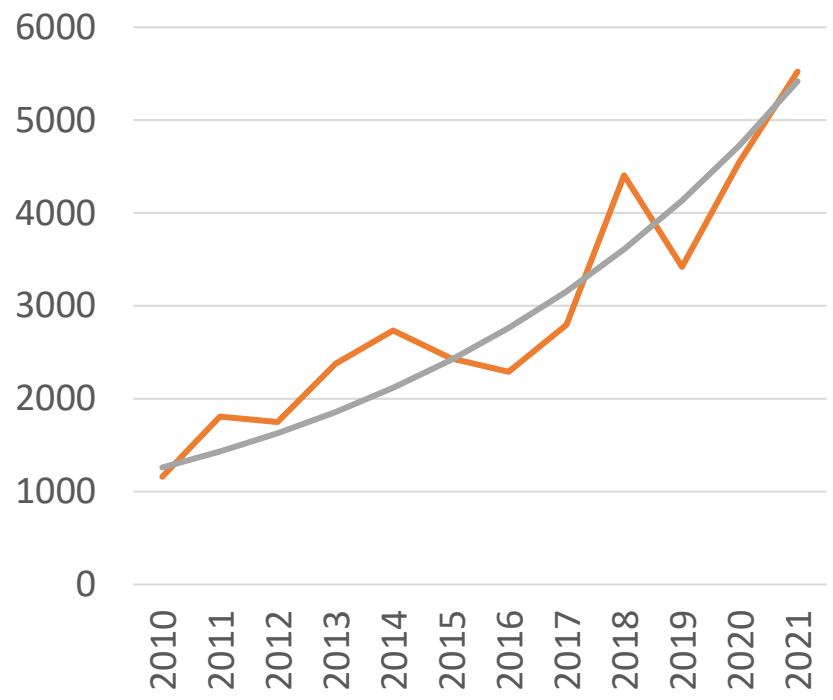
eigenfunction of \mathcal{K} ← continuous spectrum

$$g(x_n) = [\mathcal{K}^n g](x_0) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \lambda_j^n \varphi_{\lambda_j}(x_0) + \int_{-\pi}^{\pi} e^{in\theta} \phi_{\theta,g}(x_0) d\theta$$

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

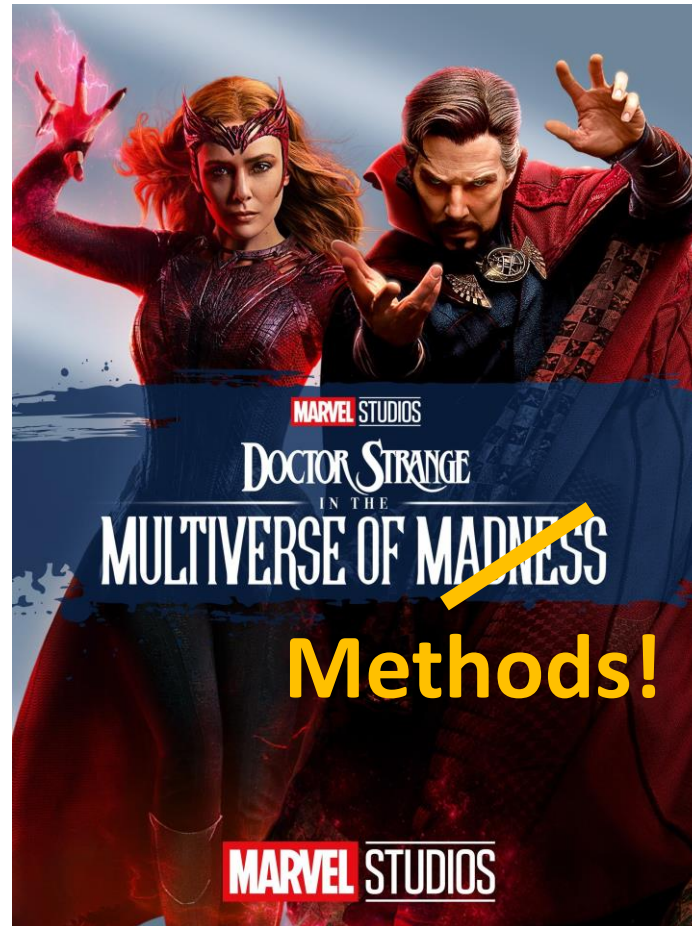
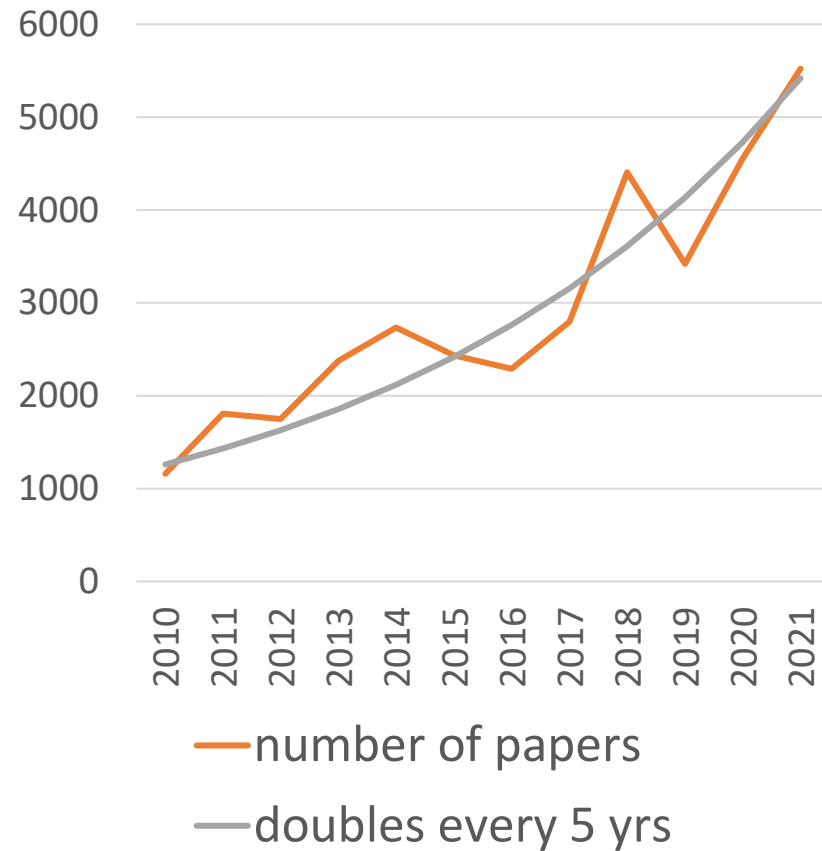
GOAL: Data-driven approximation of \mathcal{K} and its **spectral properties.**

New Papers on "Koopman Operators"



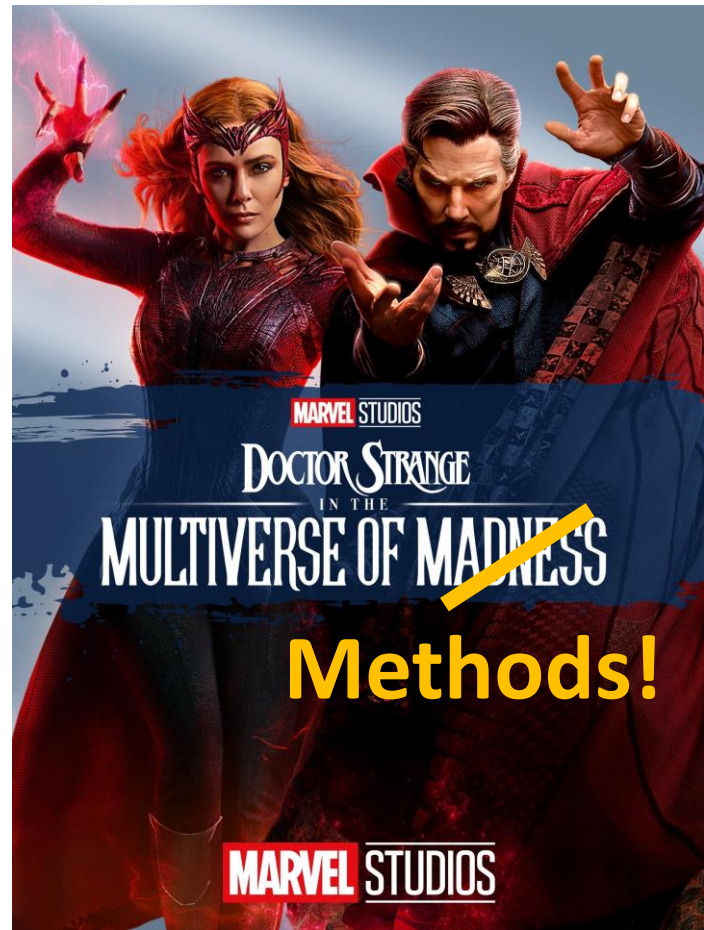
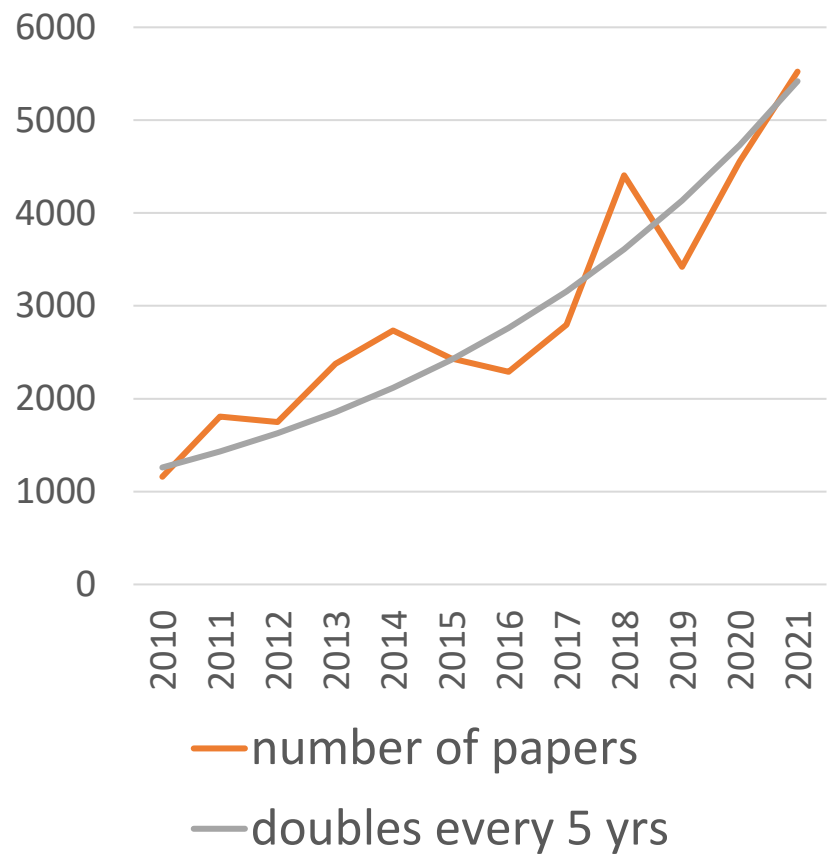
- number of papers
- doubles every 5 yrs

New Papers on “Koopman Operators”

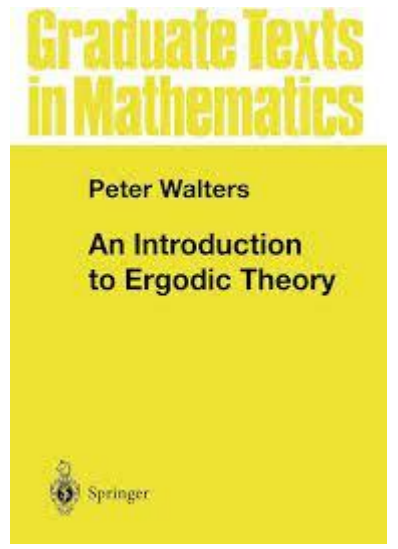


- C., “The Multiverse of Dynamic Mode Decomposition Algorithms,” **Handbook of Numerical Analysis, 2024.**

New Papers on "Koopman Operators"



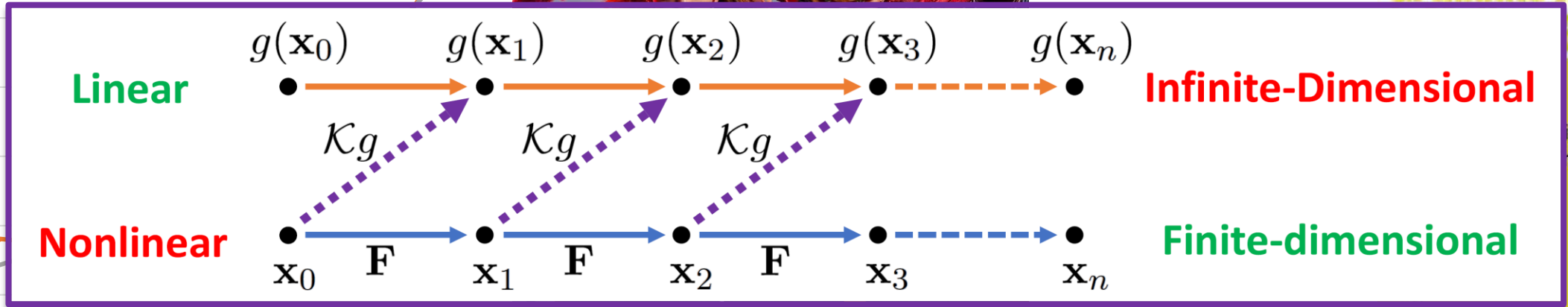
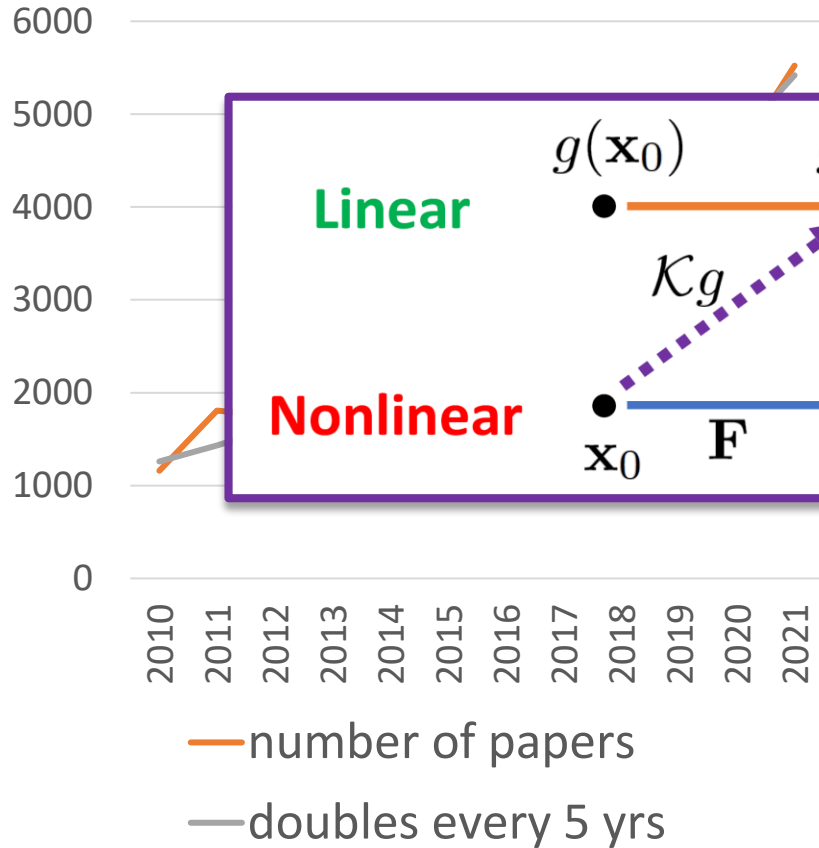
Koopman operators are
classical in ergodic theory.



Why all this sudden interest?

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

New Papers on "Koopman Operators"



Graduate Texts in Mathematics

on theory

Springer



Methods!

Why all this sudden interest?

- Data-driven
- Deal with nonlinearity
- Easy-to-use methods

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

$$\begin{pmatrix} \ddots & & & & & & \\ & \ddots & & & & & \\ & & 0 & 1 & & & \\ & & & 0 & 1 & & \\ & & & & 0 & 1 & \\ & & & & & 0 & 1 \\ & & & & & & 0 & \ddots \\ & & & & & & & 0 & \ddots \end{pmatrix} \xrightarrow{\text{Two-way infinite}} \begin{pmatrix} 0 & 1 & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & 1 & \\ & & & & 1 & 0 \end{pmatrix} \in \mathbb{C}^{N \times N}$$

- 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 $\mathcal{K} \rightarrow \mathbb{K} \in \mathbb{C}^{N \times N}$

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

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



Caution

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

Outline

- General systems:
 - Residual Dynamic Mode Decomposition.
- Measure-preserving systems:
 - Measure-Preserving Extended Dynamic Mode Decomposition.
 - Rigged Dynamic Mode Decomposition.
- The **Solvability Complexity Index** – *classification* of problems and *optimality* of algorithms.



**HOT OFF
THE
PRESS**

Outline

- General systems:
 - **Residual Dynamic Mode Decomposition.**
- Measure-preserving systems:
 - Measure-Preserving Extended Dynamic Mode Decomposition.
 - Rigged Dynamic Mode Decomposition.
- The **Solvability Complexity Index** – *classification* of problems and *optimality* of algorithms.



**HOT OFF
THE
PRESS**

Extended Dynamic Mode Decomposition (EDMD)

Functions $\psi_j: \Omega \rightarrow \mathbb{C}, j = 1, \dots, N$

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

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

Extended Dynamic Mode Decomposition (EDMD)

Functions $\psi_j: \Omega \rightarrow \mathbb{C}, j = 1, \dots, N$

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

quadrature points

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

quadrature weights

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

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

Extended Dynamic Mode Decomposition (EDMD)

Functions $\psi_j: \Omega \rightarrow \mathbb{C}, j = 1, \dots, N$

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

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

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

Galerkin
Approximation

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

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

Extended Dynamic Mode Decomposition (EDMD)

Functions $\psi_j: \Omega \rightarrow \mathbb{C}, j = 1, \dots, N$

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

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

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



Caution

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

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

Residual DMD (ResDMD)

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

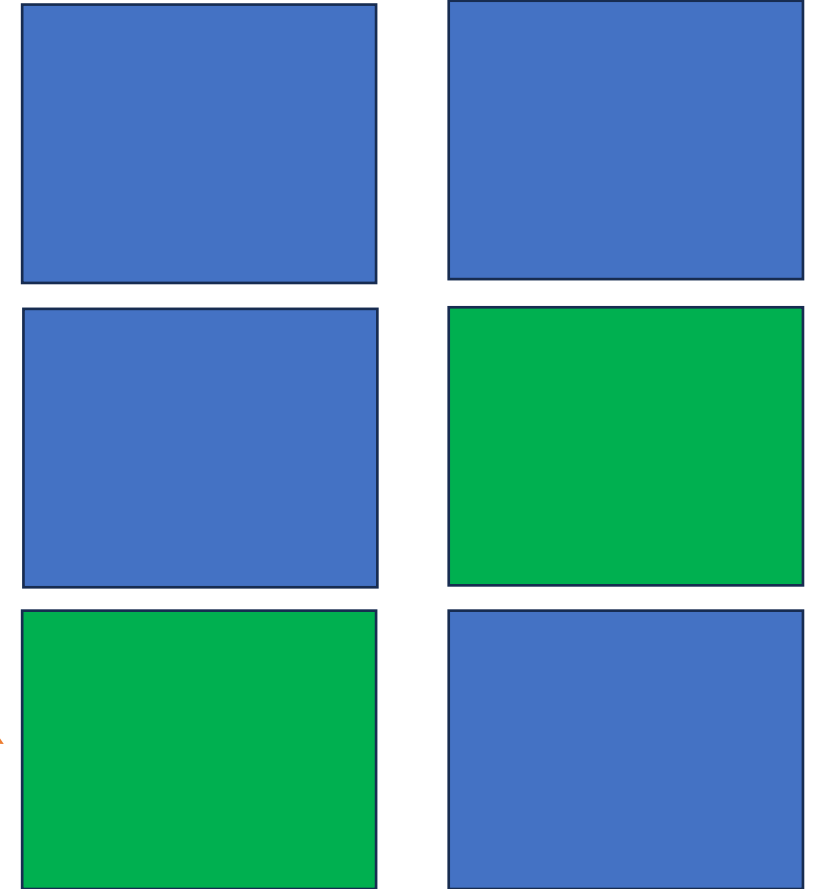
$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," **J. Fluid Mech.**, 2023.
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

Residual DMD (ResDMD)

