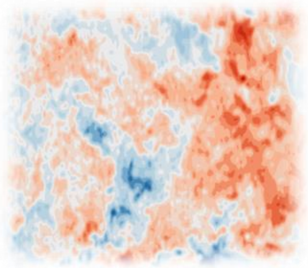
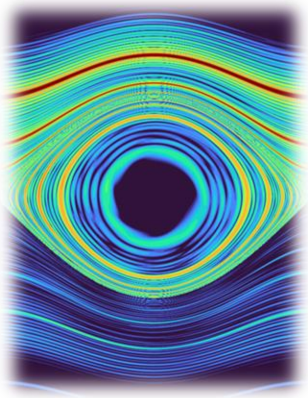




Unitary Approximations of Koopman Operators

Matthew Colbrook
University of Cambridge

20/03/2024

C., "The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems," **SIAM Journal on Numerical Analysis**, 61(3), 2023.

Motivation

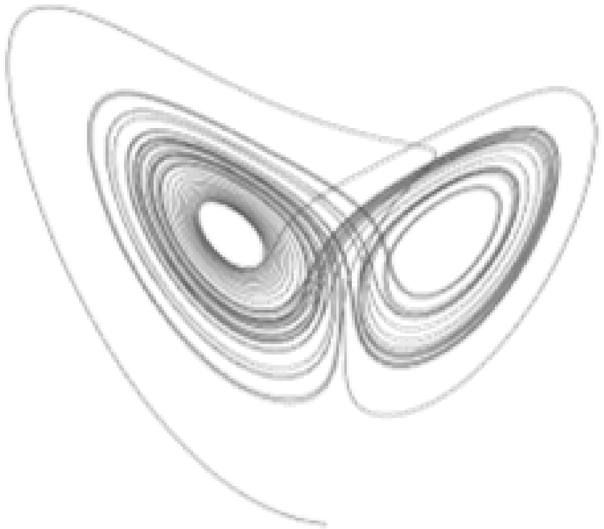
Data-driven dynamical systems

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

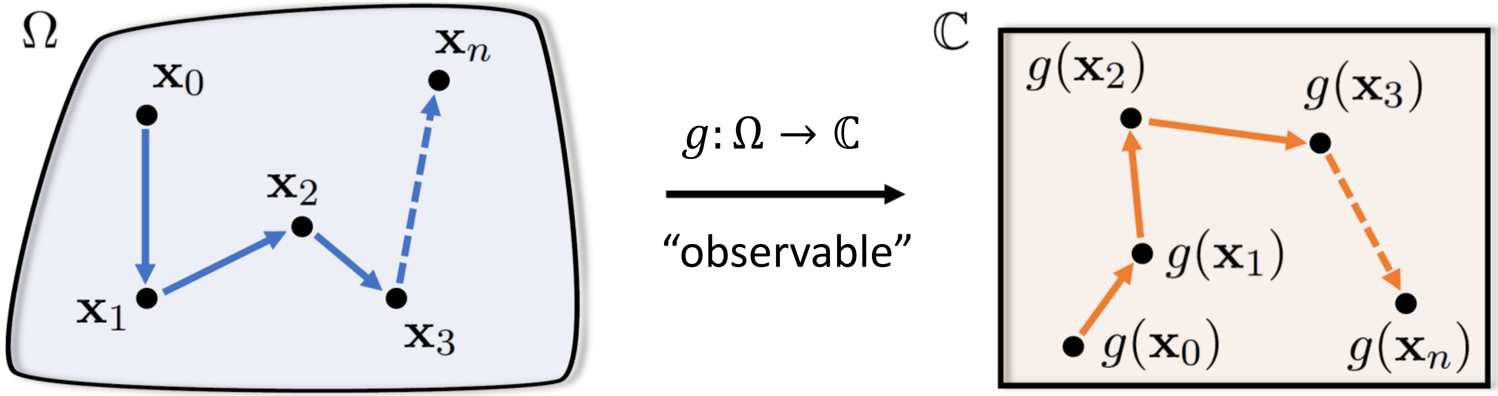
Unknown function $F: \Omega \rightarrow \Omega$ governs dynamics: $x_{n+1} = F(x_n)$

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

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



Koopman Operator $\mathcal{K}$: A global linearization



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

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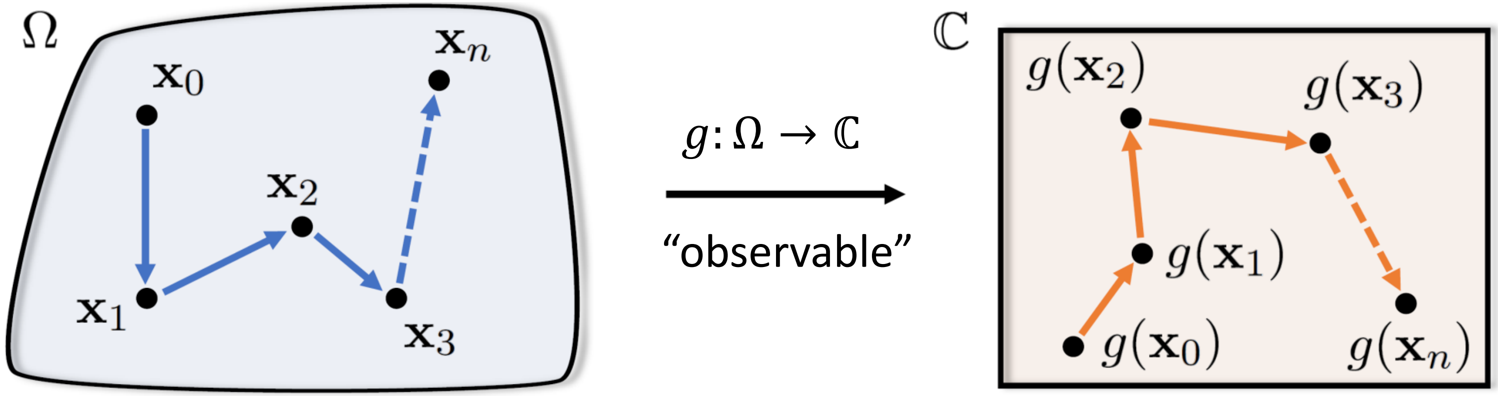

- $\mathcal{K}$ acts on functions $g: \Omega \to \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- Function space: $g \in L^2(\Omega, \omega)$, positive measure ω, inner product $\langle \cdot,\cdot \rangle$.

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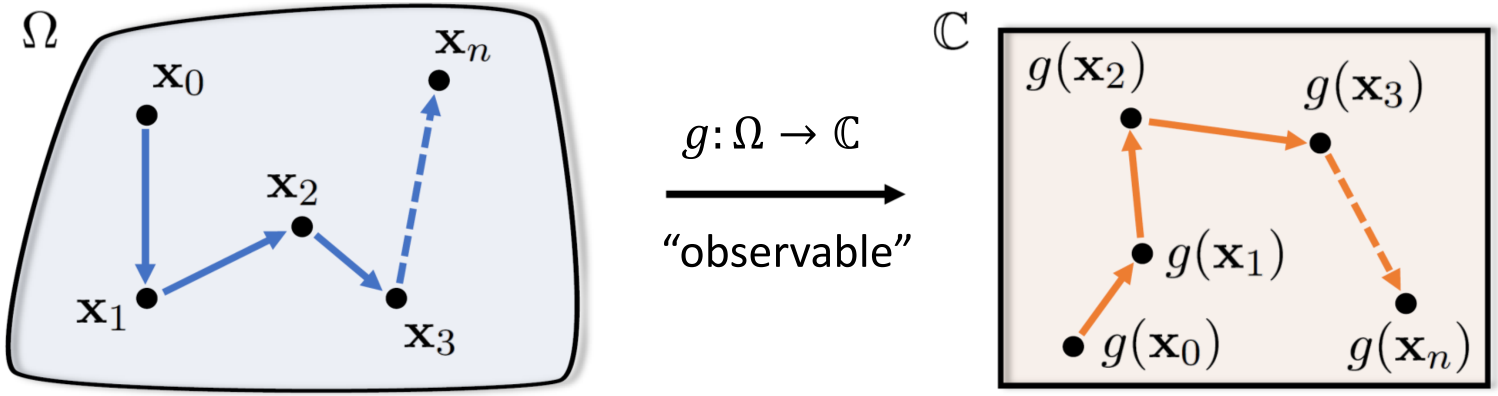