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

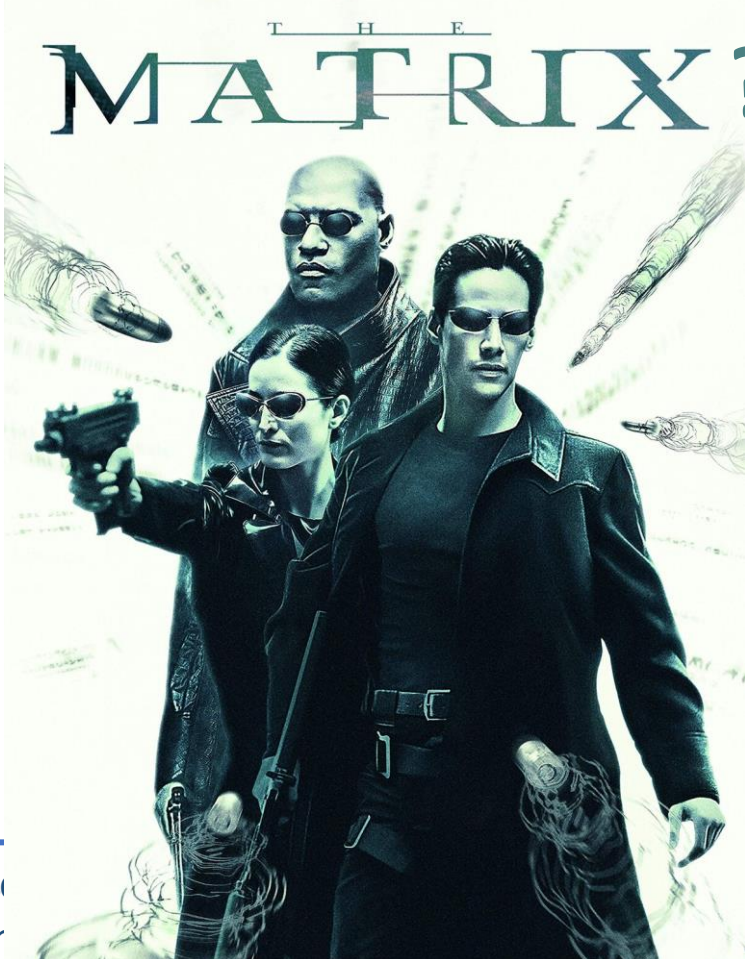
$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$



- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," **J. Fluid Mech.**, 2023.
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

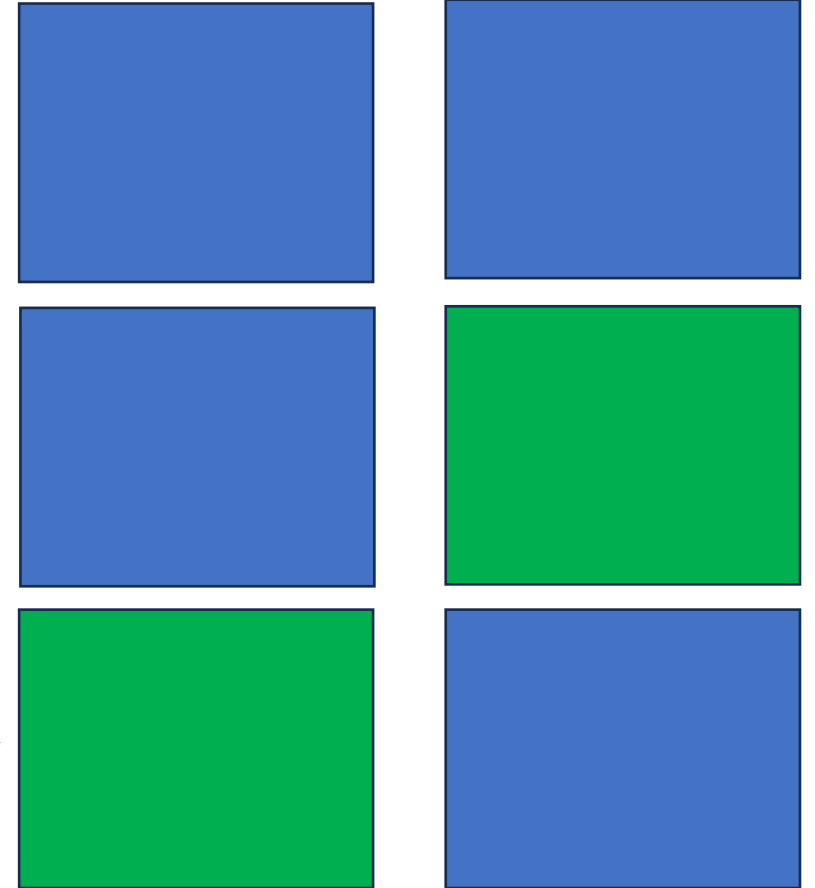
Residual DMD (ResDMD)

What's the missing



$$= \left[\underbrace{\Psi_X^* W \Psi_X}_G \right]_{jk}$$

$$= \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$



- C., Towns
- C., Aytor
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>
- "Central properties of Koopman operators for dynamical systems," *Commun. Pure Appl. Math.*, 2023.
- "Composition," *J. Fluid Mech.*, 2023.

Residual DMD (ResDMD)

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

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \underbrace{[\Psi_X^* W \Psi_Y]}_{K_1}]_{jk}$$

$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(y^{(m)})} \psi_k(y^{(m)}) = \underbrace{[\Psi_Y^* W \Psi_Y]}_{K_2}]_{jk}$$



- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," **J. Fluid Mech.**, 2023.
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

Residual DMD (ResDMD)

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

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(y^{(m)})} \psi_k(y^{(m)}) = \left[\underbrace{\Psi_Y^* W \Psi_Y}_{K_2} \right]_{jk}$$

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

- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," **J. Fluid Mech.**, 2023.
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

Residual DMD (ResDMD)

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

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(y^{(m)})} \psi_k(y^{(m)}) = \left[\underbrace{\Psi_Y^* W \Psi_Y}_{K_2} \right]_{jk}$$

Residuals: $g = \sum_{j=1}^N \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 = \sum_{k,j=1}^N \mathbf{g}_k \overline{\mathbf{g}_j} \langle \mathcal{K}\psi_k - \lambda \psi_k, \mathcal{K}\psi_j - \lambda \psi_j \rangle$

- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," **J. Fluid Mech.**, 2023.
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

Residual DMD (ResDMD)

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

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(y^{(m)})} \psi_k(y^{(m)}) = \left[\underbrace{\Psi_Y^* W \Psi_Y}_{K_2} \right]_{jk}$$



Residuals: $g = \sum_{j=1}^N \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 = \lim_{M \rightarrow \infty} \mathbf{g}^* [K_2 - \lambda K_1^* - \bar{\lambda} K_1 + |\lambda|^2 G] \mathbf{g}$

- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," *Commun. Pure Appl. Math.*, 2023.
- C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," *J. Fluid Mech.*, 2023.
- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

ResDMD: Avoiding the dangers

If quadrature rule converges

Convergent methods for general \mathcal{K}

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

M = number of snapshots
 N = number of basis functions

ResDMD: Avoiding the dangers

If quadrature rule converges

Convergent methods for general \mathcal{K}

- **1 limit** $\lim_{M \rightarrow \infty}$: Avoid spurious eigenvalues.

- **2 limits** $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$: Compute $\text{Sp}_\varepsilon(\mathcal{K}) = \bigcup_{\|\mathcal{B}\| \leq \varepsilon} \text{Sp}(\mathcal{K} + \mathcal{B})$.

- **3 limits** $\lim_{\varepsilon \downarrow 0} \lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$: Compute $\text{Sp}(\mathcal{K})$.

M = number of snapshots
 N = number of basis functions

- Verification: dictionaries, approximate eigenfunctions, coherency,...
- Error bounds of forecasts.
- Extends to kernel methods and $M < N$ (dual residual).

ResDMD: Avoiding the dangers

If quadrature rule converges

Convergent methods for general \mathcal{K}

- **1 limit** $\lim_{M \rightarrow \infty}$: Avoid spurious eigenvalues.

- **2 limits** $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$: Compute $\text{Sp}_\varepsilon(\mathcal{K}) = \bigcup_{\|\mathcal{B}\| \leq \varepsilon} \text{Sp}(\mathcal{K} + \mathcal{B})$.

- **3 limits** $\lim_{\varepsilon \downarrow 0} \lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$: Compute $\text{Sp}(\mathcal{K})$.

M = number of snapshots
 N = number of basis functions

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

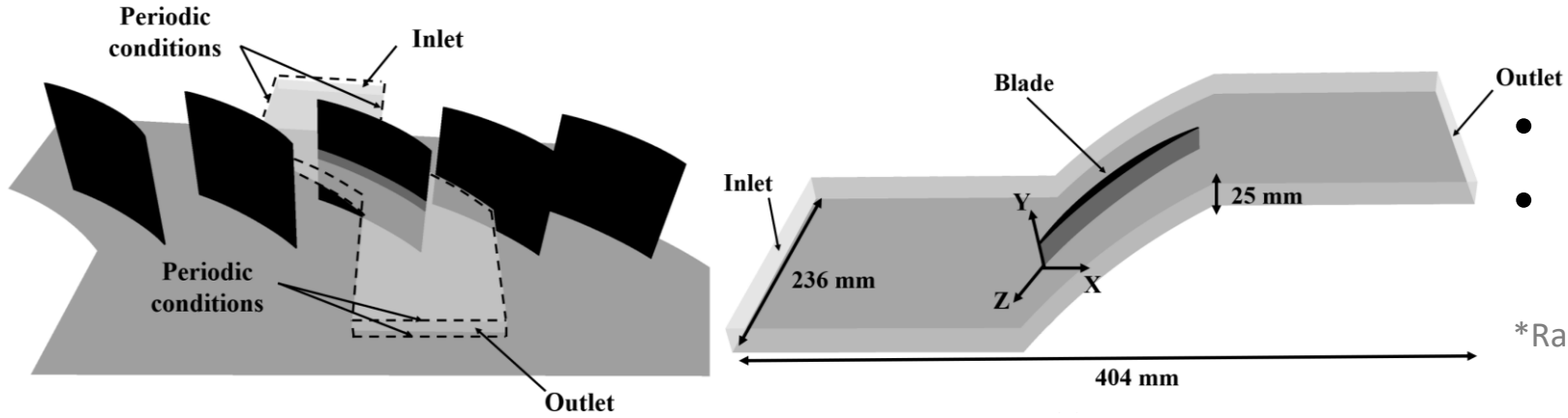
Quadrature with trajectory data

$$\text{E.g., } \langle \mathcal{K}\psi_k, \psi_j \rangle = \lim_{M \rightarrow \infty} \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})}$$

Three examples:

- **High-order quadrature:** $\{x^{(m)}, w_m\}_{m=1}^M$ M -point quadrature rule.
 Rapid convergence. Requires free choice of $\{x^{(m)}\}_{m=1}^M$ and small d .
- **Random sampling:** $\{x^{(m)}\}_{m=1}^M$ selected at random. ← Most common
 Large d . Slow Monte Carlo $O(M^{-1/2})$ rate of convergence.
- **Ergodic sampling:** $x^{(m+1)} = F(x^{(m)})$. ↙
 Single trajectory, large d . Requires ergodicity, convergence can be slow.

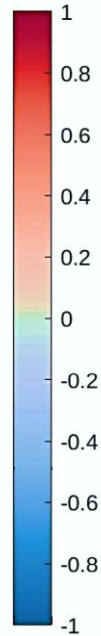
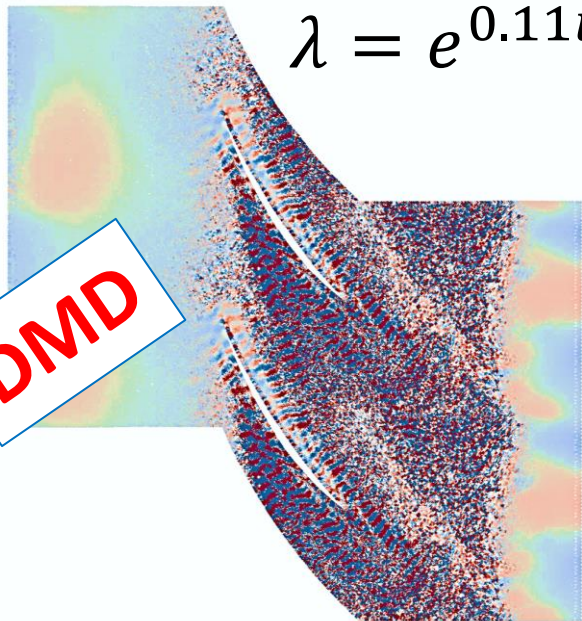
Example: Verified spectra and modes



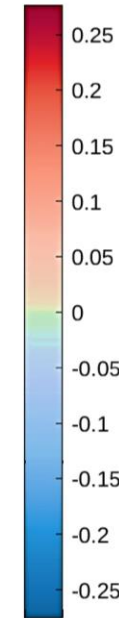
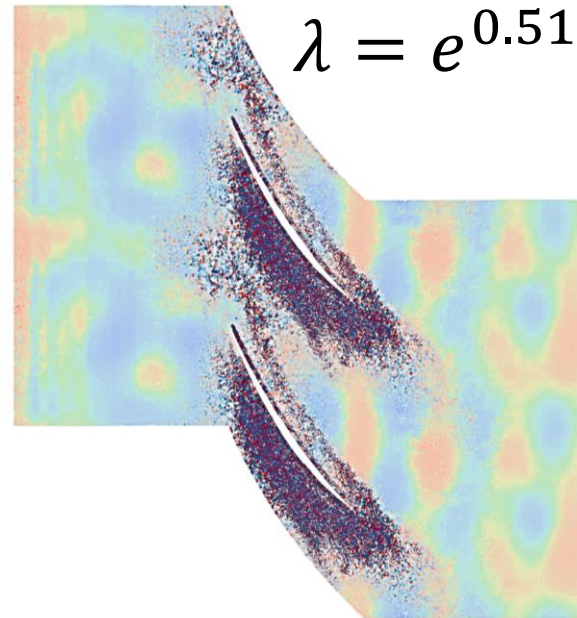
- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension (d) $\approx 300,000$ (number of measurement points)

*Raw measurements provided by Stephane Moreau (Sherbrooke)

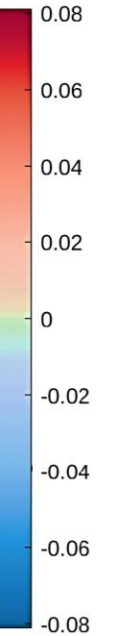
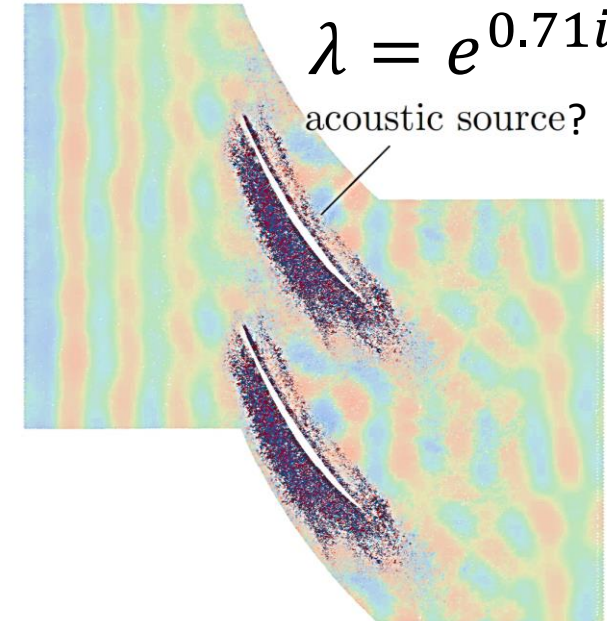
Rel. Error = ?
 $\lambda = e^{0.11i}$



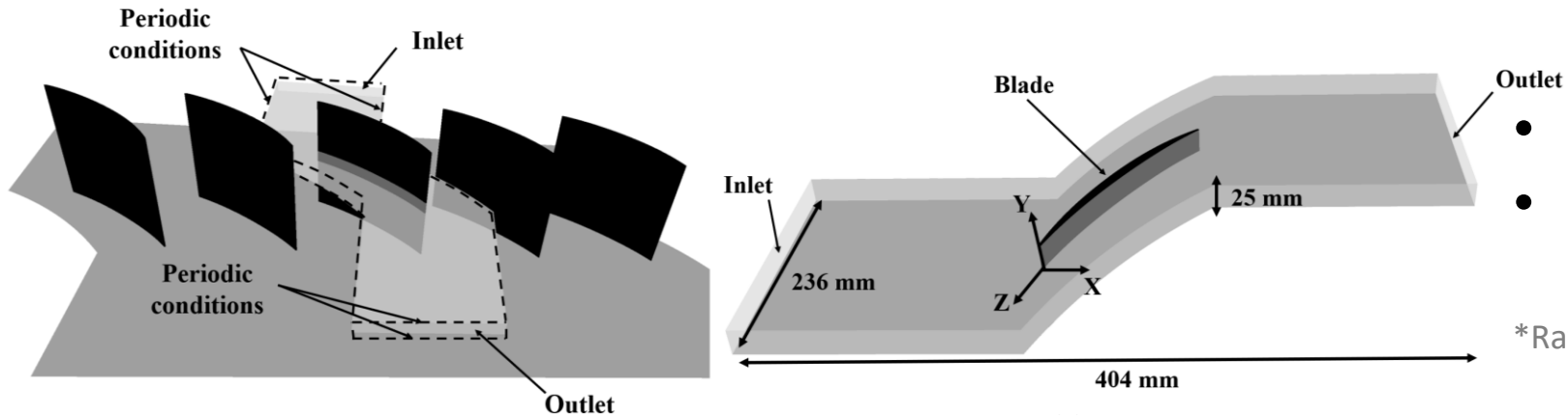
Rel. Error = ?
 $\lambda = e^{0.51i}$



Rel. Error = ?
 $\lambda = e^{0.71i}$
 acoustic source?



Example: Verified spectra and modes

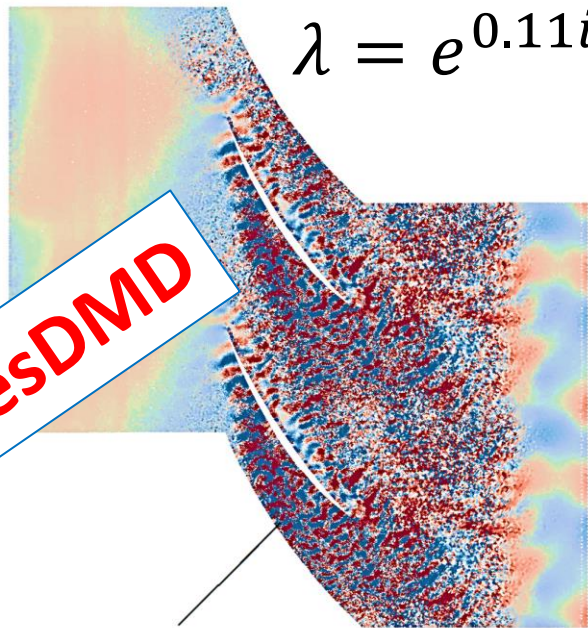


- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension (d) $\approx 300,000$ (number of measurement points)

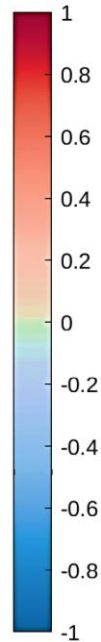
*Raw measurements provided by Stephane Moreau (Sherbrooke)