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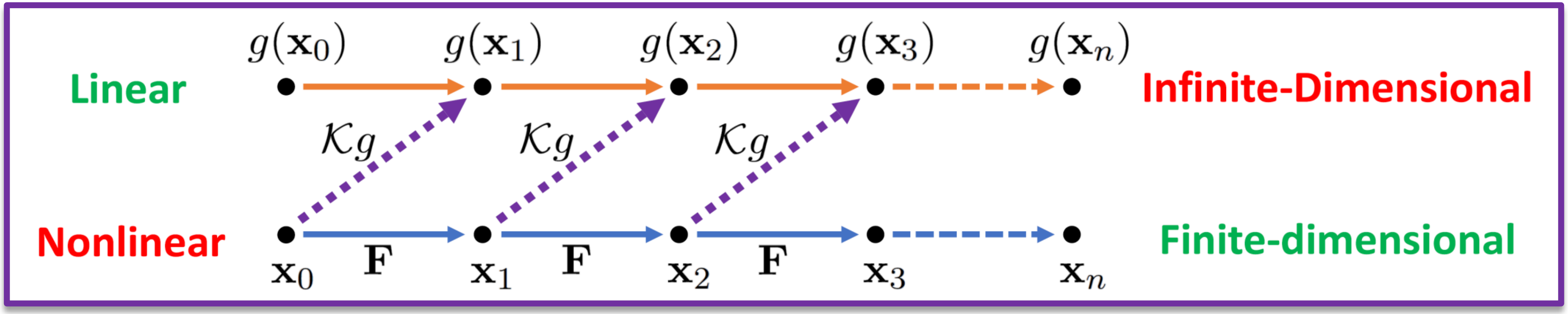

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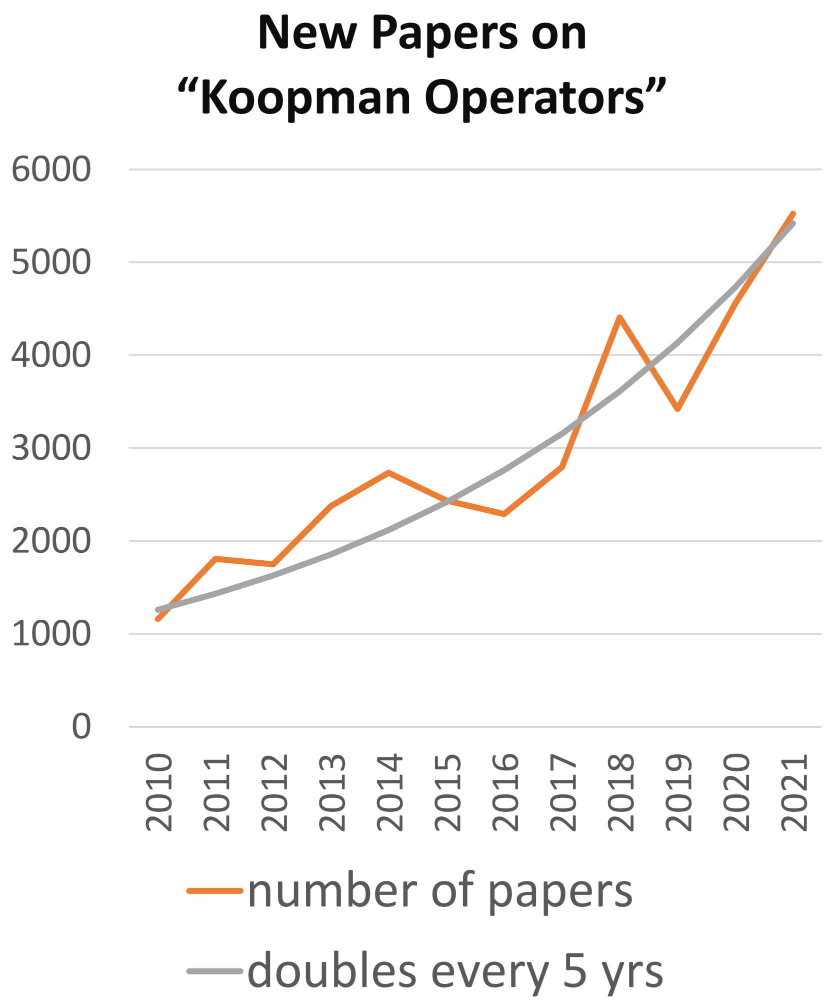
New Papers on
“Koopman Operators”
6000
5000
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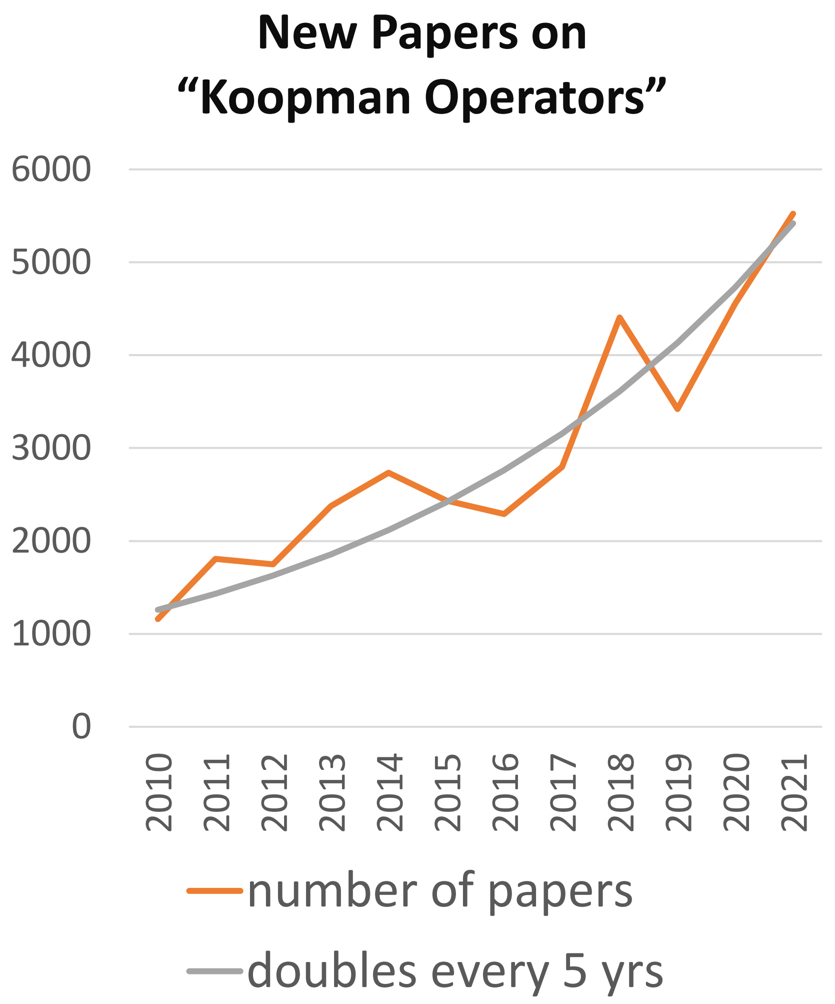
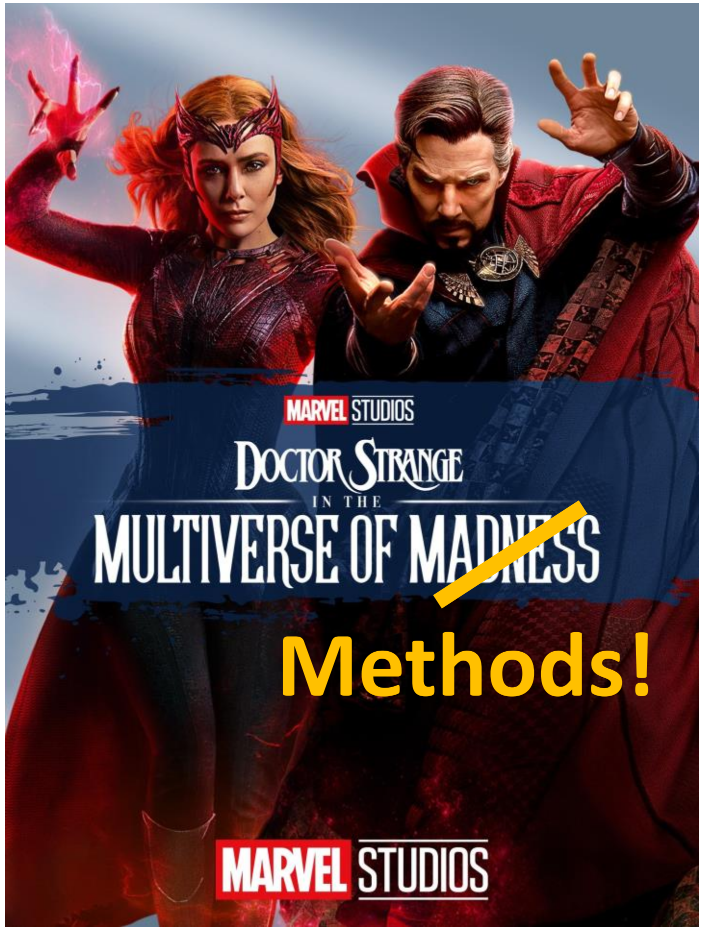
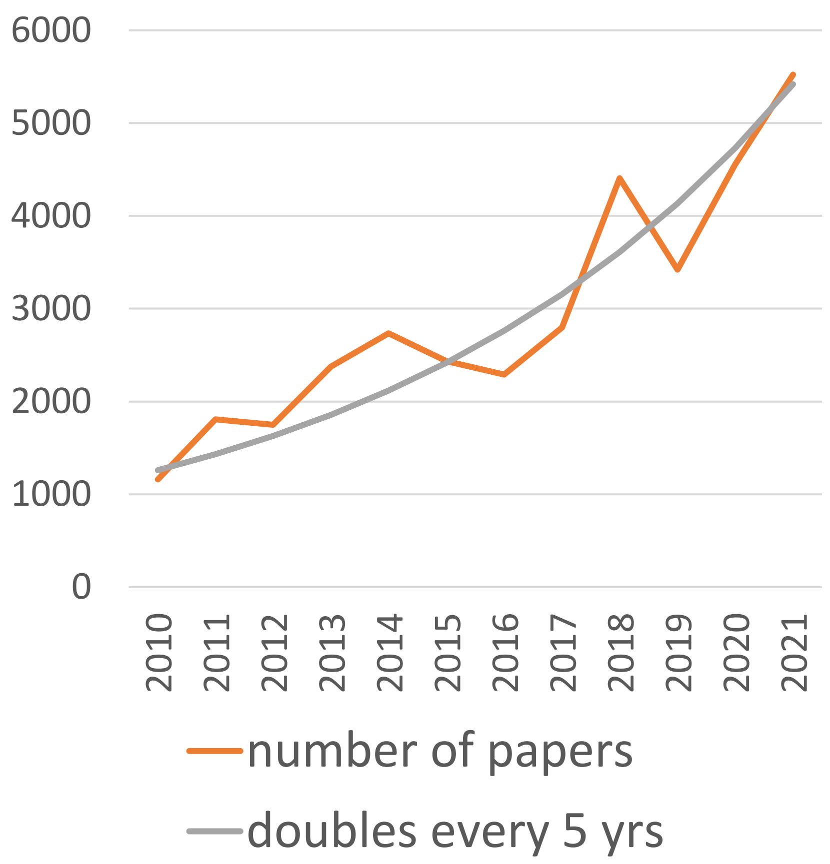
number of papers
doubles every 5 yrs

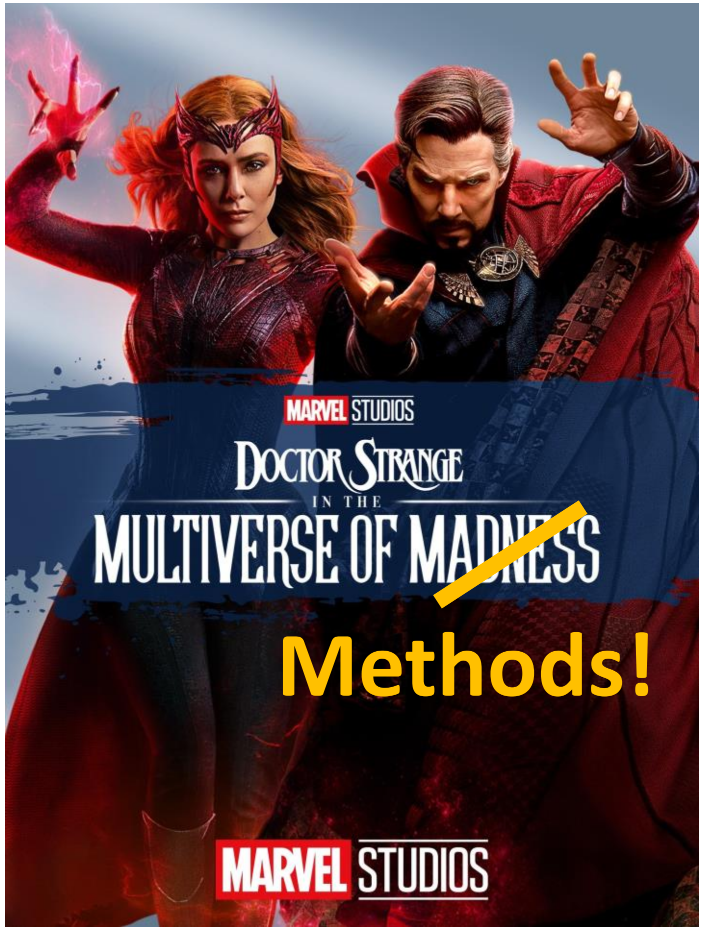




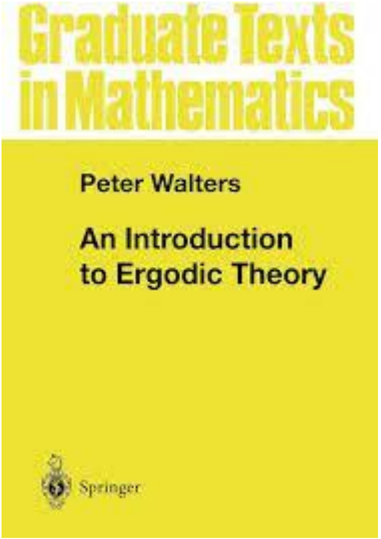
- C., *“The Multiverse of Dynamic Mode Decomposition Algorithms,”* **Handbook of Numerical Analysis**, 2024.

New Papers on "Koopman Operators"





Koopman operators are classical in ergodic theory.



Why all this sudden interest?

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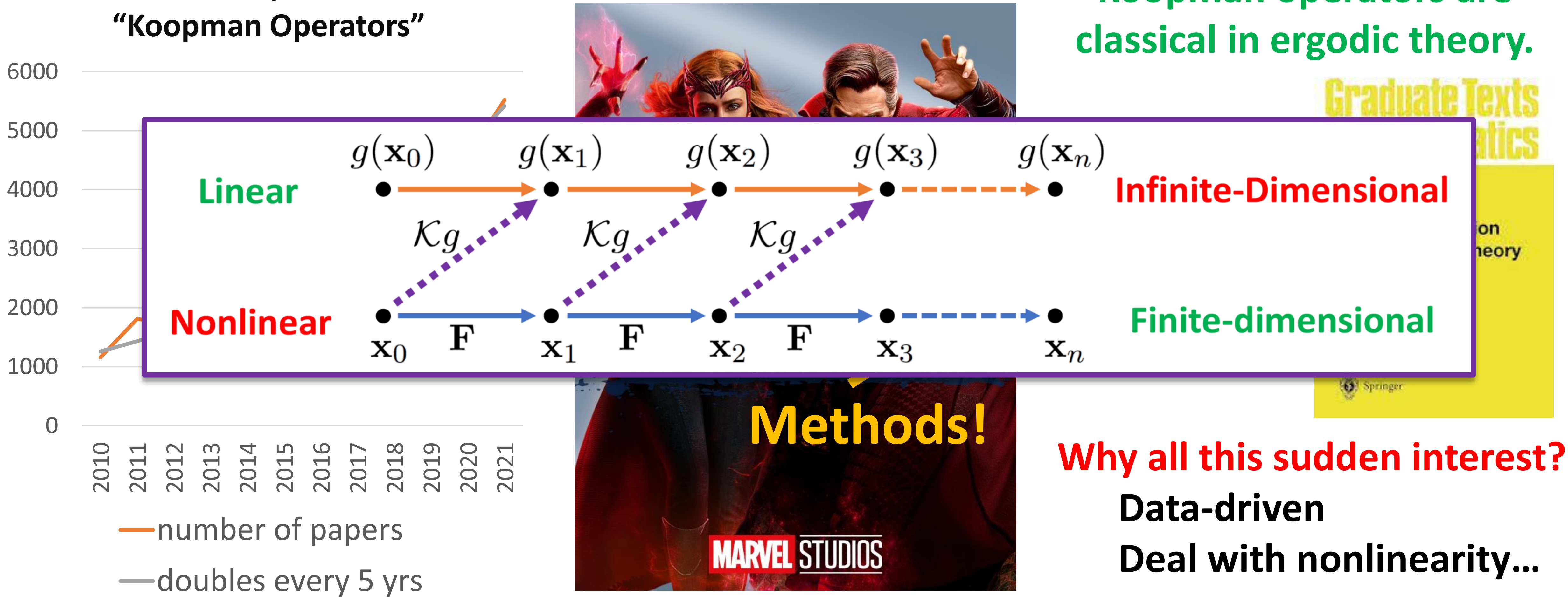


Why all this sudden interest?