Rel. Error ≤ 0.0054

$$\lambda = e^{0.11i}$$

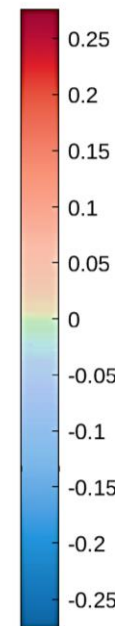
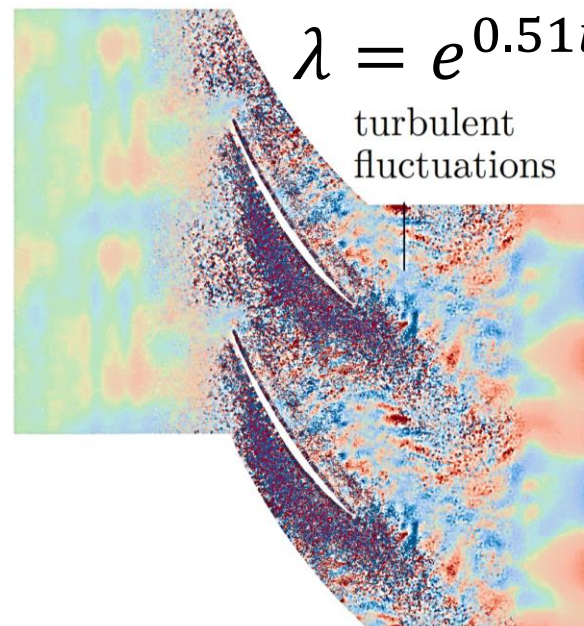


acoustic vibrations



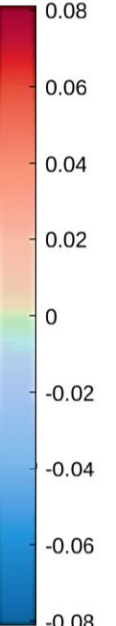
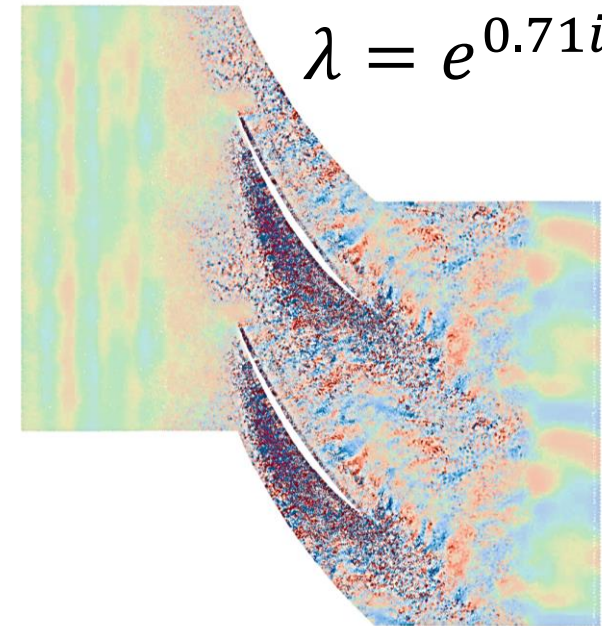
Rel. Error ≤ 0.0128

$$\lambda = e^{0.51i}$$

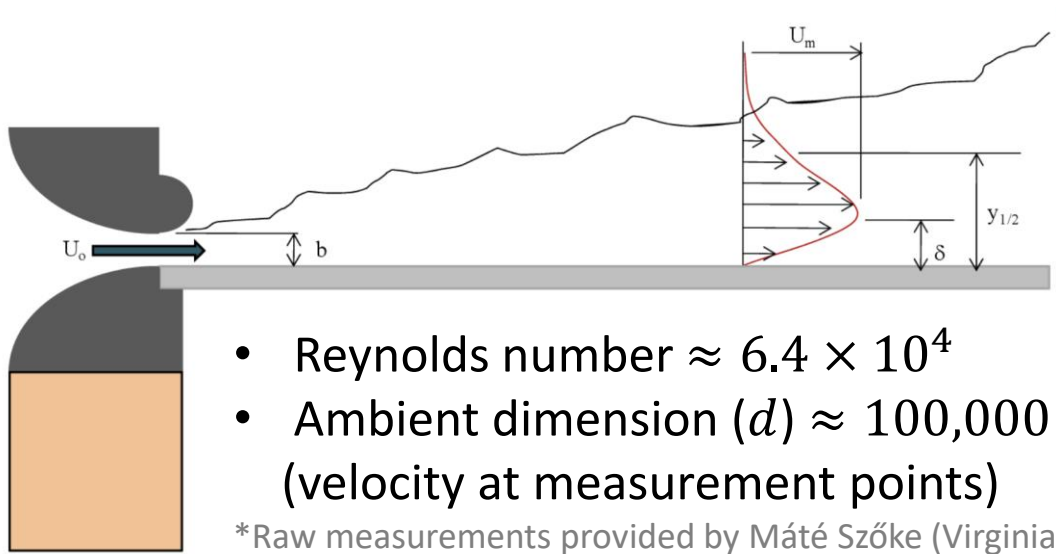


Rel. Error ≤ 0.0196

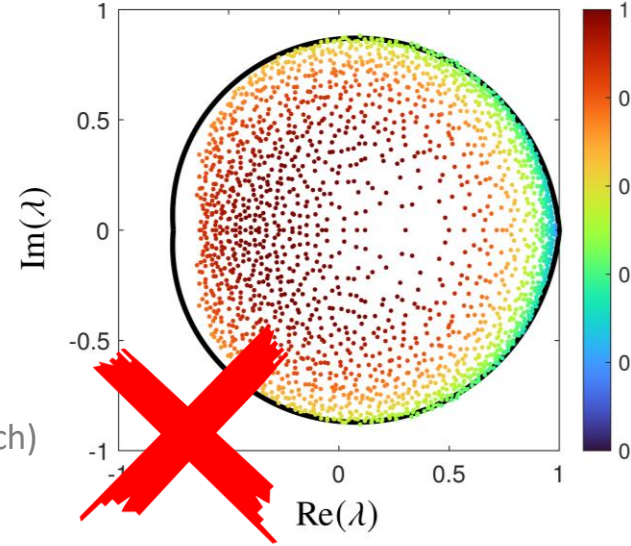
$$\lambda = e^{0.71i}$$



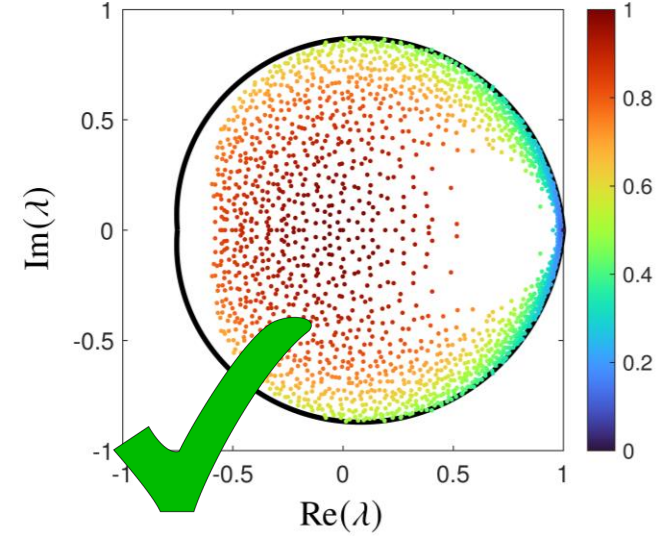
Example: Verified dictionary



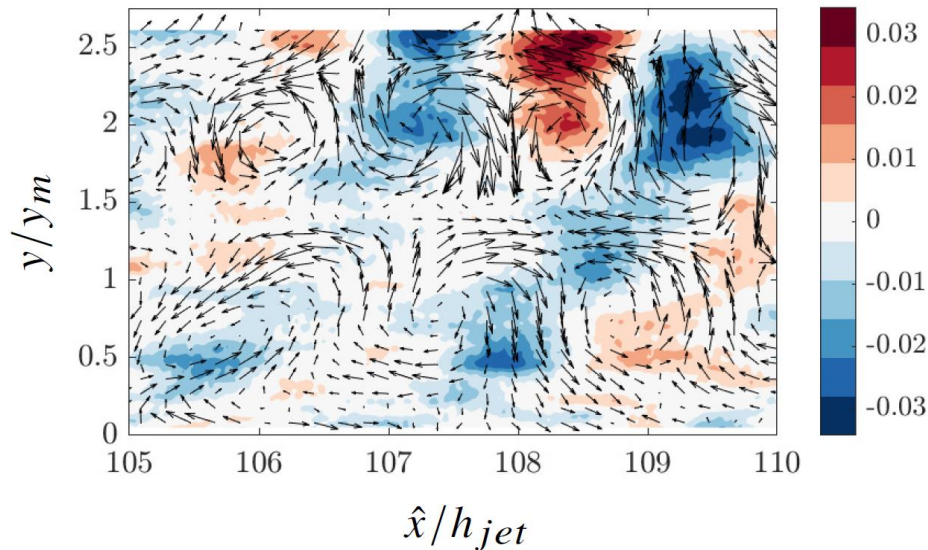
Residuals using
Truncated SVD (linear)



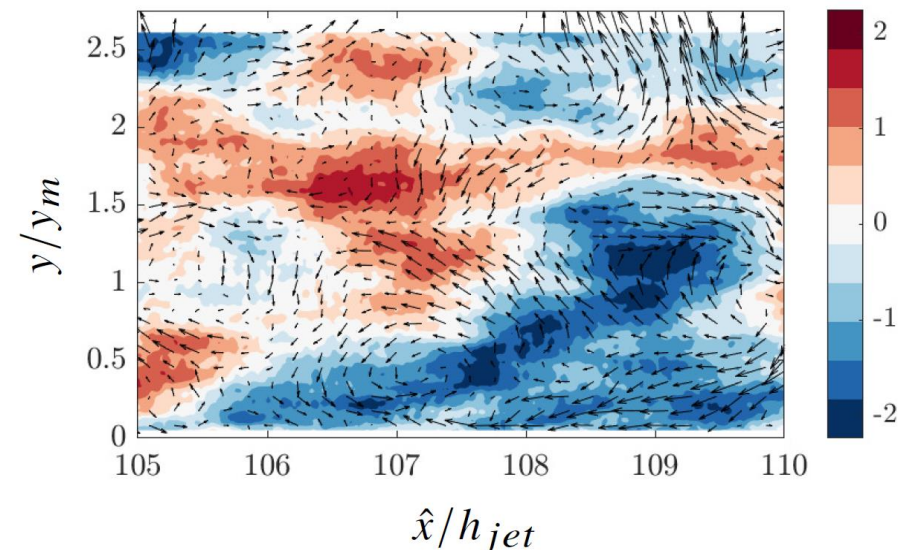
Residuals using
Gaussian kernel method



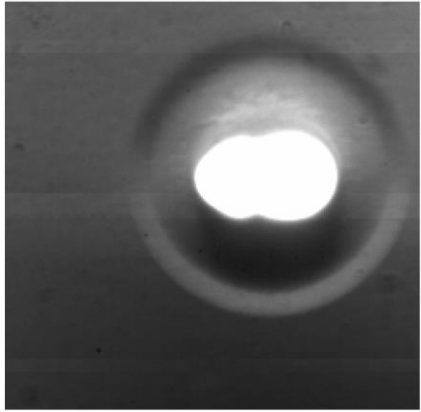
$$\lambda = 0.9439 + 0.2458i, \text{ error} \leq 0.0765$$



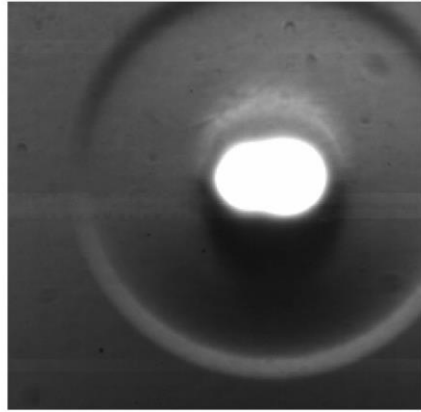
$$\lambda = 0.8948 + 0.1065i, \text{ error} \leq 0.1105$$



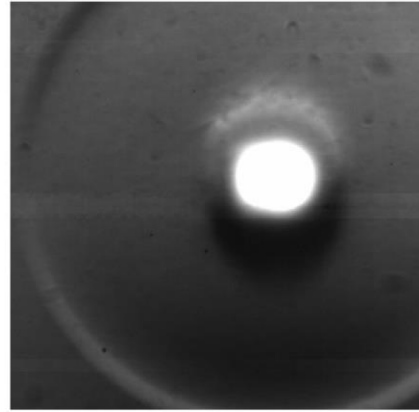
Example: Verified KMD and compression



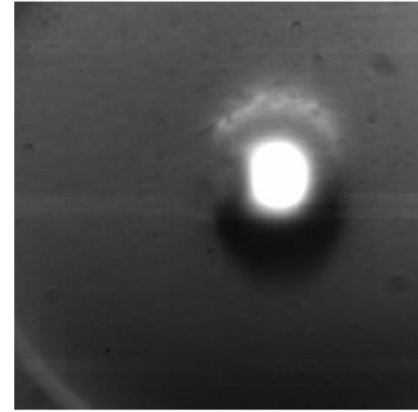
a) $t = 5 \mu\text{s}$



b) $t = 10 \mu\text{s}$



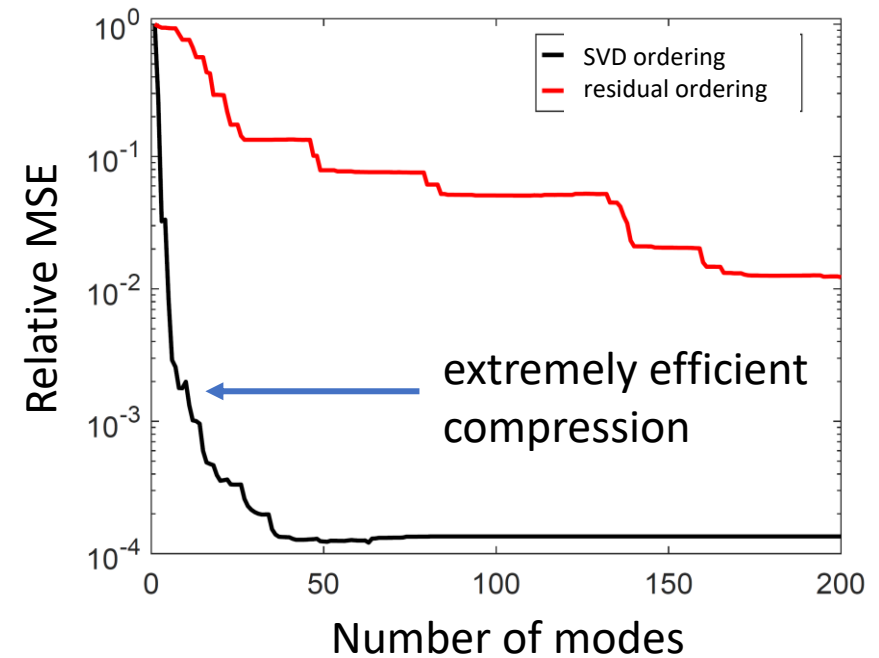
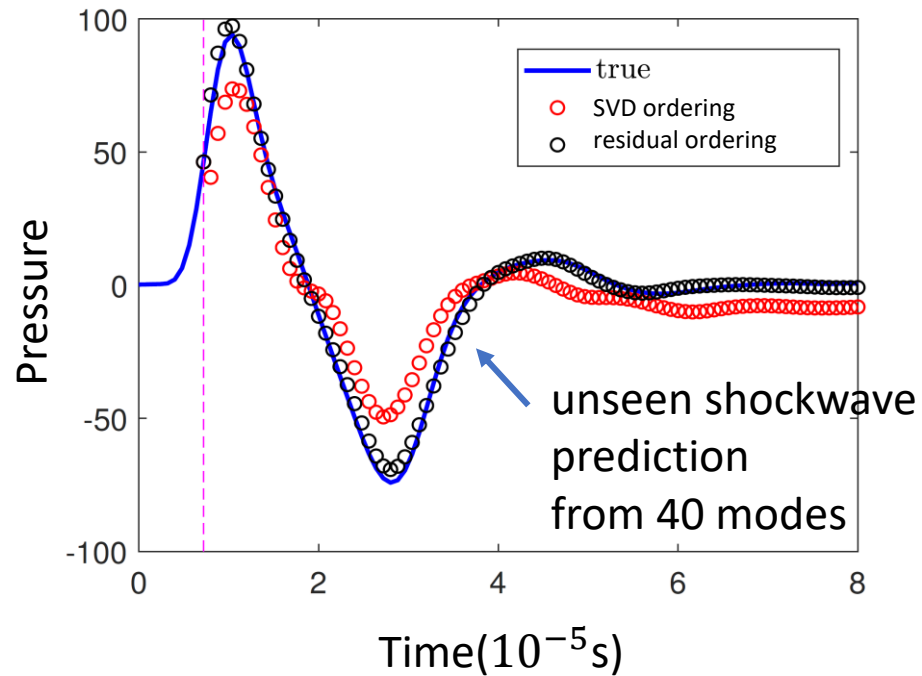
c) $t = 15 \mu\text{s}$



d) $t = 20 \mu\text{s}$



Matt Szóke's laser cannon!



Outline

- General systems:
 - Residual Dynamic Mode Decomposition.
- Measure-preserving systems:
 - **Measure-Preserving Extended Dynamic Mode Decomposition.**
 - Rigged Dynamic Mode Decomposition
- The **Solvability Complexity Index** – *classification* of problems and *optimality* of algorithms.



**HOT OFF
THE
PRESS**

Measure-preserving systems

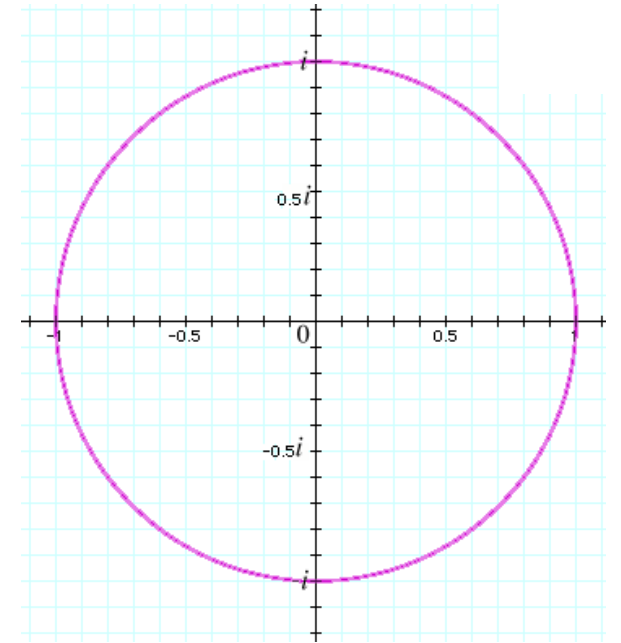
$$[\mathcal{K}g](x) = g(F(x)), \quad g \in L^2(\Omega, \omega)$$

F preserves $\omega \iff \|\mathcal{K}g\| = \|g\|$ (isometry)

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

$$\implies \text{Sp}(\mathcal{K}) \subseteq \{z: |z| \leq 1\}$$

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



Problem: We want our discretization to respect this property!



Structure-preserving DMD methods

- Enforce DMD matrix to lie on a manifold.
- **NB:** This is much easier for DMD which uses a linear choice of basis functions (which acts in state-space) than EDMD (which acts in coefficient space).
- We need something different....

royalsocietypublishing.org/journal/rspa

PROCEEDINGS A

royalsocietypublishing.org/journal/rspa

Research  

Cite this article: Baddoo PJ, Herrmann B, McKeon BJ, Nathan Kutz J, Brunton SL. 2023 Physics-informed dynamic mode decomposition. *Proc. R. Soc. A* **479**: 20220576. <https://doi.org/10.1098/rspa.2022.0576>

Received: 1 September 2022
Accepted: 23 January 2023


Subject Areas:
applied mathematics, computational mathematics, fluid mechanics

Keywords:
machine learning, dynamic mode decomposition, data-driven dynamical systems

Physics-informed dynamic mode decomposition

Peter J. Baddoo¹, Benjamin Herrmann²,
Beverley J. McKeon³, J. Nathan Kutz⁴ and
Steven L. Brunton⁵

¹Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
²Department of Mechanical Engineering, University of Chile, Beauchef 851, Santiago, Chile
³Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, CA 91125, USA
⁴Department of Applied Mathematics, and ⁵Department of Mechanical Engineering, University of Washington, Seattle, WA 98195, USA

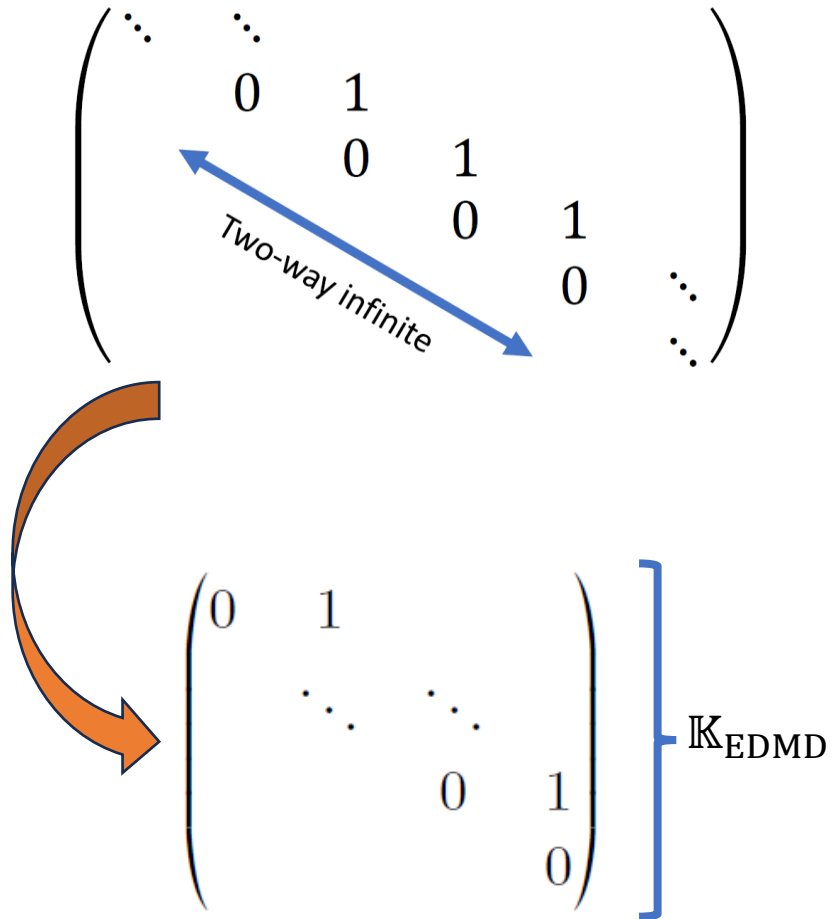
 PJB, 0000-0002-8671-6952; BJM, 0000-0003-4220-1583; JNK, 0000-0002-6004-2275; SLB, 0000-0002-6565-5118

In this work, we demonstrate how physical principles—such as symmetries, invariances and conservation laws—can be integrated into the *dynamic mode decomposition* (DMD). DMD is a widely used data analysis technique that extracts low-rank modal structures and dynamics from high-dimensional

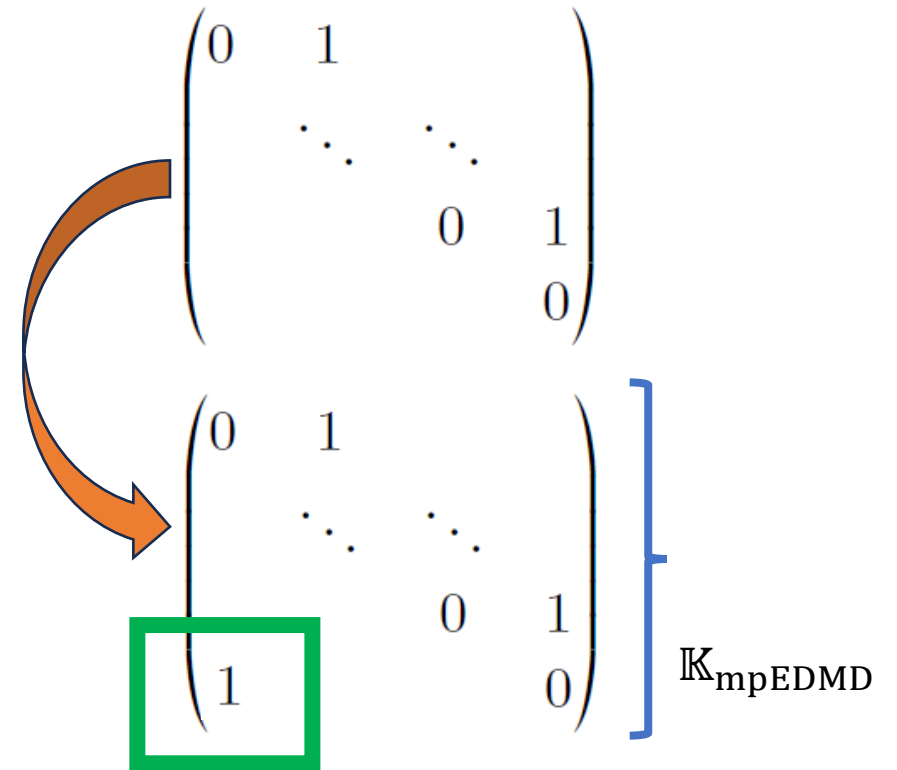
royalsocietypublishing.org/ on 21 May 2024

Back to the shift!