Data-driven

Deal with nonlinearity…

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

Linear is much easier?

- Suppose $\Omega = \mathbb{R}^d, F(x) = Ax, A \in \mathbb{R}^{d\times d}, A = V\Lambda V^{-1}$.
- Set $\xi = V^{-1}x$,

$$\xi_n = V^{-1}x_n = V^{-1}A^n x_0 = \Lambda^n V^{-1} x_0 = \Lambda^n \xi_0$$

Trivial dynamics!

- For $w^\mathrm{T} A = \lambda w$, set $g(x) = w^\mathrm{T} x$,

$$[\mathcal{K}g](x) = w^\mathrm{T} A x = \lambda g(x)$$

Eigenfunction

$$[\mathcal{K}g^n](x) = (w^\mathrm{T} A x)^n = \lambda^n g^n(x)$$

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

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

Much more general (non-linear and even chaotic F) …

Koopman mode decomposition

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

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

eigenfunction of $\mathcal{K}$

generalized eigenfunction of $\mathcal{K}$

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

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

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.

- Mezić, "*Spectral properties of dynamical systems, model reduction and decompositions,*" **Nonlinear Dynamics**, 2005.

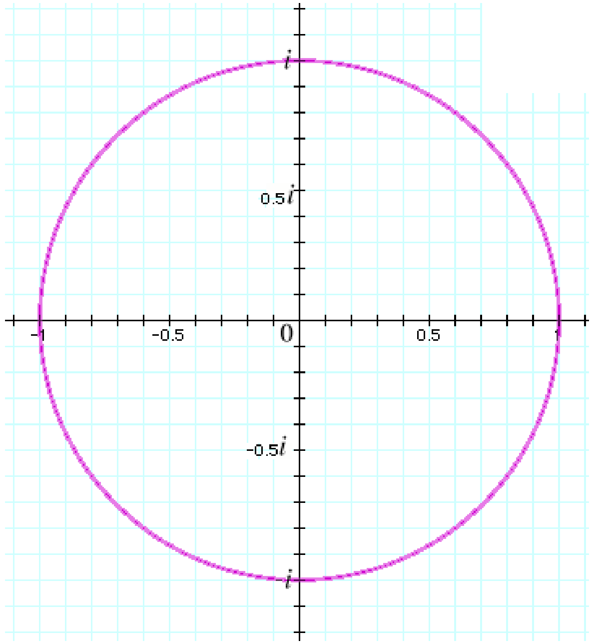
Our setting – unitary evolution

$$[\mathcal{K}g](x) = g(F(x)), \qquad g \in L^2(\Omega, \omega)$$
$$g(x_n) = [\mathcal{K}^n g](x_0)$$

Assume: System is **measure-preserving** (F preserves ω)

$$\Leftrightarrow \|\mathcal{K}g\| = \|g\| \text{ (isometry)}$$
$$\Leftrightarrow \mathcal{K}^*\mathcal{K} = I$$
$$\Rightarrow \mathrm{Spec}(\mathcal{K}) \subseteq \{z: |z| \leq 1\}$$

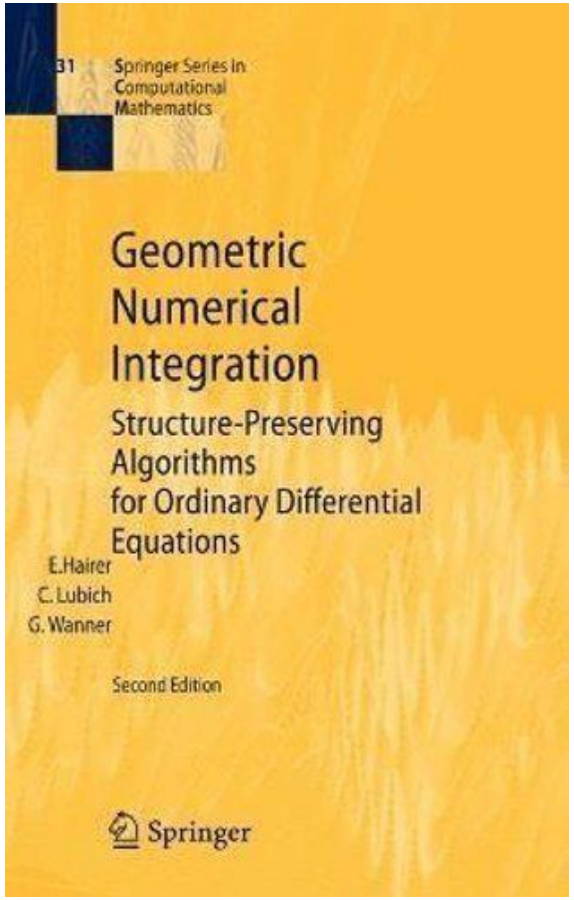
(NB: consider unitary extensions of $\mathcal{K}$ via Wold decomposition.)



Spectral measure (see later) on boundary

Our setting – unitary evolution

$$[\mathcal{K}g](x) = g\big(F(x)\big), \qquad g \in L^2(\Omega, \omega)$$
$$g(x_n) = [\mathcal{K}^n g](x_0)$$



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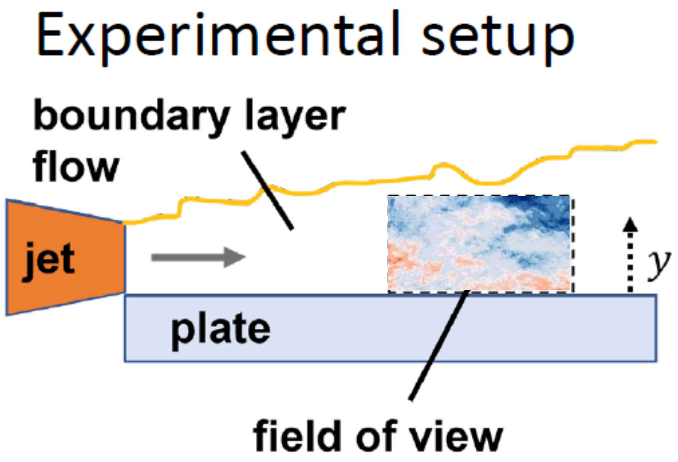
(NB: consider unitary extensions of $\mathcal{K}$ via Wold decomposition.)

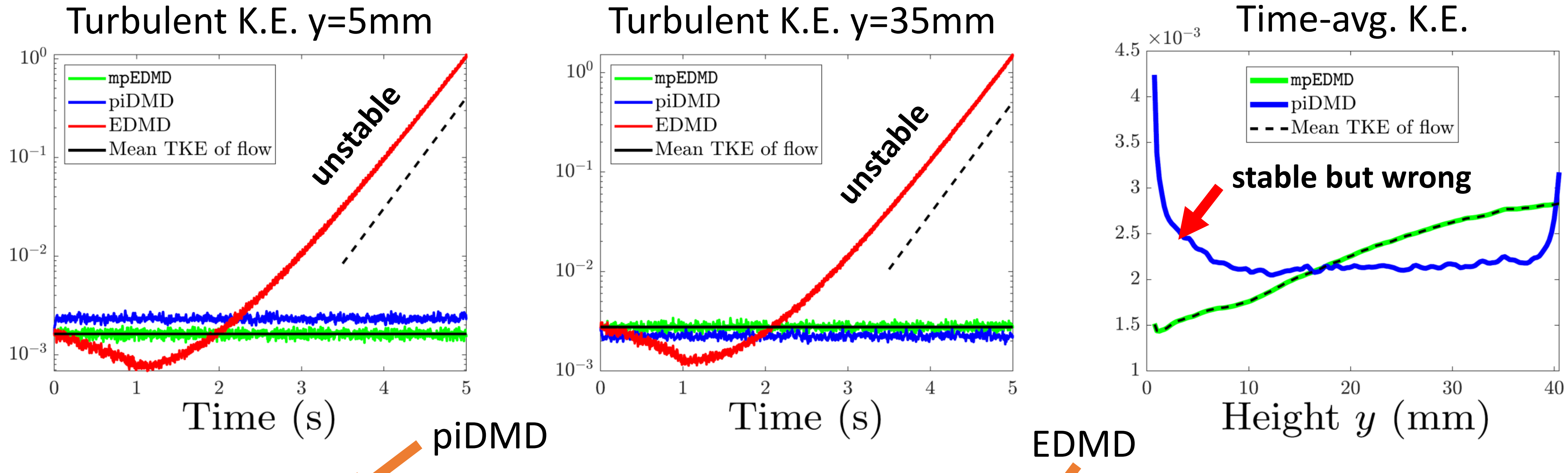
WANT: Approximation of $\mathcal{K}$ that preserves $\|\cdot\|$ (e.g., stability, long-time behavior etc.)...

Motivating example



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

*PIV data provided by Máté Szőke (Virginia Tech)



- Baddoo, Herrmann, McKeon, Kutz, Brunton, *"Physics-informed dynamic mode decomposition (piDMD),"* preprint.
- Williams, Kevrekidis, Rowley *"A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition,"* **J. Nonlinear Sci.**, 2015.

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

$$e_j \to e_{j-1}$$

Jordan block!

$$\begin{pmatrix} \ddots & \ddots & & & \\ & 0 & 1 & & \\ & & 0 & 1 & \\ & & & 0 & 1 \\ & & & & 0 & \ddots \\ & & & & & \ddots \end{pmatrix} \xrightarrow{\text{truncate /discretize}} \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{N\times N}$$

Two-way infinite

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

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

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

The most important slide

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

polar decomposition →

Circulant matrix

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

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

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

The mpEDMD algorithm

Extended Dynamic Mode Decomposition (EDMD)

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

Given dictionary $\{\psi_1, \dots, \psi_N\}$ of functions $\psi_j : \Omega \to \mathbb{C}$,

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

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

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

Galerkin method!

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

Least-squares route

feature map

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

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

quadrature

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

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

A simple alteration

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

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

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

A simple alteration

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

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

quadrature

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

orthogonal Procrustes problem

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 $\mathbf{\Psi}_X$ and $\mathbf{\Psi}_Y$ and $\mathbf{W} = \mathrm{diag}(w_1, \ldots, w_M)$.
2: Compute an economy QR decomposition $\mathbf{W}^{1/2}\mathbf{\Psi}_X = \mathbf{QR}$, where $\mathbf{Q} \in \mathbb{C}^{M\times N}$, $\mathbf{R} \in \mathbb{C}^{N\times N}$.
3: Compute an SVD of $(\mathbf{R}^{-1})^*\mathbf{\Psi}_Y^*\mathbf{W}^{1/2}\mathbf{Q} = \mathbf{U}_1\mathbf{\Sigma}\mathbf{U}_2^*$.
4: Compute the eigendecomposition $\mathbf{U}_2\mathbf{U}_1^* = \hat{\mathbf{V}}\mathbf{\Lambda}\hat{\mathbf{V}}^*$ (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 $\mathbf{\Lambda}$.

$V_N = \mathrm{span}\,\{\psi_1, \ldots, \psi_N\}$
$\mathcal{P}_{V_N}: L^2(\Omega, \omega) \to V_N$
orthogonal projection

Some initial properties:

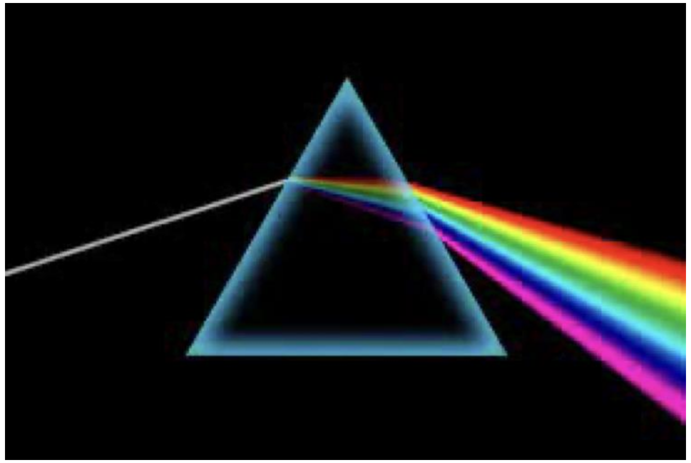
- As $M \to \infty$, EDMD: $\mathcal{P}_{V_N}\mathcal{K}\mathcal{P}_{V_N}^*$, mpEDMD: unitary part of polar decomp. of $\mathcal{P}_{V_N}\mathcal{K}\mathcal{P}_{V_N}^*$.
- Orthogonal Procrustes = constrained total least squares $\Longrightarrow$ better stability to noise!

Convergence theory

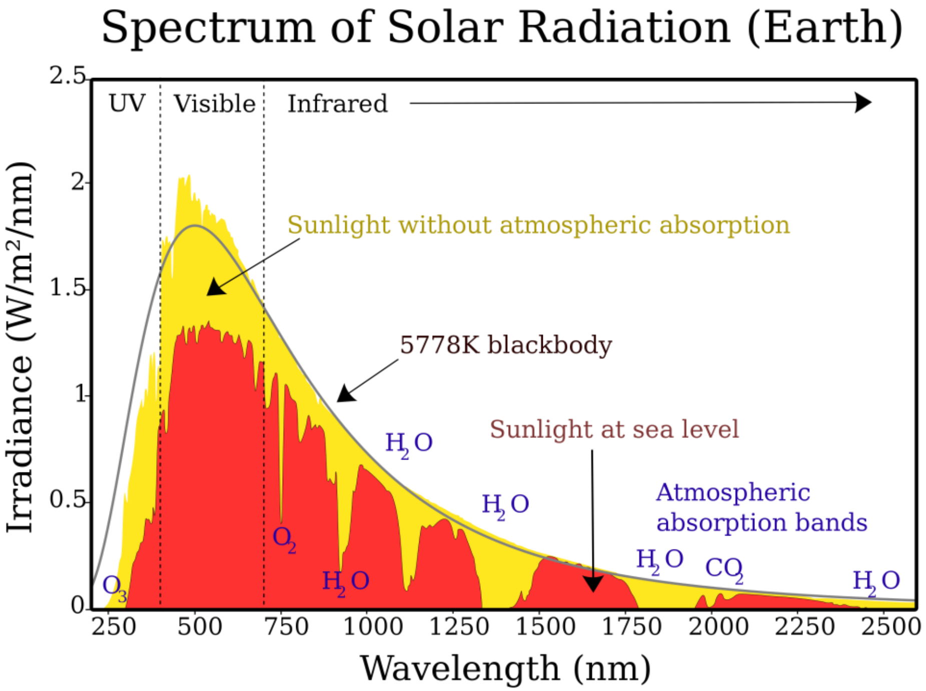
Key ingredient: **unitary** discretization.

Spectral measures

White light contains a continuous spectra



Often interesting to look at
the intensity of each wavelength



Spectral measures → diagonalisation

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

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

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

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

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

Simple way to understand spectral measures

μ_g probability measures on $\mathbb{T}$

moments

$$\widehat{\mu_g}(n) = \frac{1}{2\pi}\int_{\mathbb{T}} \lambda^n \, \mathrm{d}\mu_g(\lambda) = \frac{1}{2\pi}\langle \mathcal{K}^n g, g\rangle$$

$\lambda = \exp(i\theta)$ so Fourier coefficients in disguise.

Characterize forward-time dynamics and give back Koopman mode decomposition.

Convergence of projection-valued measures

$$\mathrm{d}\mathcal{E}_{N,M}(\lambda) = \sum_{j=1}^{N} v_j\, v_j^* G\delta(\lambda - \lambda_j)\mathrm{d}\lambda$$

This assumption cannot be dropped in general!

Theorem: Suppose that the quadrature rule converges, $\mathcal{K}$ is unitary, $\lim_{N\to\infty} \mathrm{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega,\omega)$. Then for any continuous function $\varphi: \mathbb{T} \to \mathbb{C}$, $g \in L^2(\Omega,\omega)$ and $\boldsymbol{g}_N \in \mathbb{C}^N$ with $\lim_{N\to\infty} \|g - \Psi \boldsymbol{g}_N\| = 0$,

$$\lim_{N\to\infty} \limsup_{M\to\infty} \left\| \int_{\mathbb{T}} \varphi(\lambda)\mathrm{d}\mathcal{E}(\lambda) g - \Psi \int_{\mathbb{T}} \varphi(\lambda)\mathrm{d}\mathcal{E}_{N,M}(\lambda)\boldsymbol{g}_N \right\| = 0$$

$\mathbb{K}$: mpEDMD matrix

λ_j: eigenvalues of $\mathbb{K}$

v_j: eigenvectors of $\mathbb{K}$

$V_N = \mathrm{span}\{\psi_1, \dots, \psi_N\}$

Key ingredients:

- Strong convergence of Galerkin approximation.
- Polar decomposition $\Longrightarrow$ normal operators (allow Stone-Weierstrass).