EDMD diverges:



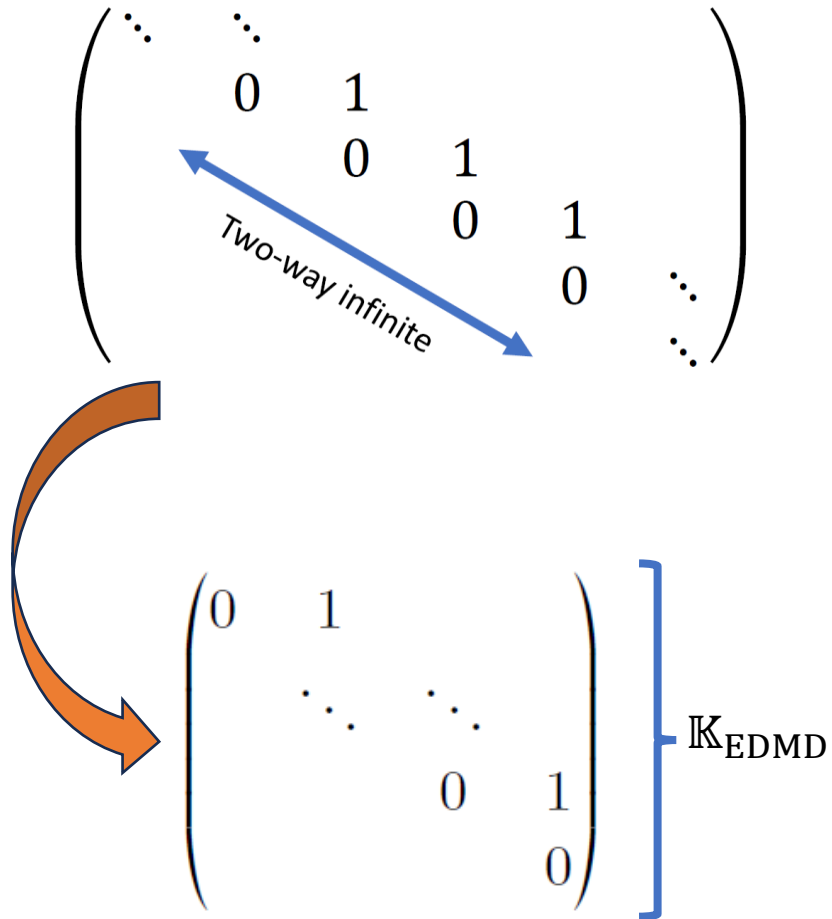
mpEDMD converges:



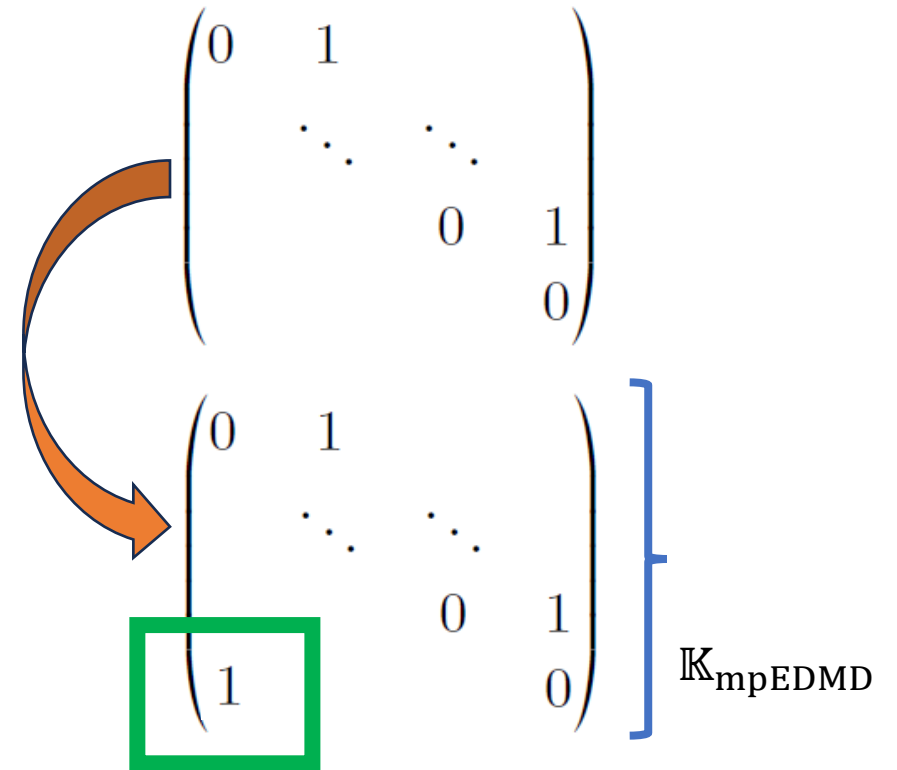
- C., "The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems," **SINUM**, 2023.
- Code: <https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition>

Back to the shift!

EDMD diverges:



mpEDMD converges:



Let's make this into a general method...

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

Back to EDMD!

$$\Psi(x) = [\psi_1(x) \ \dots \ \psi_N(x)], \quad g = \sum_{j=1}^N \mathbf{g}_j \psi_j = \Psi \mathbf{g} \in \text{span} \{\psi_1, \dots, \psi_N\}$$

$$\min_{\mathbb{K} \in \mathbb{C}^{N \times N}} \left\{ \int_{\Omega} \max_{\|\mathbf{g}\|_2=1} |\Psi(x) \mathbb{K} \mathbf{g} - [\mathcal{K}g](x)|^2 d\omega(x) = \int_{\Omega} \|\Psi(x) \mathbb{K} - \Psi(F(x))\|_2^2 d\omega(x) \right\}$$

quadrature

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

$$\min_{\mathbb{K} \in \mathbb{C}^{N \times N}} \sum_{m=1}^M w_m \|\Psi(x^{(m)}) \mathbb{K} - \Psi(y^{(m)})\|_2^2$$

Least-squares problem

A simple alteration

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

A simple alteration

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

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

A simple alteration

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

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

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

A simple alteration

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

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

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

quadrature

**Orthogonal
Procrustes problem**

$$\min_{\substack{\mathbb{K} \in \mathbb{C}^{N \times N} \\ G = \mathbb{K}^* G \mathbb{K}}} \sum_{m=1}^M w_m \|\Psi(x^{(m)}) \mathbb{K} G^{-1/2} - \Psi(y^{(m)}) G^{-1/2}\|_2^2$$

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 $\mathbf{W} = \text{diag}(w_1, \dots, w_M)$.
- 2: Compute an economy QR decomposition $\mathbf{W}^{1/2} \Psi_X = \mathbf{Q} \mathbf{R}$, 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 Λ .

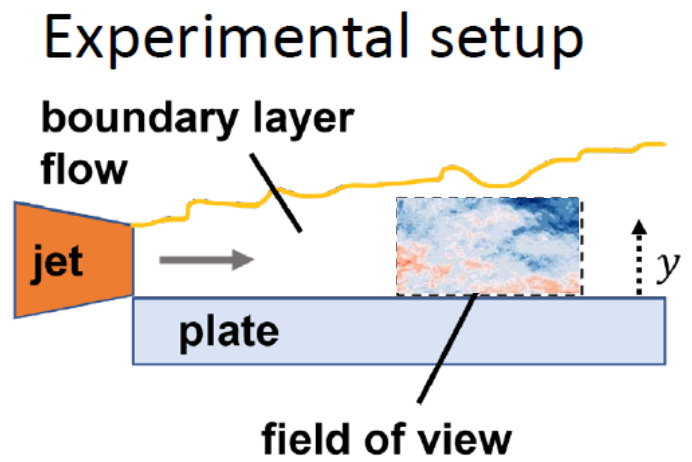
$V_N = \text{span} \{\psi_1, \dots, \psi_N\}$
 $\mathcal{P}_{V_N}: L^2(\Omega, \omega) \rightarrow V_N$
 orthogonal projection

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

Convergence: spectral measures (see later), Koopman mode decomposition,...

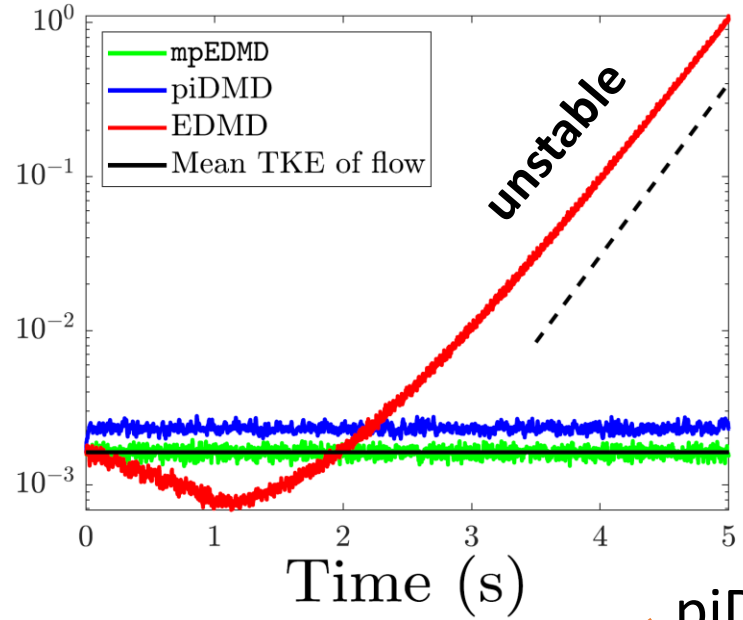
- C., "The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems," **SINUM**, 2023.
- Code: <https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition>

Turbulence (real data)

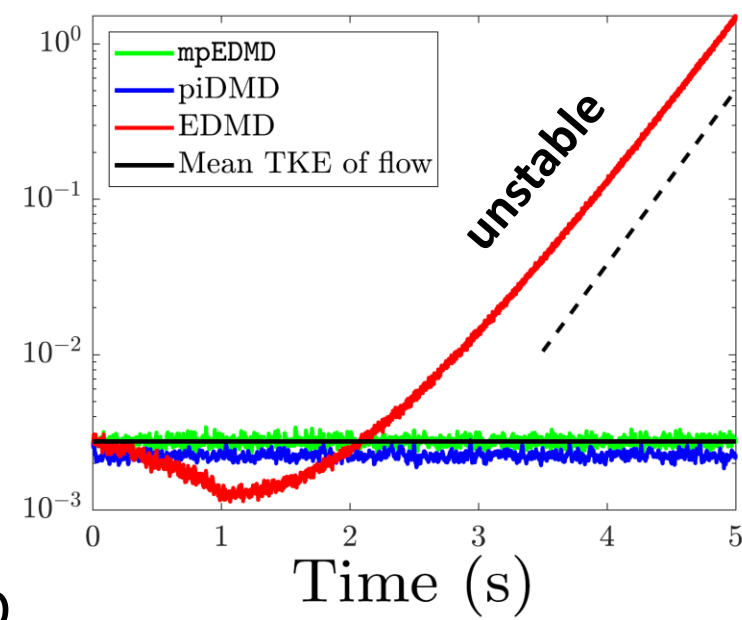


- Reynolds number $\approx 6.4 \times 10^4$
 - Ambient dimension (d) $\approx 100,000$ (velocity at measurement points)
- *PIV data provided by Máté Szőke (Virginia Tech)

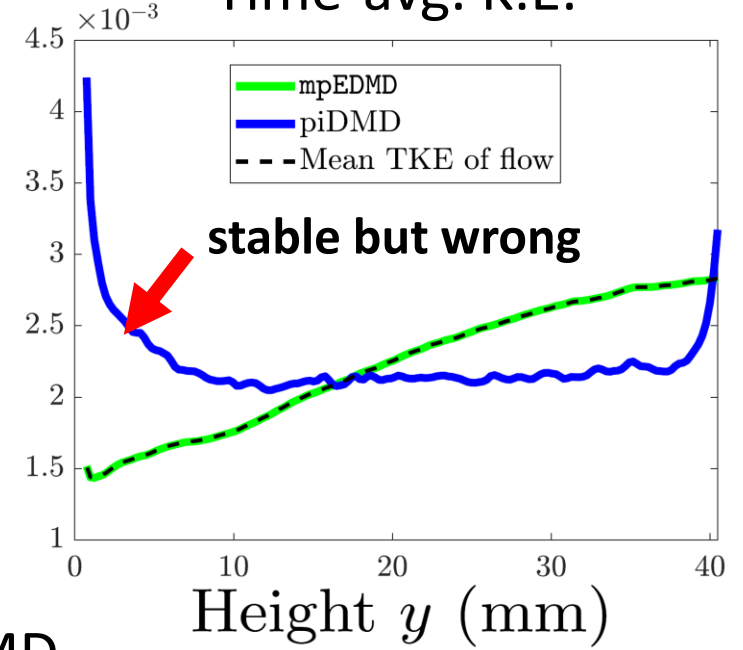
Turbulent K.E. $y=5\text{mm}$



Turbulent K.E. $y=35\text{mm}$



Time-avg. K.E.



piDMD

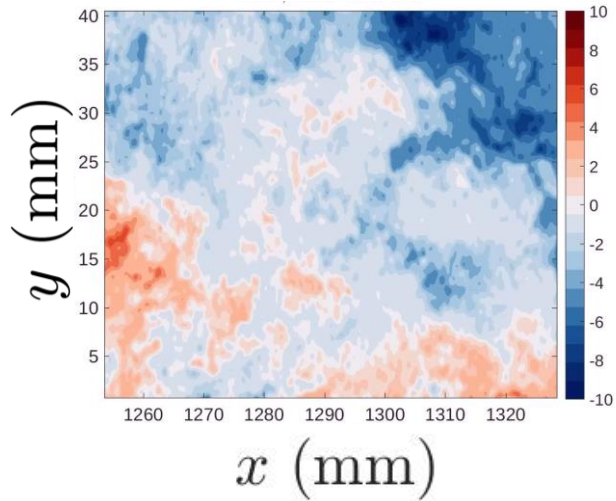
EDMD

- 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.

Turbulence statistics

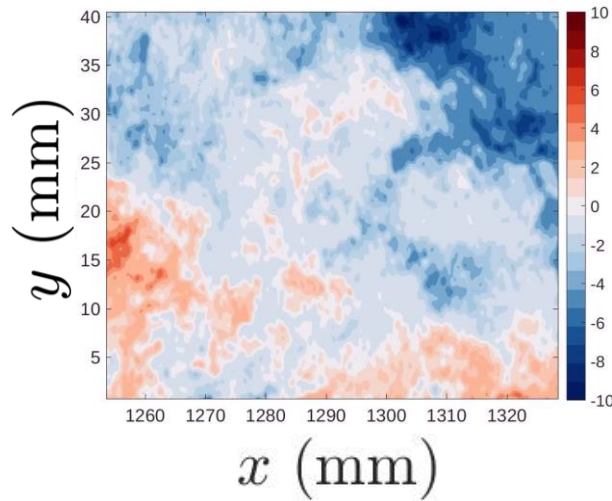
Flow

time=0.001000



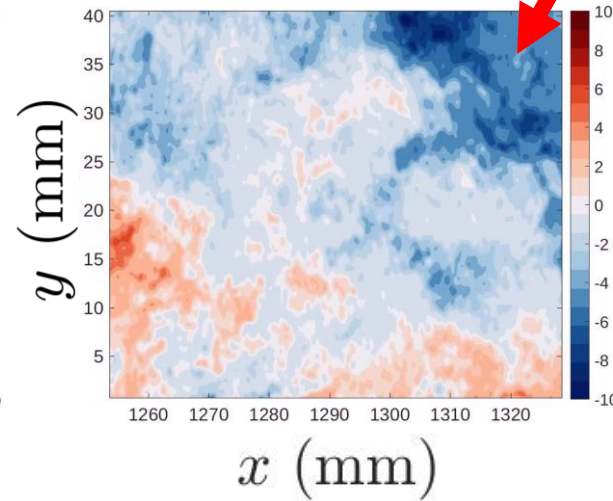
mpEDMD

time=0.001000



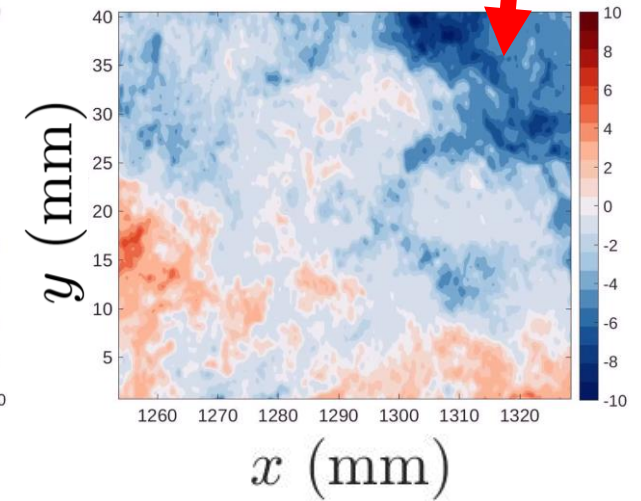
piDMD

time=0.001000



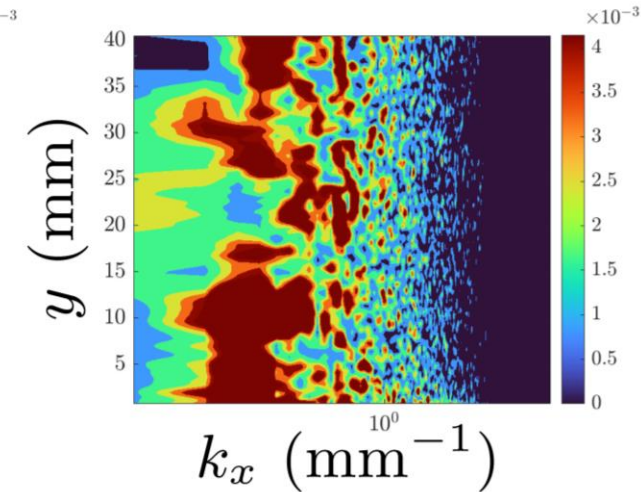
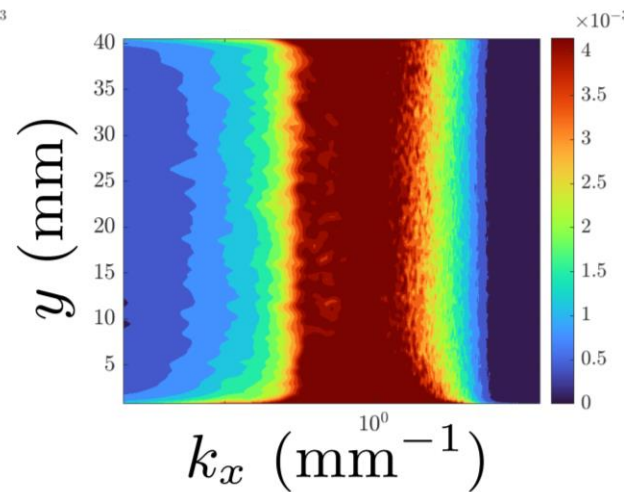
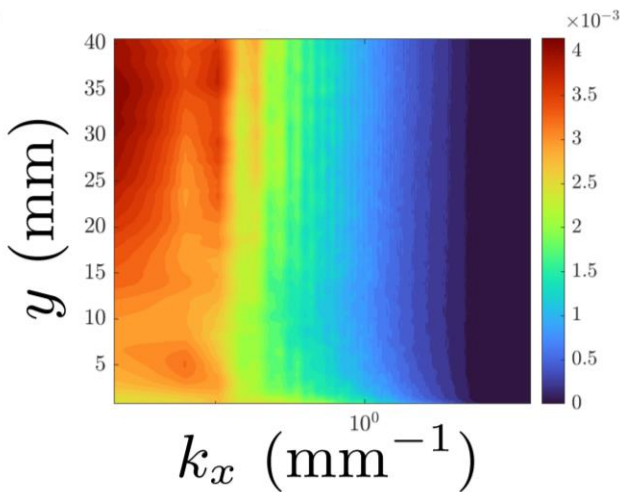
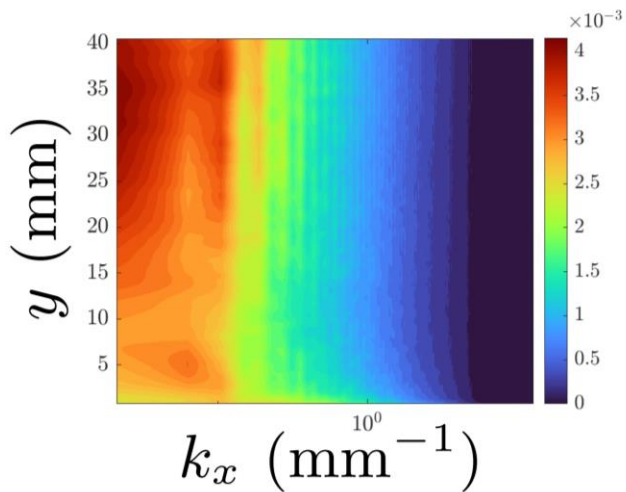
EDMD

time=0.001000



stable but
wrong

unstable



Outline

- General systems:
 - Residual Dynamic Mode Decomposition.
- Measure-preserving systems:
 - Measure-Preserving Extended Dynamic Mode Decomposition.
 - **Rigged Dynamic Mode Decomposition.**
- The **Solvability Complexity Index** – *classification* of problems and *optimality* of algorithms.