Convergence of scalar-valued measures

$$\mu_{\boldsymbol{g}}^{(N,M)}(U) = \boldsymbol{g}^* G \mathcal{E}_{N,M}(U)\boldsymbol{g} = \sum_{\lambda_j \in U} \left|v_j^* G \boldsymbol{g}\right|^2$$

$$W_1(\mu,\nu) = \sup\left\{\int_{\mathbb{T}} \varphi(\lambda)\mathrm{d}(\mu-\nu)(\lambda) : \varphi \text{ Lipschitz } 1\right\}$$

Captures weak convergence of measures

Theorem: Suppose quad. rule converges, $\lim_{N\to\infty} \mathrm{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega,\omega)$. Then for $g \in L^2(\Omega,\omega)$ and $\boldsymbol{g}_N \in \mathbb{C}^N$ with $\lim_{N\to\infty} \|g - \Psi \boldsymbol{g}_N\| = 0$,

$$\lim_{N\to\infty} \limsup_{M\to\infty} W_1\left(\mu_g, \mu_{\boldsymbol{g}}^{(N,M)}\right) = 0.$$

If $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$ and $g = \Psi\boldsymbol{g}$, then

$$\limsup_{M\to\infty} W_1\left(\mu_g, \mu_{\boldsymbol{g}}^{(N,M)}\right) \lesssim \frac{\log(N)}{N}.$$

Matching autocorrelations!

$\mathbb{K}$: mpEDMD matrix

λ_j: eigenvalues of $\mathbb{K}$

v_j: eigenvectors of $\mathbb{K}$

$V_N = \mathrm{span}\{\psi_1, \dots, \psi_N\}$

Approximate all the spectrum

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

(This is all the spectrum if $\mathcal{K}$ unitary.)

Theorem: Suppose quad. rule converges, $\lim_{N\to\infty} \mathrm{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega, \omega)$. Then

$$\lim_{N\to\infty} \limsup_{M\to\infty} \sup_{\lambda\in\mathrm{Spec}_{\mathrm{ap}}(\mathcal{K})} \mathrm{dist}(\lambda, \mathrm{Spec}(\mathbb{K})) = 0.$$

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

Approximate all the spectrum

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

(This is all the spectrum if $\mathcal{K}$ unitary.)

Theorem: Suppose quad. rule converges, $\lim_{N\to\infty} \mathrm{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega, \omega)$. Then

$$\lim_{N\to\infty} \limsup_{M\to\infty} \sup_{\lambda\in \mathrm{Spec}_{\mathrm{ap}}(\mathcal{K})} \mathrm{dist}(\lambda, \mathrm{Spec}(\mathbb{K})) = 0.$$

Are there spurious eigenvalues?

$\mathbb{K}$: mpEDMD matrix
λ_j: eigenvalues of $\mathbb{K}$
v_j: eigenvectors of $\mathbb{K}$
$V_N = \mathrm{span}\,\{\psi_1, \ldots, \psi_N\}$

Residuals ⇒ avoid spurious eigenvalues!

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

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

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

Suitable conditions $\Longrightarrow \lim_{N\to\infty} \min_{g\in V_N} \|(\mathcal{K}-\lambda)\Psi \boldsymbol{g}\| / \|g\| = \mathrm{dist}(\lambda, \mathrm{Spec_{ap}}(\mathcal{K}))$

Two methods:

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

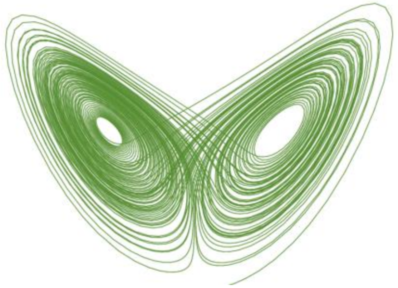
$\mathrm{Spec_{ap}}(\mathcal{K}) = \left\{\lambda : \exists u_n, \|u_n\| = 1, \lim_{n\to\infty} \|(\mathcal{K}-\lambda)u_n\| = 0\right\}$

Generalizes to general $\mathcal{K}$.

- C., Townsend, *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,"* **CPAM**,2024.
- C., Ayton, Szőke, *"Residual Dynamic Mode Decomposition,"* **J. Fluid Mech.,** 2023.

Numerical examples

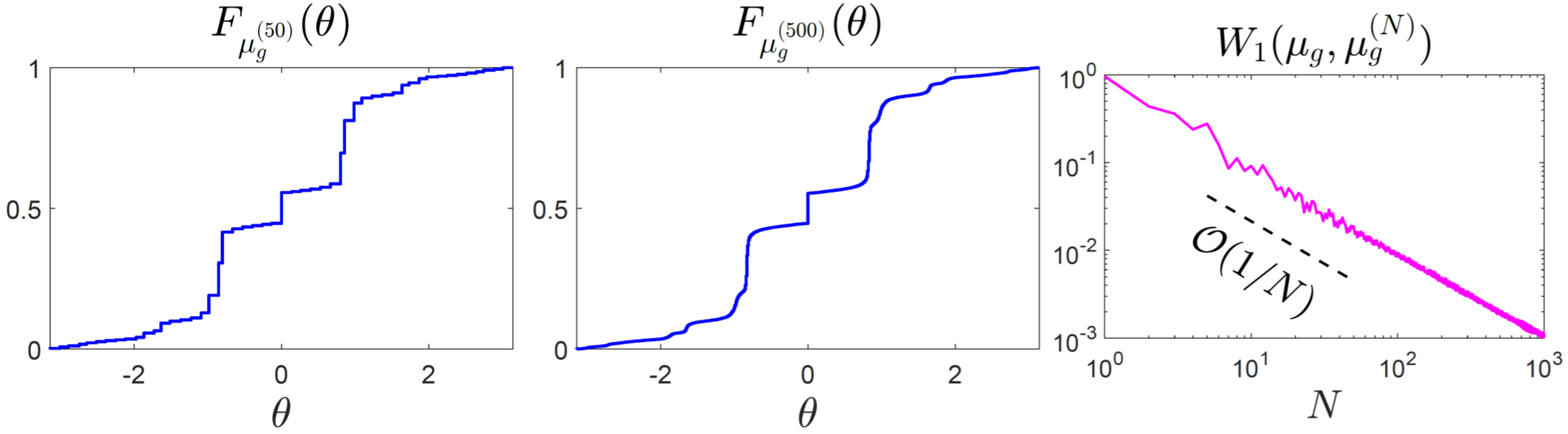
Lorenz system



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

$$g(x_1, x_2, x_3) = c \tanh((x_1 x_2 - 3x_3)/5), \qquad V_N = \mathrm{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$$

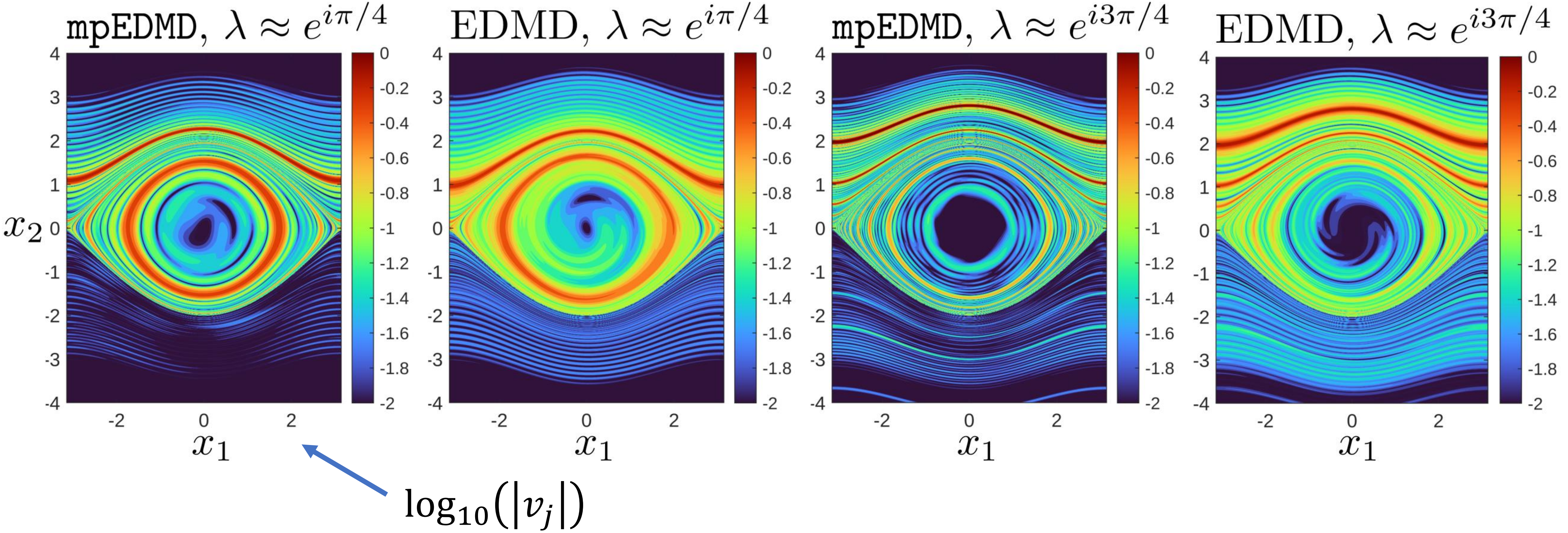
Cdf: $F_\mu(\theta) = \mu(\{\exp(it) : -\pi \le t \le \theta\})$