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



Back to the shift!

“Solve” $(U - zI)u_z = 0$

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

$$U = \begin{pmatrix} \ddots & & & & & & \\ & \ddots & & & & & \\ & & 0 & 1 & & & \\ & & & 0 & 1 & & \\ & & & & 0 & 1 & \\ & & & & & 0 & 1 & \ddots \\ & & & & & & & 0 & \ddots \\ & & & & & & & & & \ddots \end{pmatrix}$$

$e_j \rightarrow e_{j-1}$

Two-way infinite

Back to the shift!

“Solve” $(U - zI)u_z = 0$

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

Doesn't live in $\ell^2(\mathbb{Z})!!!$

$$U = \begin{pmatrix} \ddots & \ddots & & & & & \\ & 0 & 1 & & & & \\ & & 0 & 1 & & & \\ & & & 0 & 1 & & \\ & & & & 0 & 1 & \\ & & & & & 0 & \ddots \\ & & & & & & \ddots \end{pmatrix}$$

$e_j \rightarrow e_{j-1}$

Two-way infinite

Back to the shift!

“Solve” $(U - zI)u_z = 0$

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

Doesn't live in $\ell^2(\mathbb{Z})!!!$

Let $|z| = 1$, $\phi = \sum_{j=-\infty}^{\infty} \phi_j e_j$ where ϕ_j decay faster than any inverse polynomial.

Test functions

$$U = \begin{pmatrix} \ddots & \ddots & & & & & \\ & 0 & 1 & & & & \\ & & 0 & 1 & & & \\ & & & 0 & 1 & & \\ & & & & 0 & 1 & \\ & & & & & 0 & \ddots \\ & & & & & & \ddots \end{pmatrix}$$

$e_j \rightarrow e_{j-1}$

Two-way infinite

Back to the shift!

“Solve” $(U - zI)u_z = 0$

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

Doesn't live in $\ell^2(\mathbb{Z})$!!!

Let $|z| = 1$, $\phi = \sum_{j=-\infty}^{\infty} \phi_j e_j$ where ϕ_j decay faster than any inverse polynomial.

$$U = \begin{pmatrix} \ddots & \ddots & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & 0 & 1 & \\ & & & & 0 & \ddots \\ & & & & & \ddots \end{pmatrix}$$

$e_j \rightarrow e_{j-1}$

Two-way infinite

Test functions

$$\langle u_z, \phi \rangle = \sum_{j=-\infty}^{\infty} z^j \overline{\phi_j}, \quad \langle Uu_z, \phi \rangle = \langle u_z, U^* \phi \rangle = \sum_{j=-\infty}^{\infty} z^j \overline{\phi_{j-1}} = z \langle u_z, \phi \rangle$$

Back to the shift!

“Solve” $(U - zI)u_z = 0$

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

Doesn't live in $\ell^2(\mathbb{Z})!!!$

Let $|z| = 1$, $\phi = \sum_{j=-\infty}^{\infty} \phi_j e_j$ where ϕ_j decay faster than any inverse polynomial.

$$U = \begin{pmatrix} \ddots & & & & & & \\ & \ddots & & & & & \\ & & 0 & 1 & & & \\ & & & 0 & 1 & & \\ & & & & 0 & 1 & \\ & & & & & 0 & 1 \\ & & & & & & \ddots \\ & & & & & & & \ddots \end{pmatrix}$$

$e_j \rightarrow e_{j-1}$

Two-way infinite

Test functions

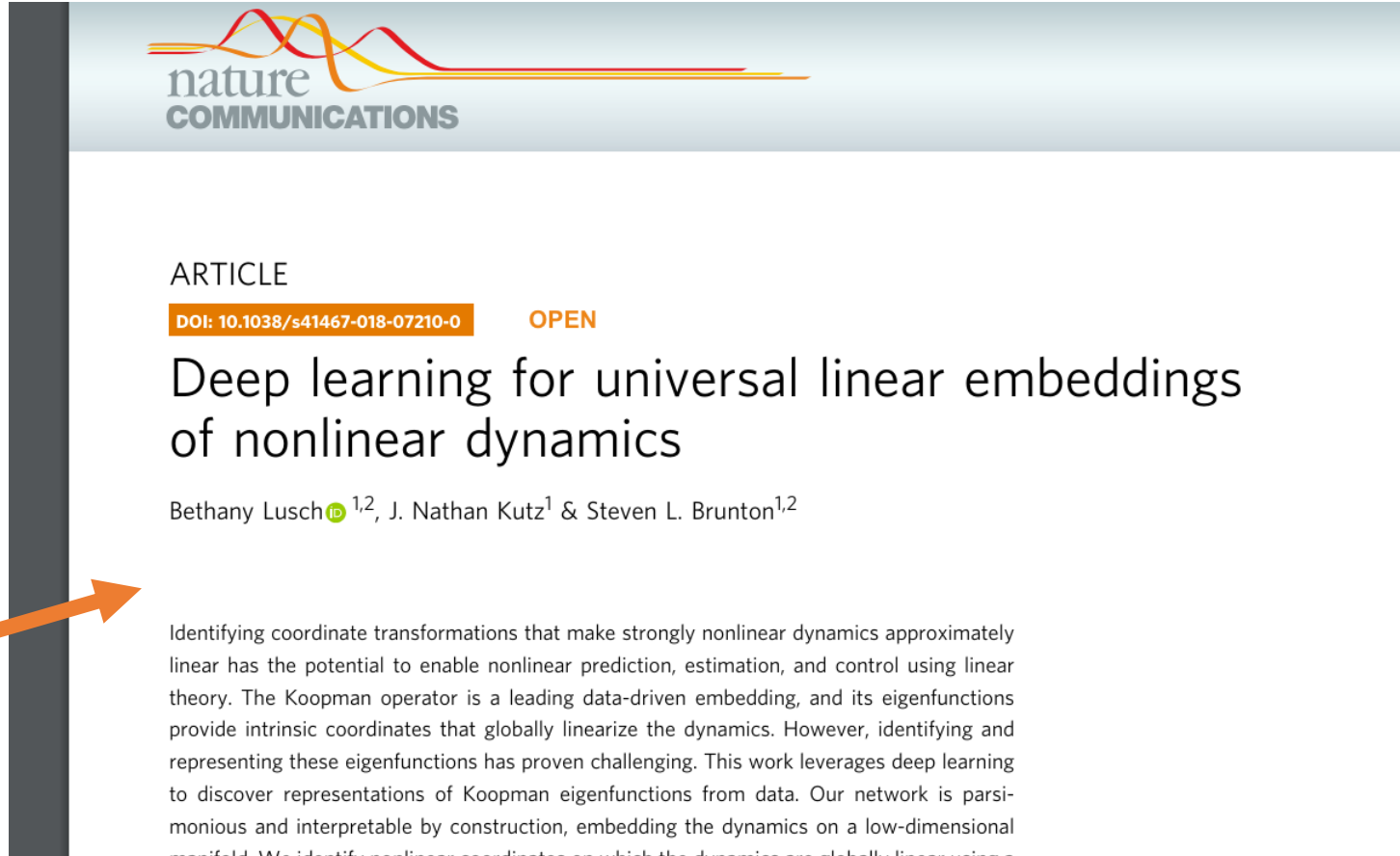
$$\langle u_z, \phi \rangle = \sum_{j=-\infty}^{\infty} z^j \overline{\phi_j}, \quad \langle Uu_z, \phi \rangle = \langle u_z, U^* \phi \rangle = \sum_{j=-\infty}^{\infty} z^j \overline{\phi_{j-1}} = z \langle u_z, \phi \rangle$$

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

Another example: Nonlinear pendulum

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

**Considered a challenge in
Koopman theory!**



nature
COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-018-07210-0 OPEN

Deep learning for universal linear embeddings of nonlinear dynamics

Bethany Lusch^{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 nonlinear coordinates on which the dynamics are globally linear using a

Explicit diagonalization using Radon transform!

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

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

Explicit diagonalization using Radon transform!

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

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

- g in Schwartz space,

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

Explicit diagonalization using Radon transform!

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

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

- g in Schwartz space,

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

$$\hat{g}_{\mathbf{k}}(\mathbf{I}) = \sum_{j=1}^{\infty} \sum_{m=-\infty}^{\infty} \int_{[-\pi, \pi]_{\text{per}}} \left\langle g_{\theta}^{(\mathbf{k}, m, j)*} \mid g \right\rangle g_{\theta}^{(\mathbf{k}, m, j)} d\theta$$

$$g_{\theta}^{(\mathbf{k}, m, j)} = \frac{1}{(2\pi)^n} \delta(\theta + 2\pi m - \Delta t \mathbf{k} \cdot \mathbf{I}) \psi_j^{(\mathbf{k})} e^{i\mathbf{k} \cdot \boldsymbol{\theta}}$$

Generalised eigenfunctions

Explicit diagonalization using Radon transform!

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

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

- g in Schwartz space,

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

$$\hat{g}_{\mathbf{k}}(\mathbf{I}) = \sum_{j=1}^{\infty} \sum_{m=-\infty}^{\infty} \int_{[-\pi, \pi]_{\text{per}}} \left\langle g_{\theta}^{(\mathbf{k}, m, j)*} \mid g \right\rangle g_{\theta}^{(\mathbf{k}, m, j)} d\theta$$

$$g_{\theta}^{(\mathbf{k}, m, j)} = \frac{1}{(2\pi)^n} \underbrace{\delta(\theta + 2\pi m - \Delta t \mathbf{k} \cdot \mathbf{I})}_{\text{Supported on hyperplane}} \underbrace{\psi_j^{(k)} e^{i\mathbf{k} \cdot \boldsymbol{\theta}}}_{\text{Orthonormal basis of hyperplane}}$$

Plane wave

Generalised eigenfunctions

Supported on
hyperplane

Orthonormal basis of
hyperplane

Gelfand's theorem \rightarrow diagonalisation

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

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

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

$$g = \int_{[-\pi, \pi]_{\text{per}}} \underbrace{\langle g_\theta^* | g \rangle}_{\text{Koopman modes}} g_\theta dv(\theta), \quad \mathcal{K}g = \int_{[-\pi, \pi]_{\text{per}}} e^{i\theta} \langle g_\theta^* | g \rangle g_\theta dv(\theta)$$

$g \in S \subset L^2(\Omega, \omega)$

generalized eigenfunctions
distributions $\in S^*$

$e^{i\theta} = \lambda$

Koopman Mode Decomposition

Rigged DMD: Smoothing

Carathéodory function:

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

Rigged DMD: Smoothing

Carathéodory function:

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

Let $r = 1 + \varepsilon > 1$, $\theta_0 \in [-\pi, \pi]_{\text{per}}$,

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

Rigged DMD: Smoothing

Carathéodory function:

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

Let $r = 1 + \varepsilon > 1$, $\theta_0 \in [-\pi, \pi]_{\text{per}}$,

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

Rigged DMD: Smoothing

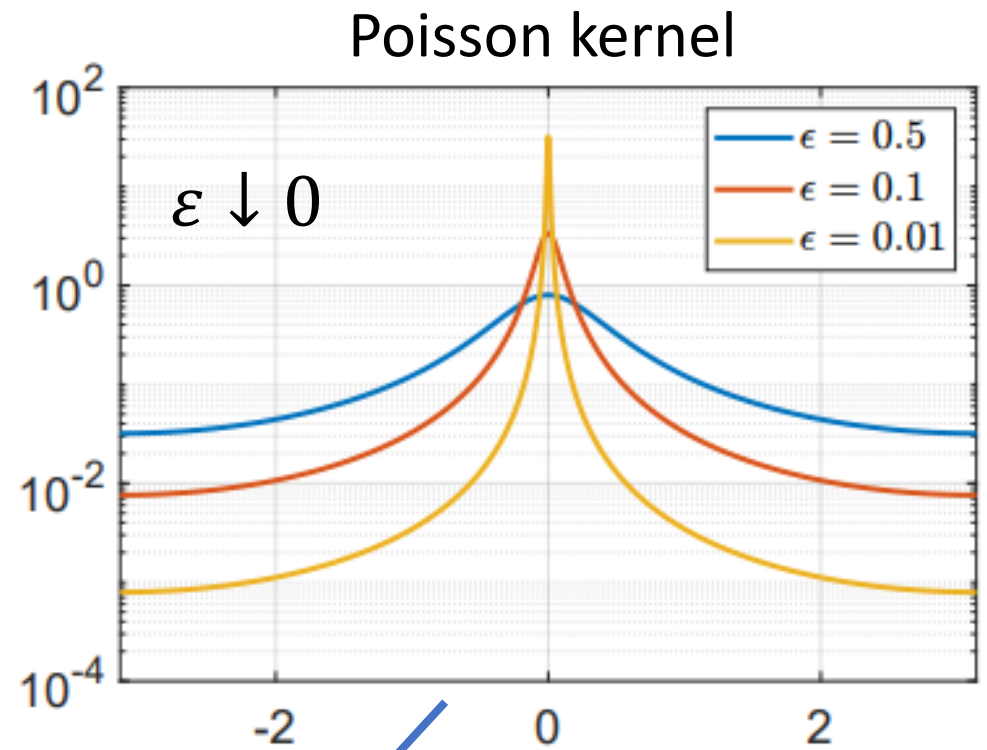
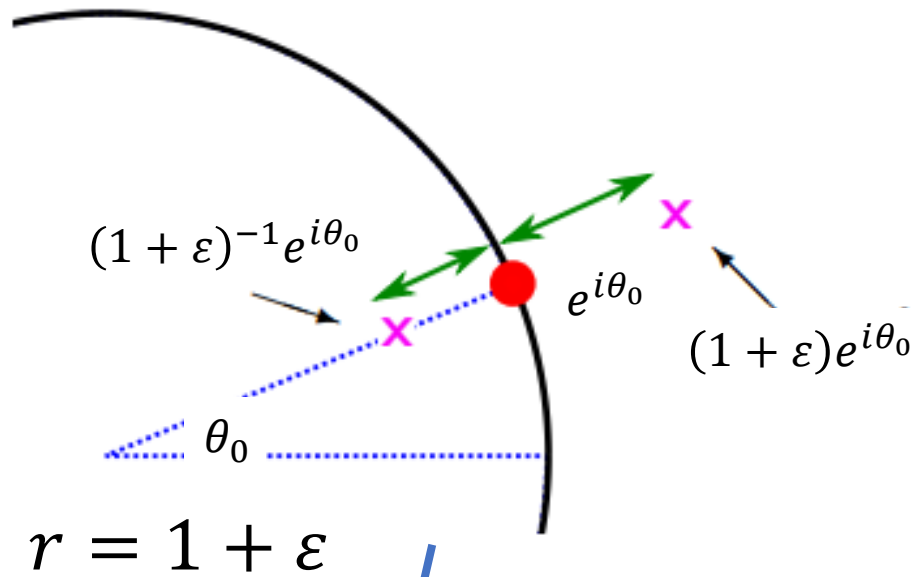
Carathéodory function:

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

Let $r = 1 + \varepsilon > 1$, $\theta_0 \in [-\pi, \pi]_{\text{per}}$,

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

Smoothed generalized eigenfunction



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

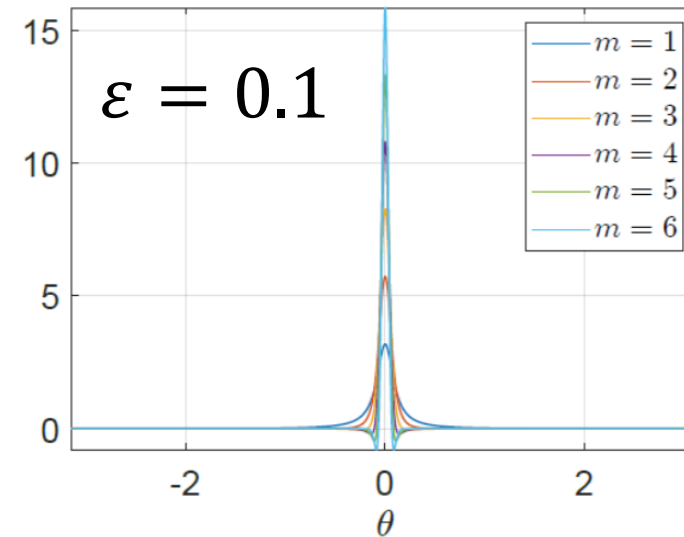
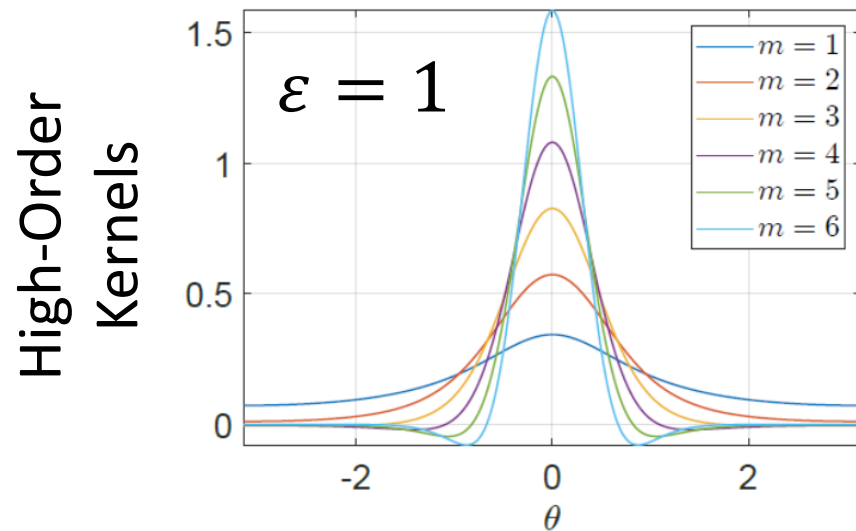
$$= \frac{1}{2\pi} \int_{[-\pi, \pi]_{\text{per}}} \underbrace{\frac{r^2 - 1}{1 + r^2 - 2r\cos(\theta_0 - \theta)}}_{\text{Poisson kernel}} \langle g_\theta^* | g \rangle g_\theta dv(\theta)$$

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 $F_g(z)$.

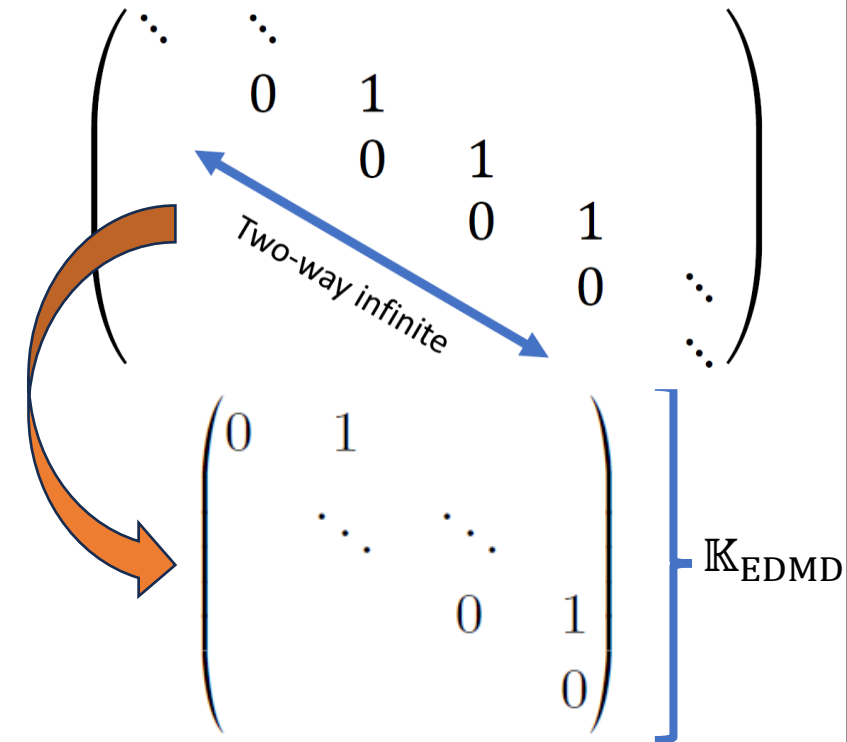
Smaller ε
requires
more data



- **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^p , weak,...
 - Forecasting (i.e., iterating Koopman mode decomposition), coherency etc.

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

EDMD diverges:



Acts on $\text{span}\{e_{-N}, \dots, e_N\}$

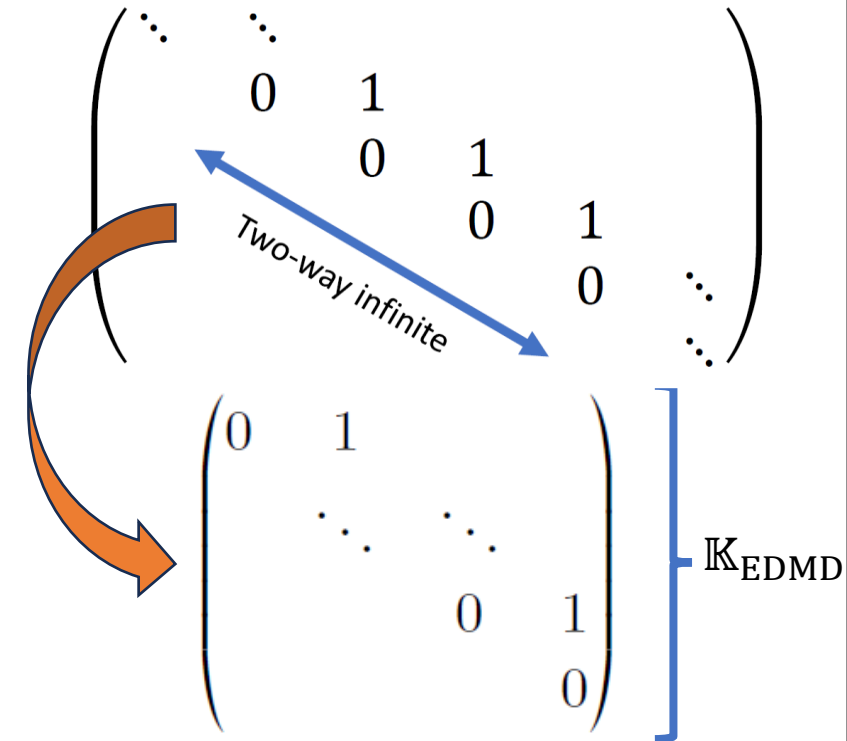
E.g., if $|z| < 1$,

$$(\mathbb{K}_{\text{EDMD}} - zI)^{-1}e_0 = \sum_{j=1}^N \frac{-1}{z^j} e_{-j}$$

Exponential
blowup
as $N \rightarrow \infty$.

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

EDMD diverges:



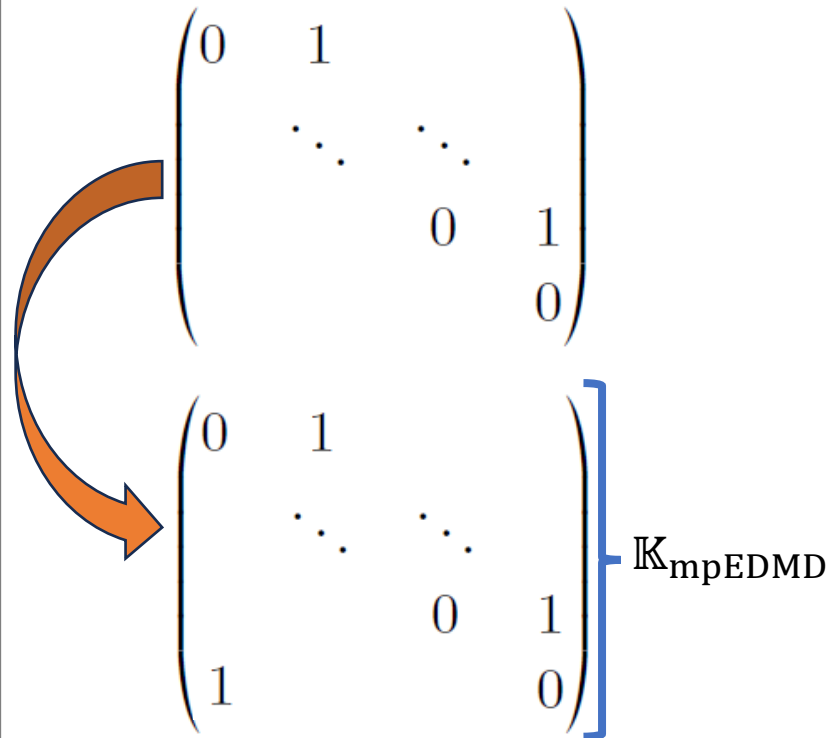
Acts on $\text{span}\{e_{-N}, \dots, e_N\}$

E.g., if $|z| < 1$,

$$(\mathbb{K}_{\text{EDMD}} - zI)^{-1}e_0 = \sum_{j=1}^N \frac{-1}{z^j} e_{-j}$$

Exponential
blowup
as $N \rightarrow \infty$.

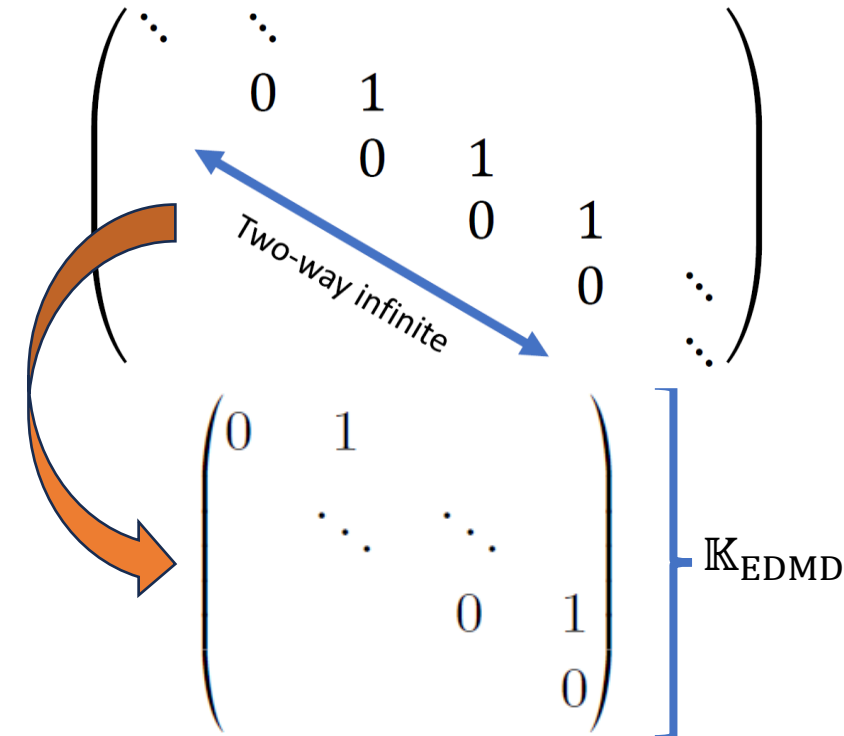
mpEDMD converges:



General method: unitary part of a
polar decomposition of EDMD!

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

EDMD diverges:



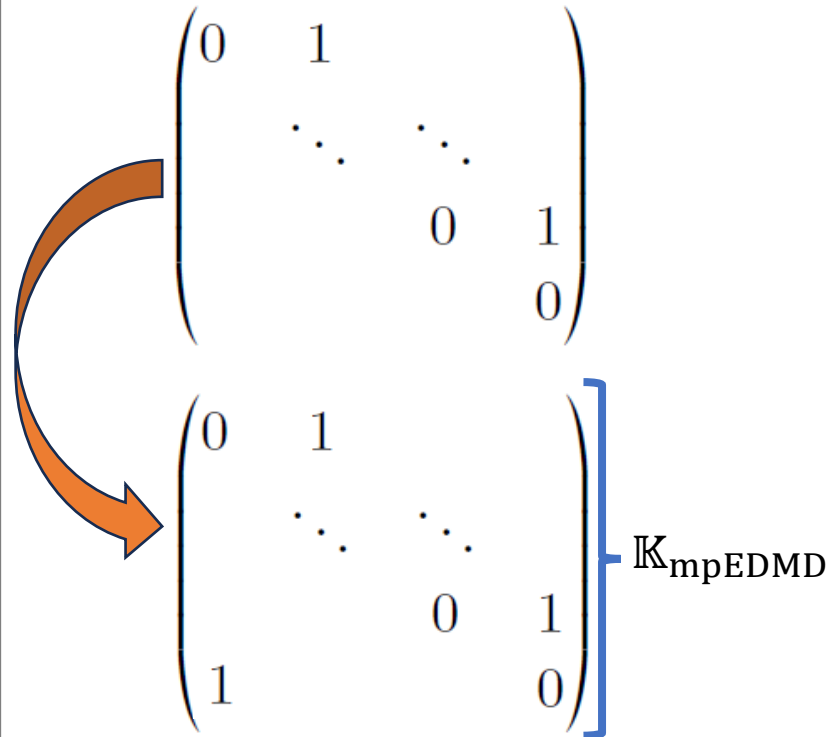
Acts on $\text{span}\{e_{-N}, \dots, e_N\}$

E.g., if $|z| < 1$,

$$(\mathbb{K}_{\text{EDMD}} - zI)^{-1}e_0 = \sum_{j=1}^N \frac{-1}{z^j} e_{-j}$$

Exponential
blowup
as $N \rightarrow \infty$.

mpEDMD converges:



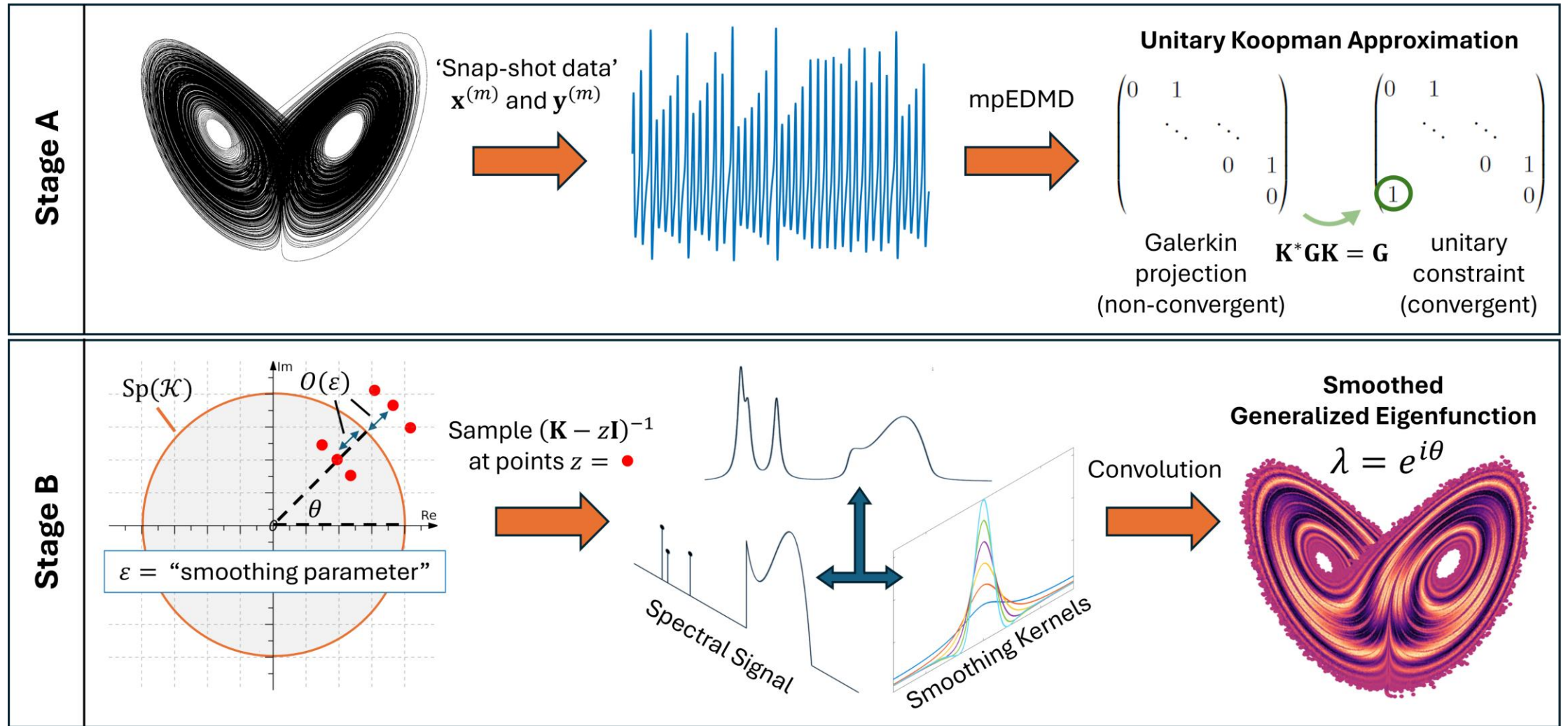
General method: unitary part of a
polar decomposition of EDMD!

Rigged DMD converges:

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



Rigged DMD

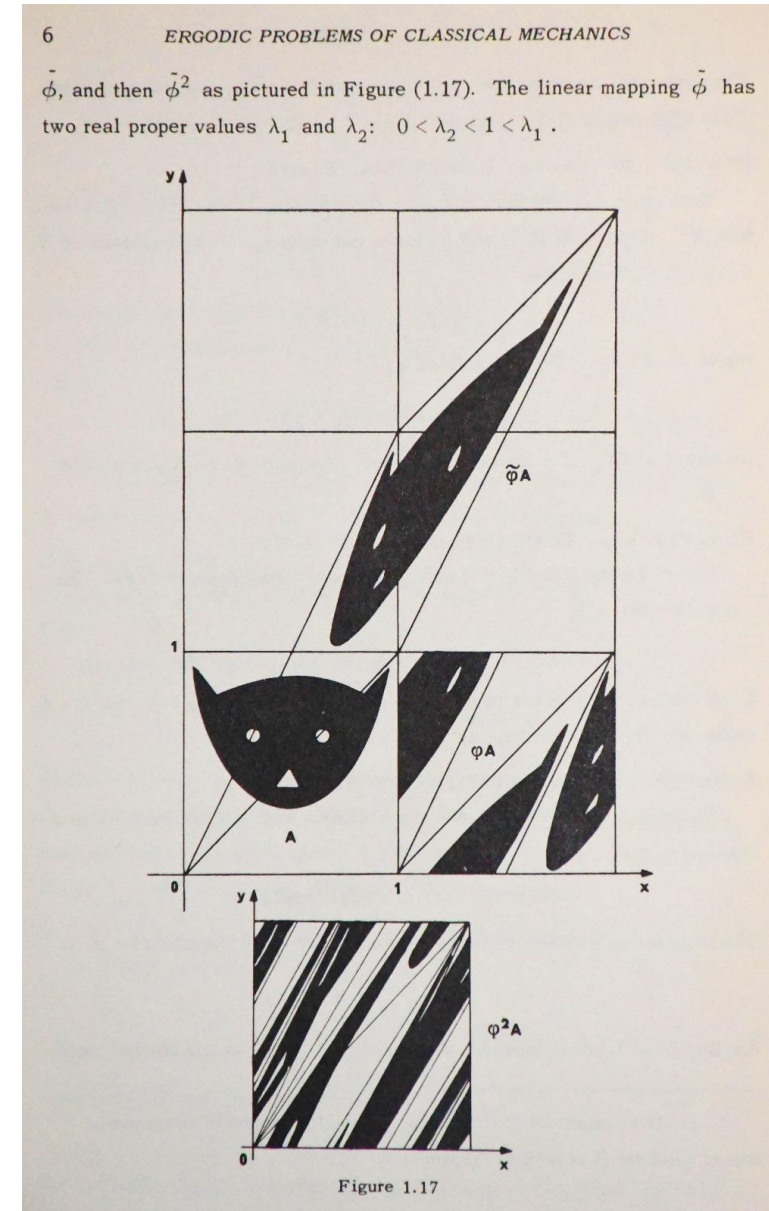


- C., Drysdale, Horning, "Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators", arxiv preprint.
- Code: <https://github.com/MColbrook/Rigged-Dynamic-Mode-Decomposition>

Example: Arnold's cat map

$$F(x, y) = (2x + y, x + y) \pmod{2\pi}$$

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



Arnold's "Ergodic Problems of Classical Mechanics"

Example: Arnold's cat map

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

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

Explicit formula: g_θ become more oscillatory as $\epsilon \downarrow 0$ (non-decaying Fourier series)

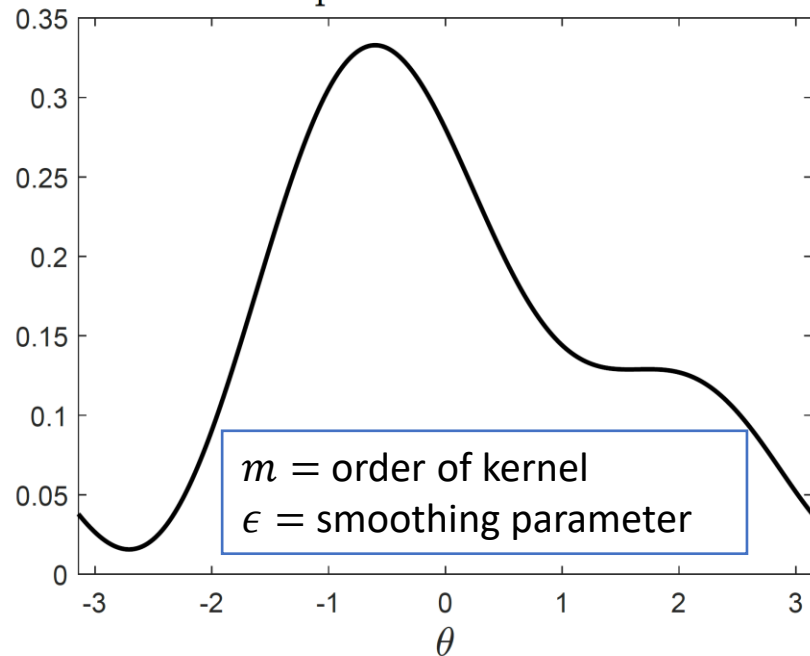
Experimental details

Length-one trajectories, $M = 50 \times 50, N = 500$

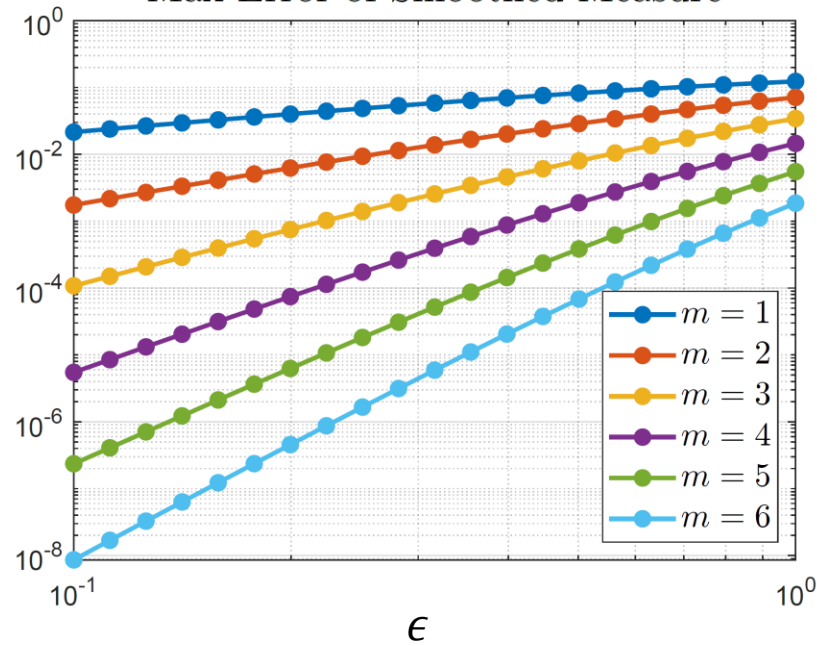
$$g(x, y) = \sin(x) + \frac{1}{2} \sin(2x + y) + \frac{i}{4} \sin(5x + 3y)$$