Nonlinear pendulum

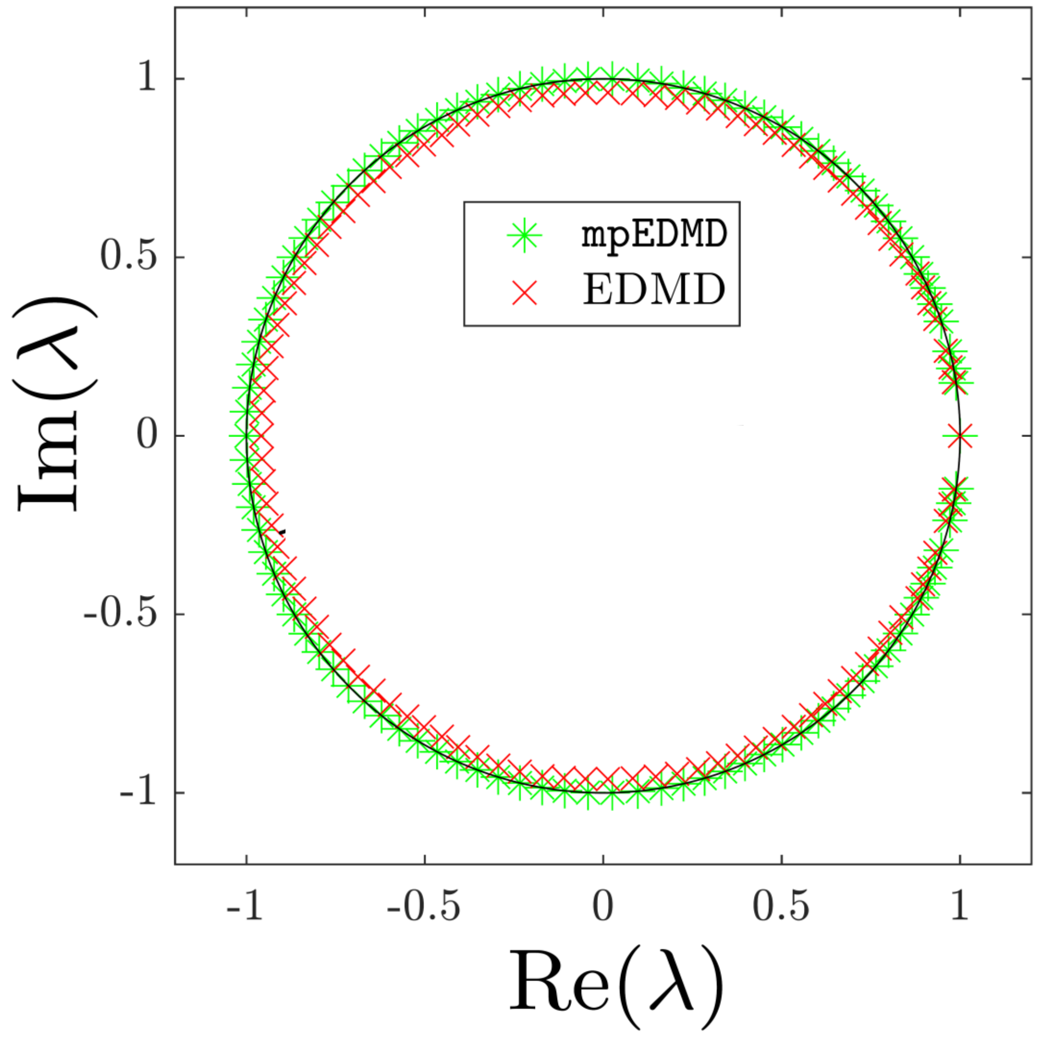
$$\dot{x}_1 = x_2, \qquad \dot{x}_2 = -\sin(x_1), \qquad \Omega = [-\pi,\pi]_{\text{per}} \times \mathbb{R}, \qquad \Delta_t = 0.5$$

$$g(x) = \exp(ix_1)\, x_2 \exp(-x_2^2/2), \qquad V_N = \text{span}\{g, \mathcal{K}g, \ldots, \mathcal{K}^{99}g\}$$