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

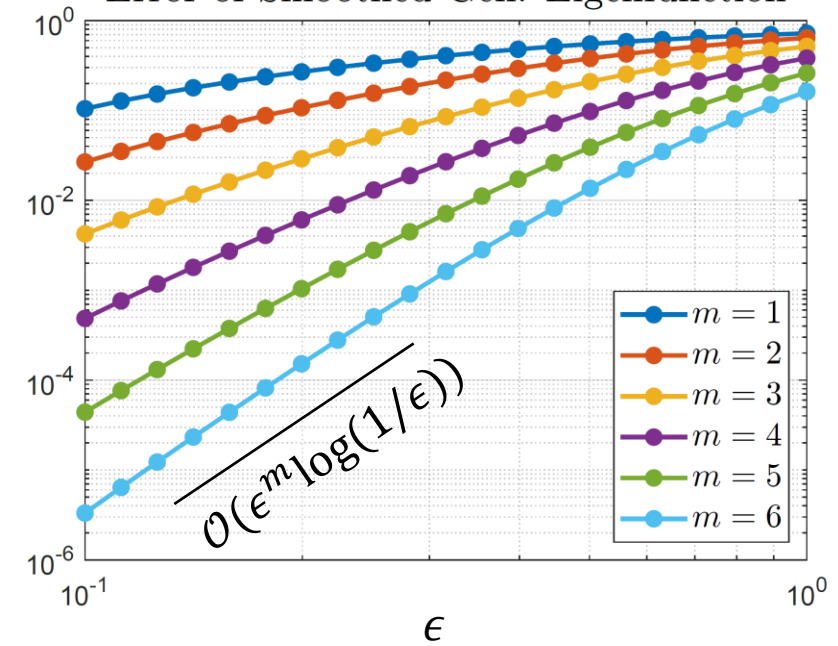
Spectral Measure



Max Error of Smoothed Measure



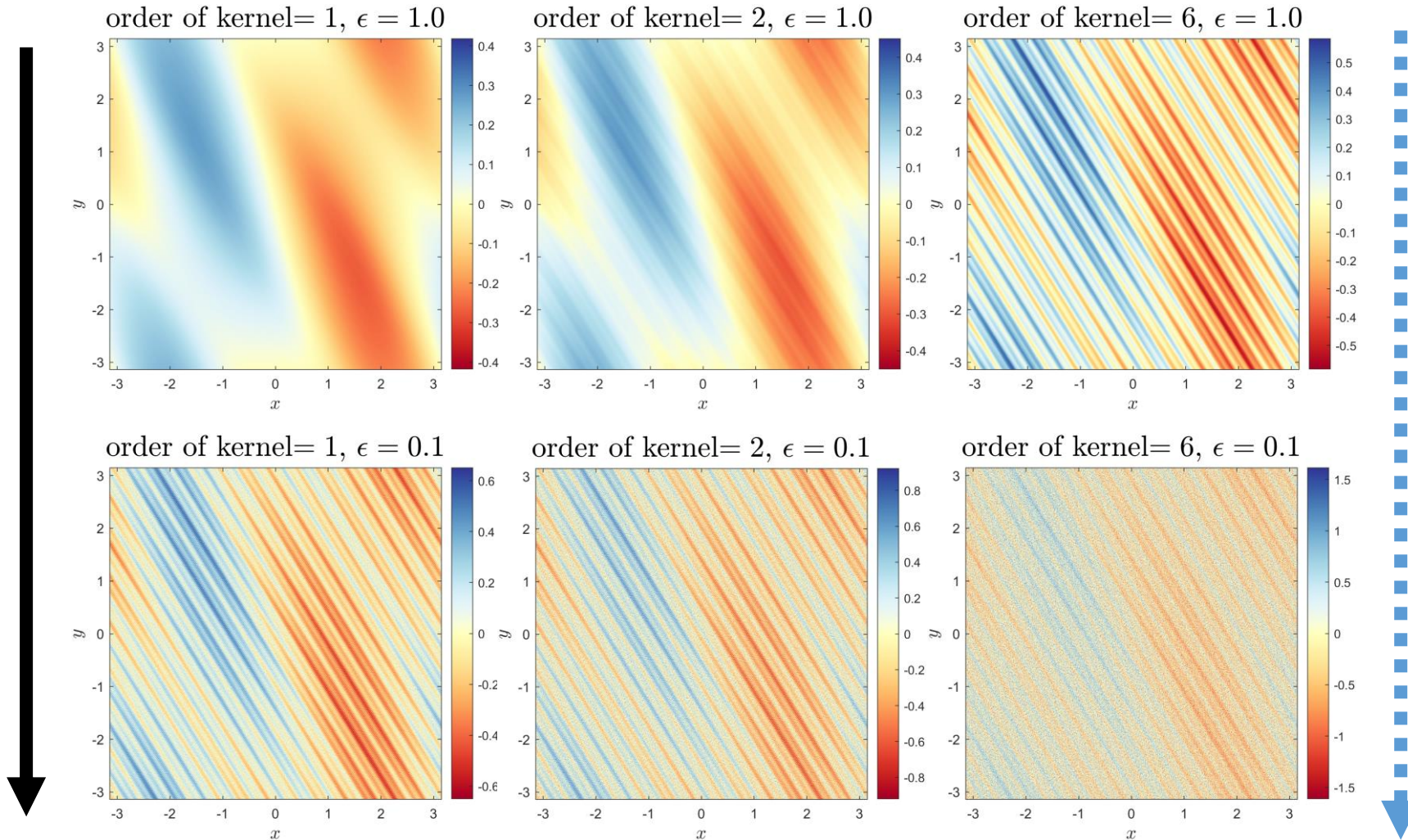
Error of Smoothed Gen. Eigenfunction



Higher kernel order (accuracy)



Higher resolution ($\epsilon \downarrow 0$)

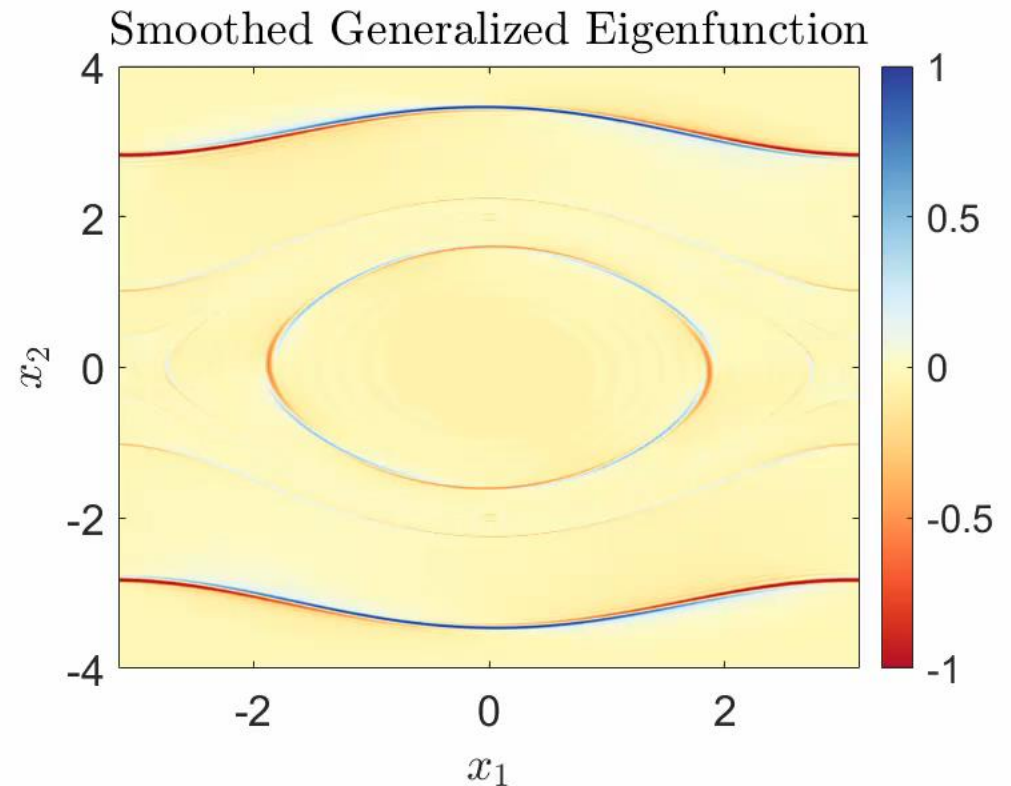
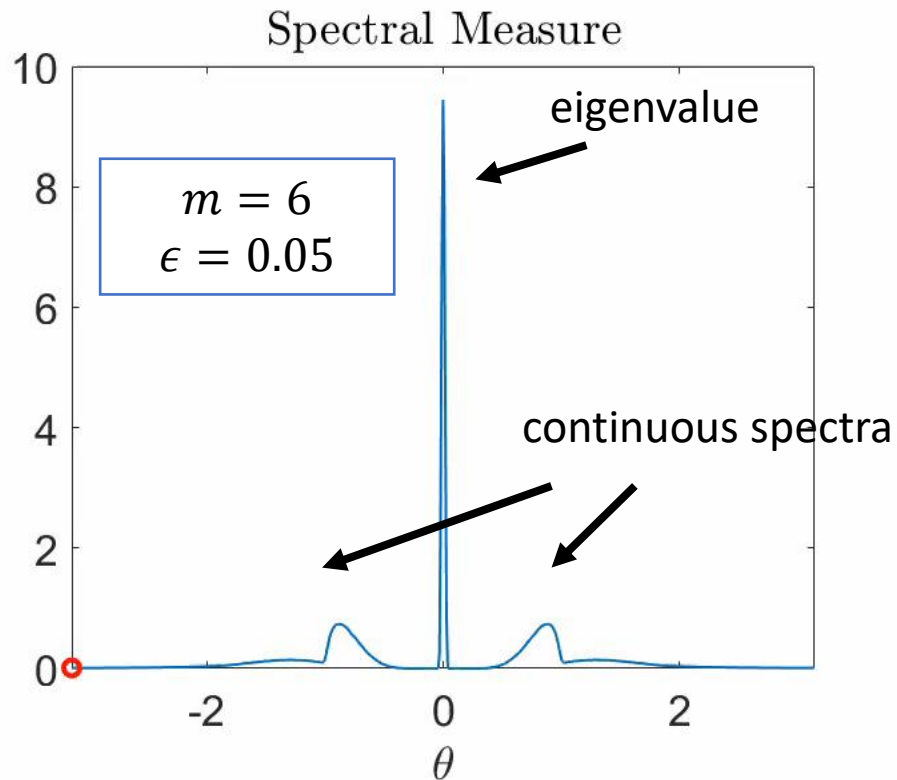


Example: Nonlinear pendulum

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: $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$

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

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



Interlude: Can we always find an \mathcal{S} ?

- 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:

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

- Generalises shift example but in coefficient space w.r.t. Krylov subspaces.

Interlude: Can we always find an \mathcal{S} ?

- 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:

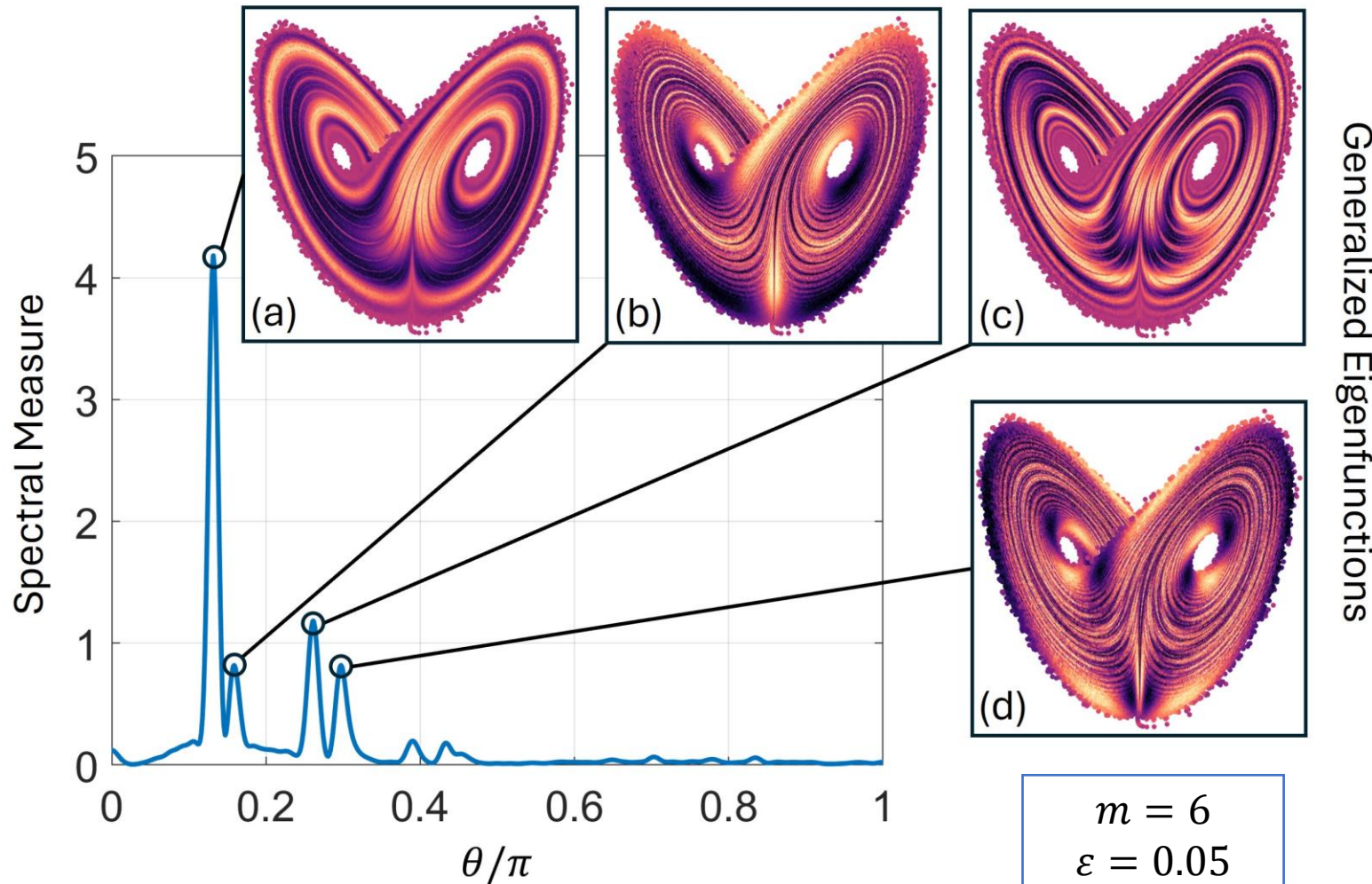
$$\{\text{Unions (different } g) \text{ of spaces } \text{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g, \dots\}\} \subset \mathcal{S}$$

- Generalises shift example but in coefficient space w.r.t. Krylov subspaces.

Let's do this for Lorenz...

Example: Lorenz system

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



Generalized Eigenfunctions

No formula for
generalized eigenfunctions!!

Experimental Details

Single trajectory (ergodic system)

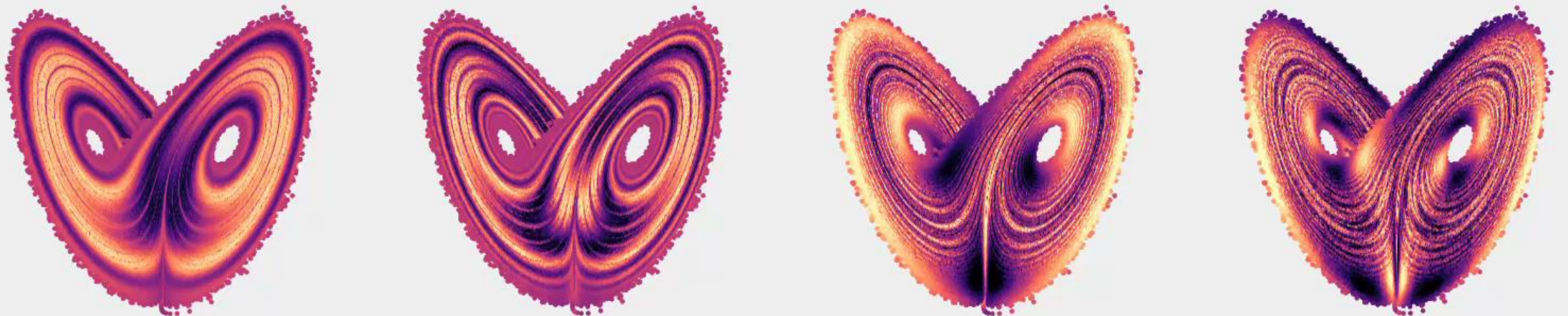
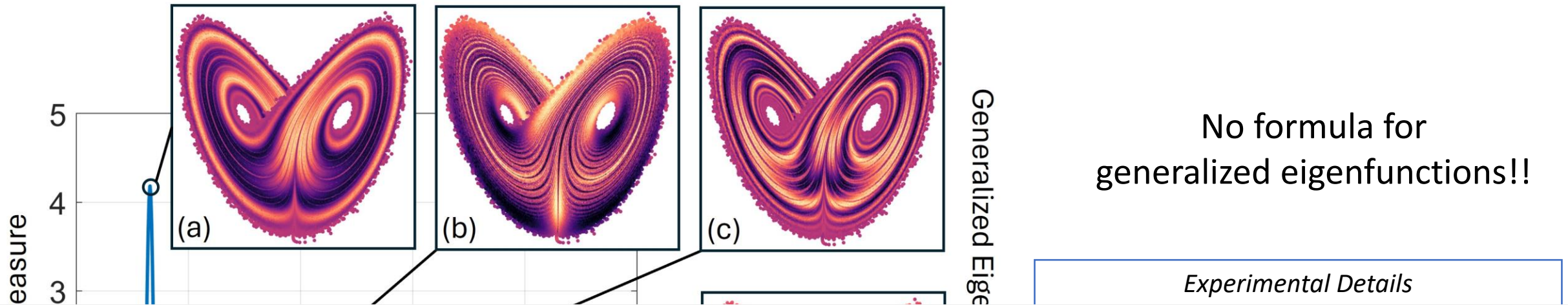
$$M = 10000, N = 1000$$

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

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

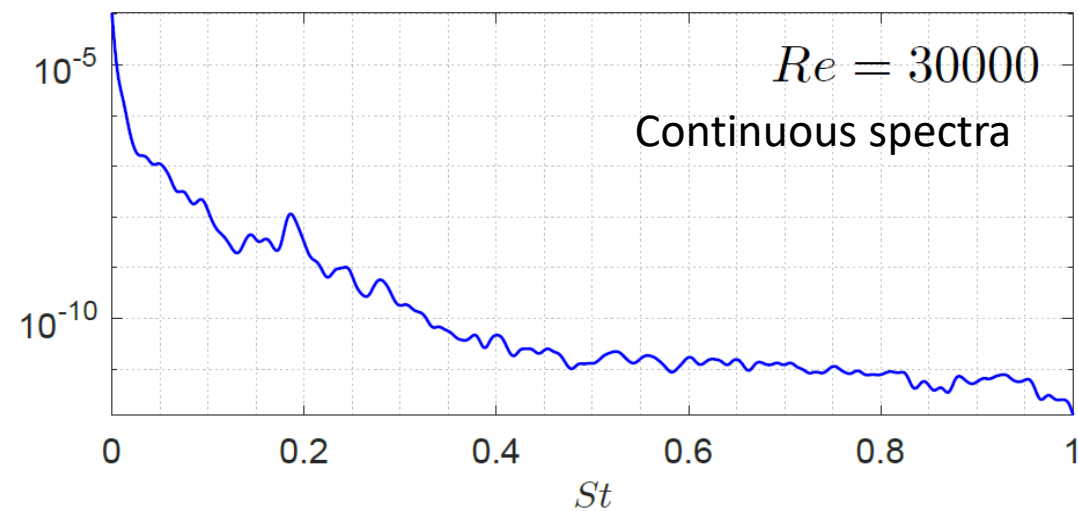
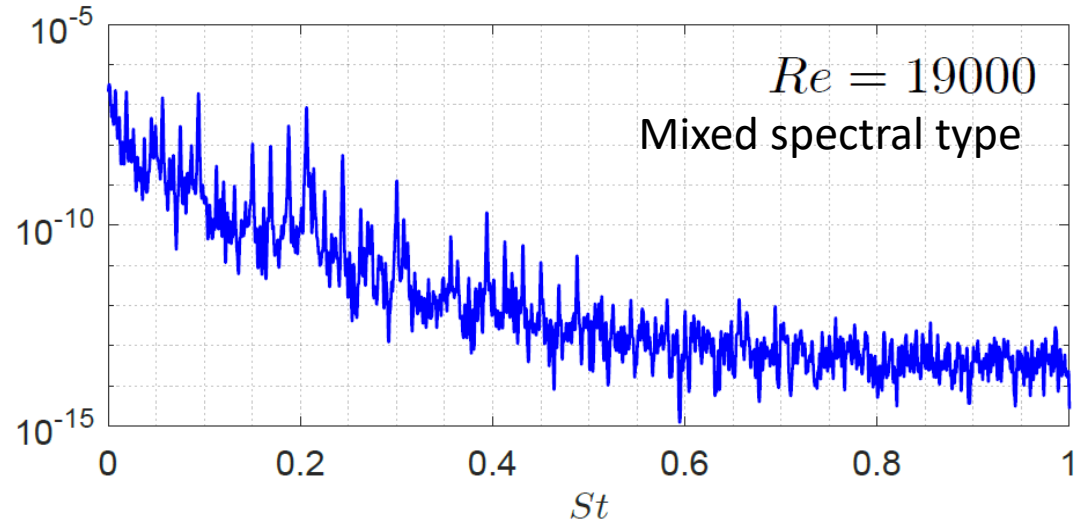
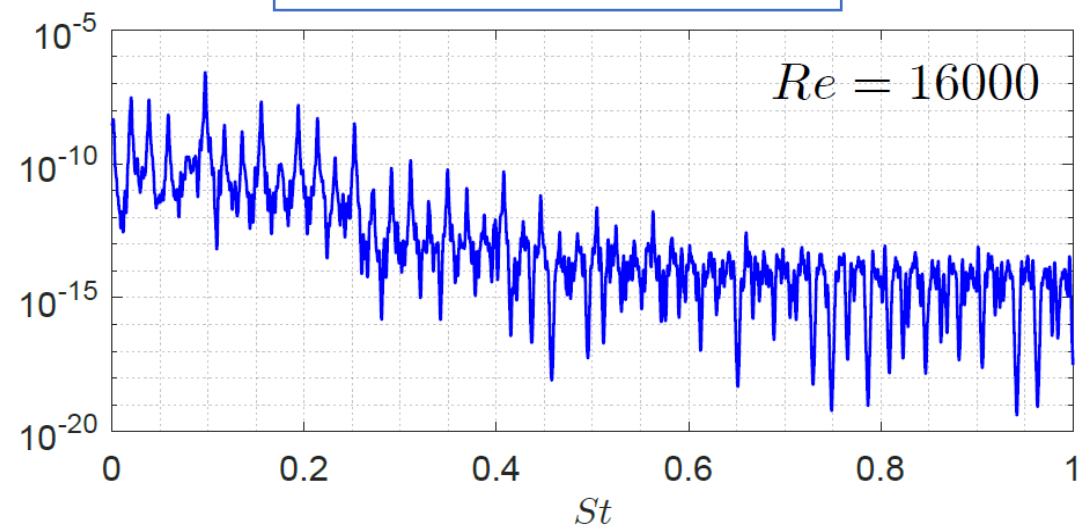
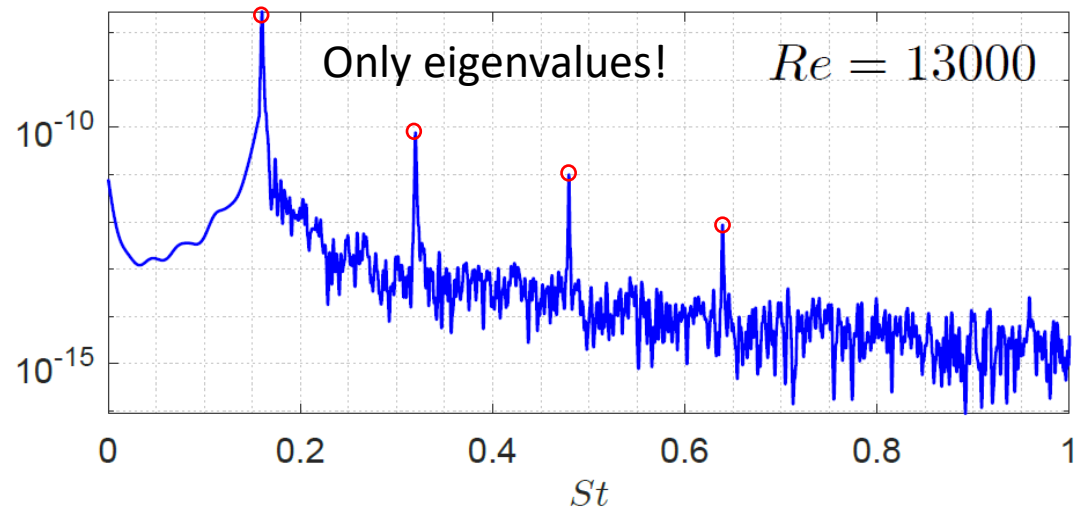
Example: Lorenz system

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



Example: Noisy cavity flow (spectral measures)

Single trajectory
 $M = 10000, N$ varies
Basis: POD modes
20% Gaussian noise
*Raw measurements provided
Arbabi and Mezić (PRF 2017)

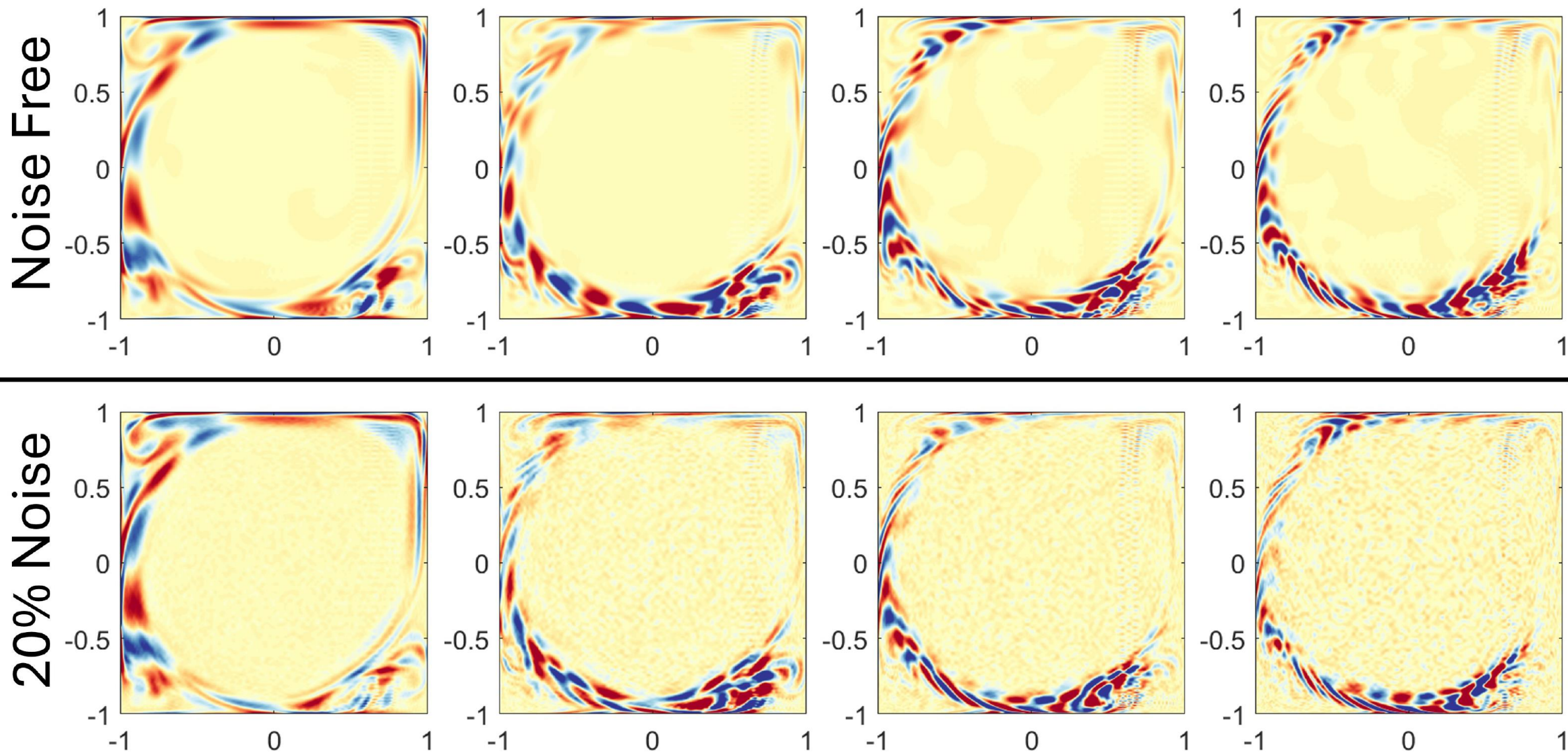


Example: Noisy cavity flow (generalized Koopman modes)

Re=30000

79

Deep in the continuous spectrum!!!



Outline

- General systems:
 - Residual Dynamic Mode Decomposition.
- Measure-preserving systems:
 - Rigged Dynamic Mode Decomposition
 - Measure-Preserving Extended Dynamic Mode Decomposition.
- The **Solvability Complexity Index** – *classification* of problems and *optimality* of algorithms.



**HOT OFF
THE
PRESS**

Wider program: Solvability Complexity Index

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

Wider program: Solvability Complexity Index

- ResDMD: convergence as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
 - Rigged DMD: convergence ($\varepsilon = \varepsilon(N)$) as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
- } Convergence in multiple successive limits

Wider program: Solvability Complexity Index

- ResDMD: convergence as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
 - Rigged DMD: convergence ($\varepsilon = \varepsilon(N)$) as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
- } Convergence in multiple successive limits
- **FACT:** Unless you have very strong assumptions (e.g., uniform ergodicity, finite-dimensional invariant subspace etc.), EVERY convergent Koopman algorithm to date needs multiple limits. These limits can be different things.

Wider program: Solvability Complexity Index

- ResDMD: convergence as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
 - Rigged DMD: convergence ($\varepsilon = \varepsilon(N)$) as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
- } Convergence in multiple successive limits
- **FACT:** Unless you have very strong assumptions (e.g., uniform ergodicity, finite-dimensional invariant subspace etc.), EVERY convergent Koopman algorithm to date needs multiple limits. These limits can be different things.
 - Solvability Complexity Index (SCI): smallest number k for which we can solve problem with $\lim_{n_k \rightarrow \infty} \dots \lim_{n_1 \rightarrow \infty}$ via an algorithm (n_1, \dots, n_k can be **anything**).

-
- C., Hansen, "The foundations of spectral computations via the solvability complexity index hierarchy," *J. Eur. Math. Soc.*, 2022.
 - C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks," *Proc. Natl. Acad. Sci. USA*, 2022.
 - Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," arXiv, 2020.

Wider program: Solvability Complexity Index

- ResDMD: convergence as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
 - Rigged DMD: convergence ($\varepsilon = \varepsilon(N)$) as $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$
- } Convergence in multiple successive limits
- **FACT:** Unless you have very strong assumptions (e.g., uniform ergodicity, finite-dimensional invariant subspace etc.), EVERY convergent Koopman algorithm to date needs multiple limits. These limits can be different things.
 - Solvability Complexity Index (SCI): smallest number k for which we can solve problem with $\lim_{n_k \rightarrow \infty} \dots \lim_{n_1 \rightarrow \infty}$ via an algorithm (n_1, \dots, n_k can be **anything**).

⇒ Classification of problems, optimality of algorithms.

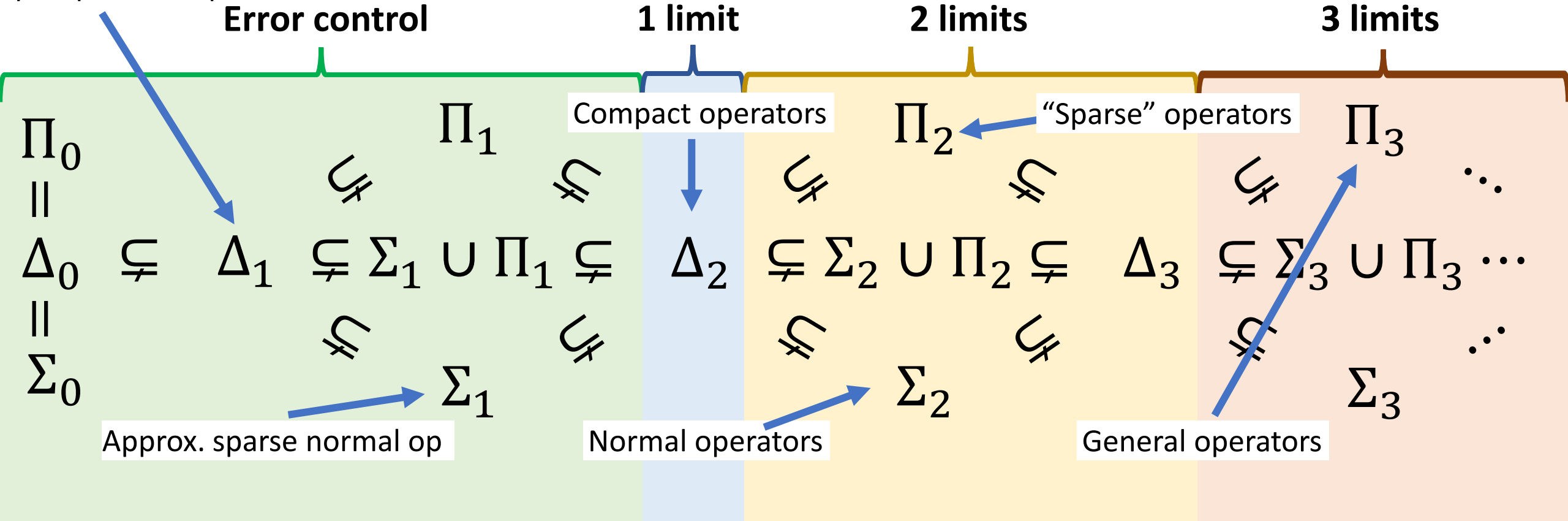


Steve Smale

- C., Hansen, "The foundations of spectral computations via the solvability complexity index hierarchy," J. Comput. Anal. Appl., 2022.
- C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks," Proc. Natl. Acad. Sci., 2022.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," arXiv, 2020.

Sample: some results for bounded op. on $l^2(\mathbb{N})$

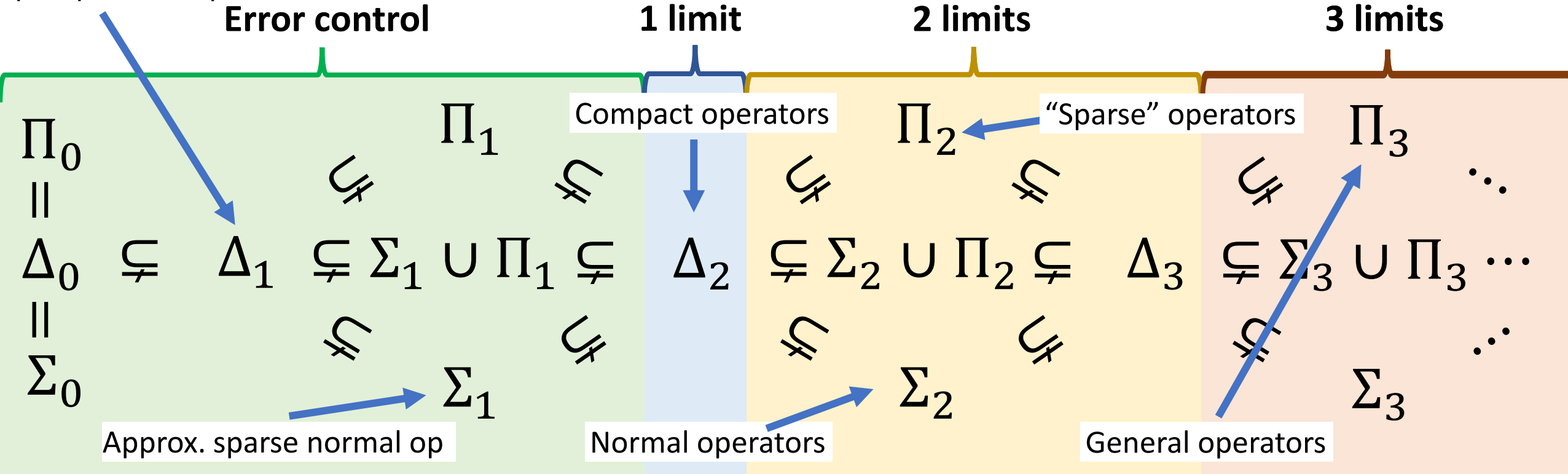
Certain self-adjoint 1D quasiperiodic operators



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 ...

Sample: some results for bounded op. on $l^2(\mathbb{N})$

Certain self-adjoint 1D quasiperiodic operators



- C., "The foundations of infinite-dimensional spectral computations," **PhD diss.**, University of Cambridge, 2020.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.
- C., Horning, Townsend, "Computing spectral measures of self-adjoint operators," **SIAM Rev.**, 2021.
- Ben-Artzi, Marletta, Rösler, "Computing the sound of the sea in a seashell," **Found. Comput. Math.**, 2022.
- Ben-Artzi, Marletta, Rösler, "Computing scattering resonances," **J. Eur. Math. Soc.**, 2022.
- C., "On the computation of geometric features of spectra of linear operators on Hilbert spaces," **Found. Comput. Math.**, 2022.
- Webb, Olver, "Spectra of Jacobi operators via connection coefficient matrices," **Commun. Math. Phys.**, 2021.
- Rösler, Stepanenko, "Computing eigenvalues of the Laplacian on rough domains," preprint.
- Rösler, Tretter, "Computing Klein-Gordon Spectra," preprint.

Coming soon... SCI for Koopman (with Igor 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.

Summary: Infinities matter

Practical + theoretical guarantees

- A complete picture has emerged on $L^2(\Omega, \omega)$
 - *General systems:* **ResDMD** compute spectral properties with error control.
CONTROL INFINITE-DIMENSIONAL RESIDUALS
 - *Measure-preserving systems:* **mpEDMD** structure-preserving
Rigged DMD continuous spectra (and generalized eigenfunctions)
SMOOTHING KERNELS and the **RESOLVENT**.

Brief Summaries



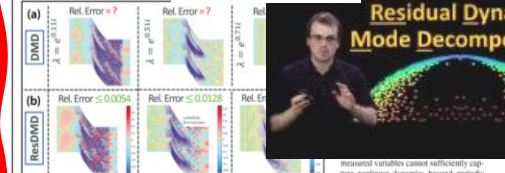
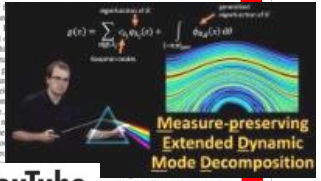
Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective

By Steven L. Brunton and Matthew J. Colbrook

Dynamical systems, which describe the evolution of systems in time, are ubiquitous in modern science and engineering. They find use in a wide variety of applications, from mechanics and circuits to climatology, neuroscience, and epidemiology. Consider a discrete-time dynamical system with state x in a state space \mathbb{R}^n that is governed by an unknown and typically nonlinear function $F: \mathbb{R}^n \rightarrow \mathbb{R}^n$:

$$x_{k+1} = F(x_k), \quad x_0 \geq 0. \quad (1)$$

on the local analysis of periodic orbits, stable or unstable, and so forth. Although this work has revolutionized the study of dynamical systems, the least two challenges in its application are: (1) Obtaining an accurate approximation of the nonlinear dynamics of the system that are of interest to analyze or otherwise control; and (2) Obtaining an accurate approximation of the evolution (i.e., the Koopman operator) associated with the system.



Summary: Infinities matter

Practical + theoretical guarantees

- A complete picture has emerged on $L^2(\Omega, \omega)$
 - *General systems:* **ResDMD** compute spectral properties with error control.
CONTROL INFINITE-DIMENSIONAL RESIDUALS
 - *Measure-preserving systems:* **mpEDMD** structure-preserving
Rigged DMD continuous spectra (and generalized eigenfunctions)
SMOOTHING KERNELS and the **RESOLVENT**.
- Convergent algorithms (provably must) use **successive limits**.
SCI hierarchy: classify problems, provably optimal algorithms.

Brief Summaries

Journal of the Society for Industrial and Applied Mathematics
siam news
Volume 56 Issue 1
January/February 2023

Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective

By Steven L. Brunton
and Matthew J. Colbrook

Dynamical systems, which describe the evolution of systems in time, are ubiquitous in modern science and engineering. They find use in a wide variety of applications, from mechanics and circuits to climatology, neuroscience, and epidemiology. Consider a discrete-time dynamical system with state x in a state space \mathbb{R}^n that is governed by an unknown and typically nonlinear function $F: \mathbb{R}^n \rightarrow \mathbb{R}^n$:

$$x_{n+1} = F(x_n), \quad n \geq 0. \quad (1)$$

The classical, geometric way to analyze such systems—which dates back to the seminal work of Henri Poincaré—is based

on the local analysis of periodic orbits, stable or unstable manifolds, and so forth. Although this work has revolutionized the study of dynamical systems, it has at least two challenges in applications: (1) Obtaining an accurate approximation of the nonlinear dynamics of the system is often difficult, and (2) Analyzing the evolution of the system is often computationally expensive.

Koopman operator theory, introduced by Bernard Koopman in 1931, provides a linear framework for analyzing the evolution of a nonlinear system. The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

$$K\phi(x) = \phi(F(x)).$$

The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

$$K\phi(x) = \phi(F(x)).$$

The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

$$K\phi(x) = \phi(F(x)).$$

The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

$$K\phi(x) = \phi(F(x)).$$

The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

$$K\phi(x) = \phi(F(x)).$$

The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

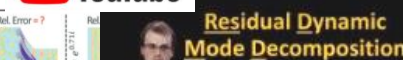
$$K\phi(x) = \phi(F(x)).$$

The Koopman operator is a linear operator on the space of bounded measurable functions on the state space, and it acts on the Koopman operator K as follows:

$$K\phi(x) = \phi(F(x)).$$



YouTube



Summary: Infinities matter

Practical + theoretical guarantees

- A complete picture has emerged on $L^2(\Omega, \omega)$
 - *General systems:* **ResDMD** compute spectral properties with error control.
CONTROL INFINITE-DIMENSIONAL RESIDUALS
 - *Measure-preserving systems:* **mpEDMD** structure-preserving
Rigged DMD continuous spectra (and generalized eigenfunctions)
SMOOTHING KERNELS and the **RESOLVENT**.
- Convergent algorithms (provably must) use **successive limits**.
SCI hierarchy: classify problems, provably optimal algorithms.

Future work

- Other uses of residuals and ResDMD (e.g., control)
- What about other function spaces?
- What further classifications can we prove?
Only starting to scratch the surface!

Brief Summaries



Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective

By Steven L. Brunton and Matthew J. Colbrook

on the local analysis of periodic orbits, stable or unstable, and so forth. Although the work has revolutionized the study of dynamical systems, the least two challenges in its application: (1) Obtaining an accurate approximation of the nonlinear Koopman operator for analyzing or otherwise understanding systems that are difficult to analyze or otherwise understand about the evolution (i.e., the Koopman operator) of the system with Bernard Koenig and von Neumann [6, 7], the

The classical, geometric way to analyze such systems—which dates back to the seminal work of Henri Poincaré—is based

Measured variables cannot sufficiently capture nonlinear dynamics beyond periodic

Measure-preserving Extended Dynamic Mode Decomposition

Residual Dynamic Mode Decomposition

YouTube

Summary: Infinities matter

Practical + theoretical guarantees

- A complete picture has emerged on $L^2(\Omega, \omega)$
 - *General systems*: **ResDMD** compute spectral properties with error control.
CONTROL INFINITE-DIMENSIONAL RESIDUALS
 - *Measure-preserving systems*: **mpEDMD** structure-preserving
Rigged DMD continuous spectra (and generalized eigenfunctions)
SMOOTHING KERNELS and the **RESOLVENT**.
- Convergent algorithms (provably must) use **successive limits**.
SCI hierarchy: classify problems, provably optimal algorithms

Future work

- Other uses of residuals and ResDMD (e.g., control)
- What about other function spaces?
- What further classifications can we prove?
Only starting to scratch the surface!

Buzz was right!



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 Szóke. "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."