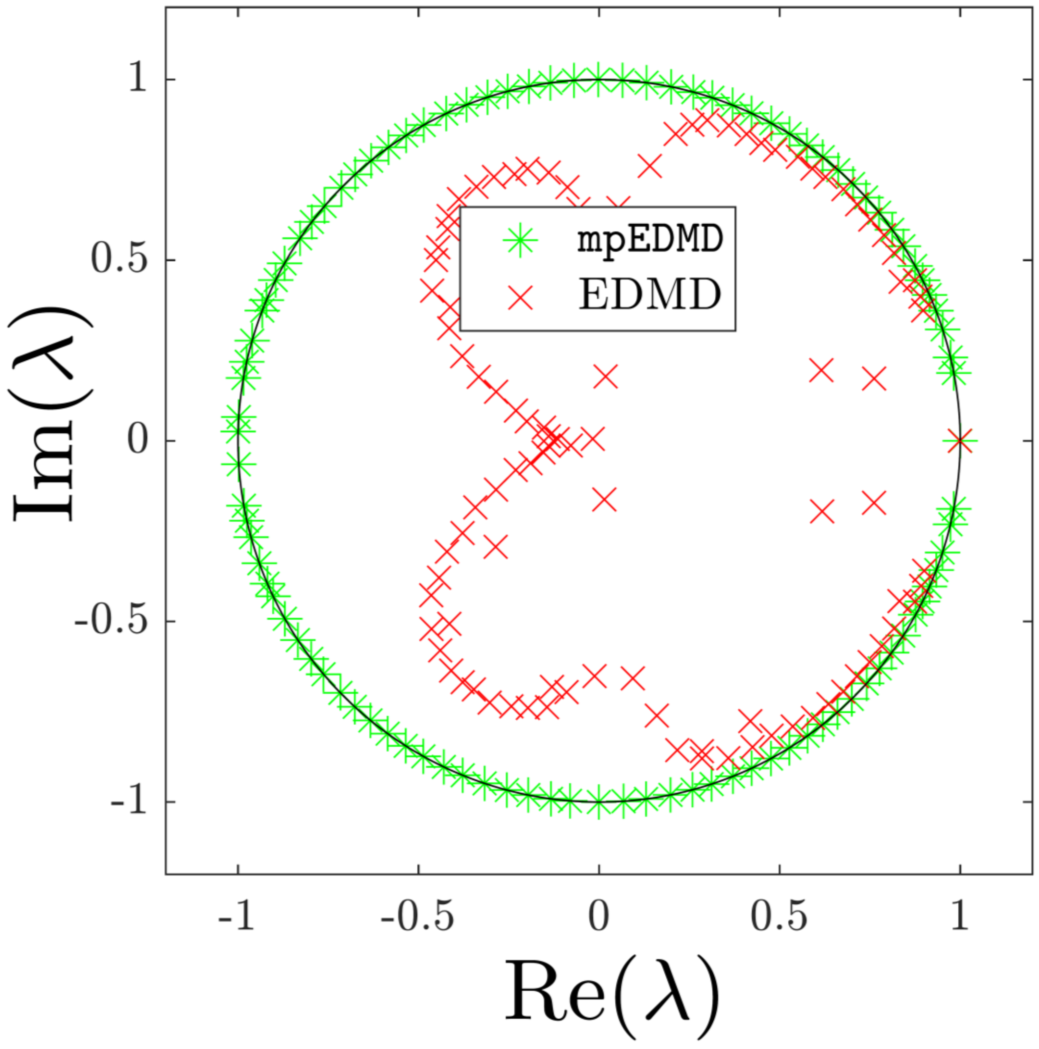


Nonlinear pendulum

Noise free

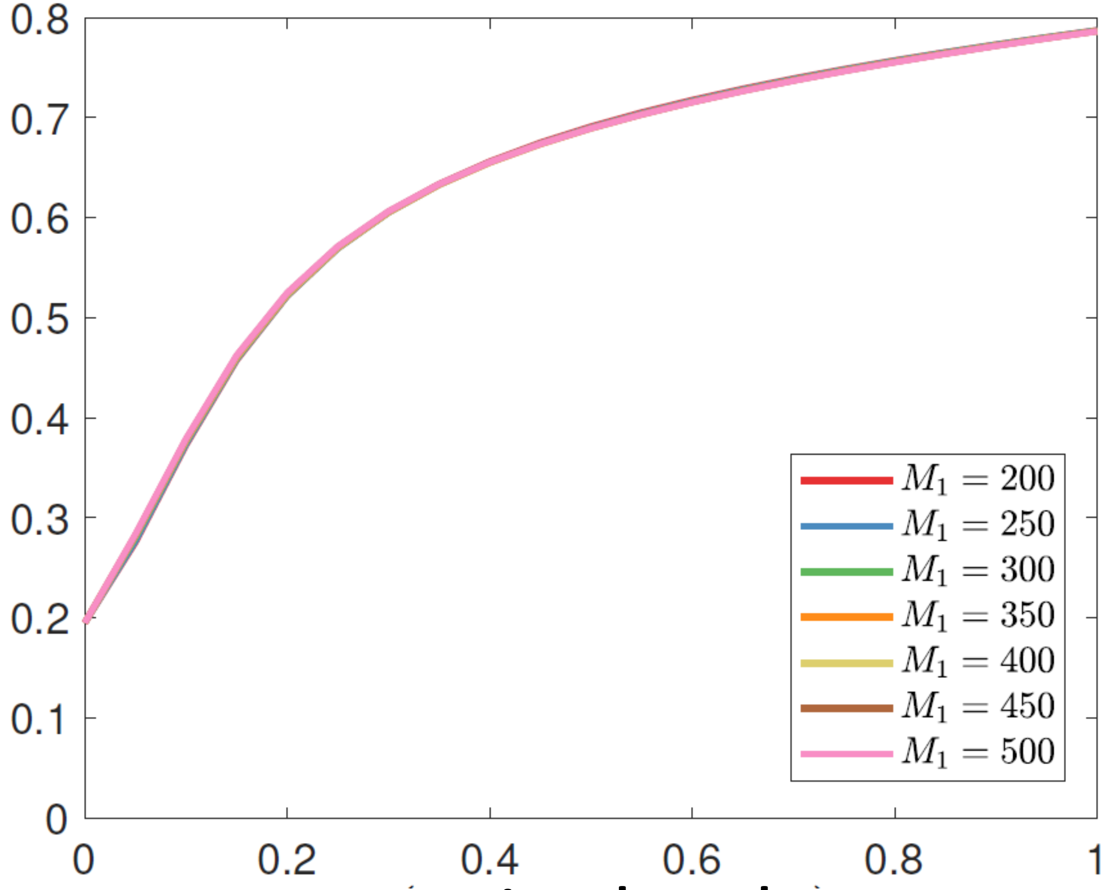


10% Gauss. noise for Ψ_X, Ψ_Y



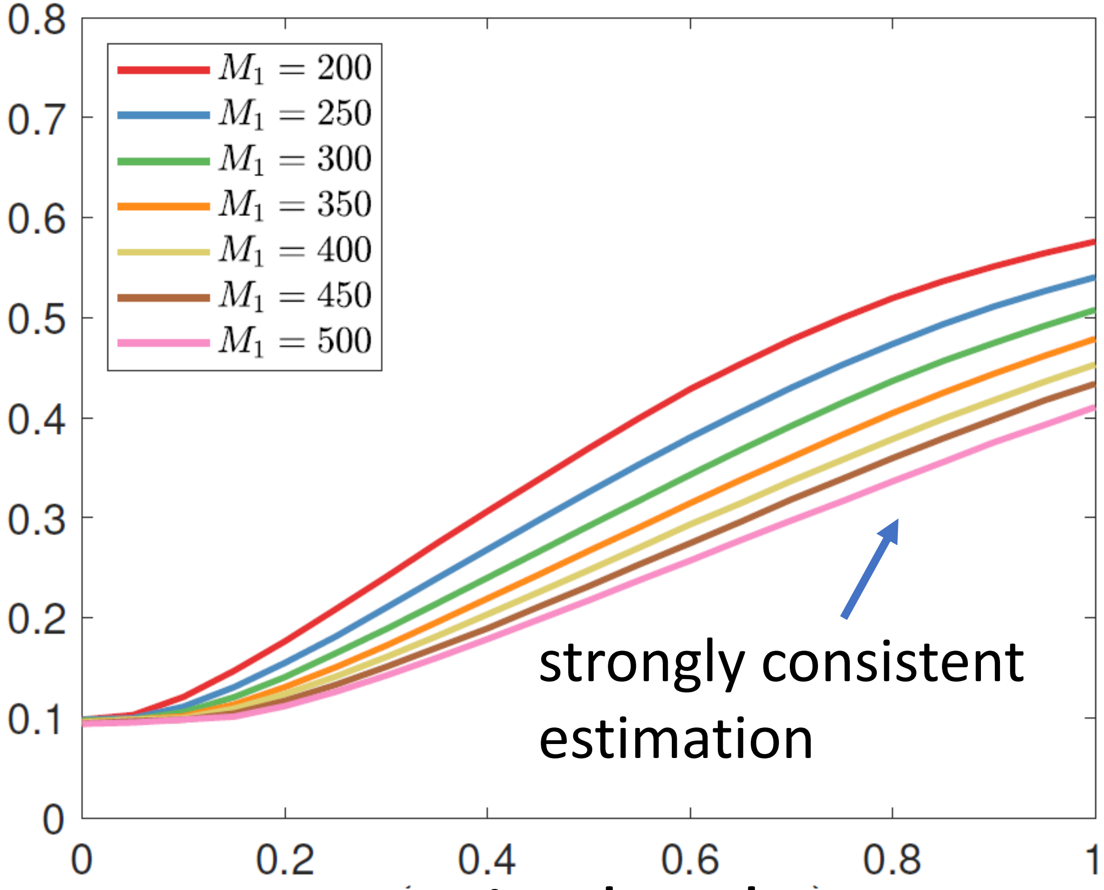
Robustness to noise: Gauss. noise for Ψ_X, Ψ_Y

Mean residual (EDMD)



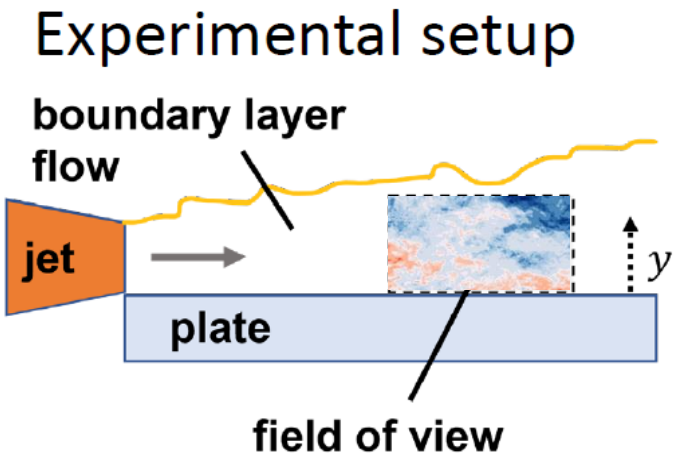
Noise level

Mean residual (mpEDMD)



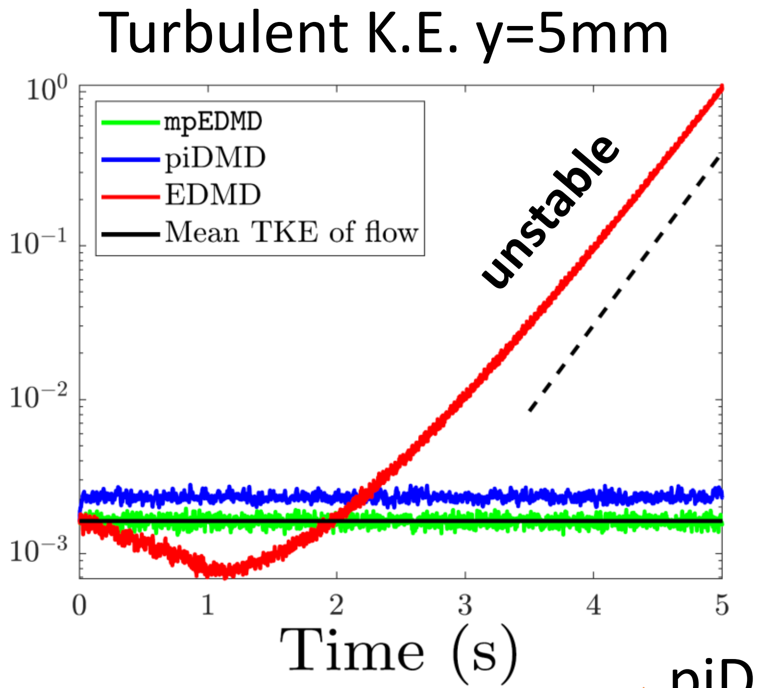
Noise level

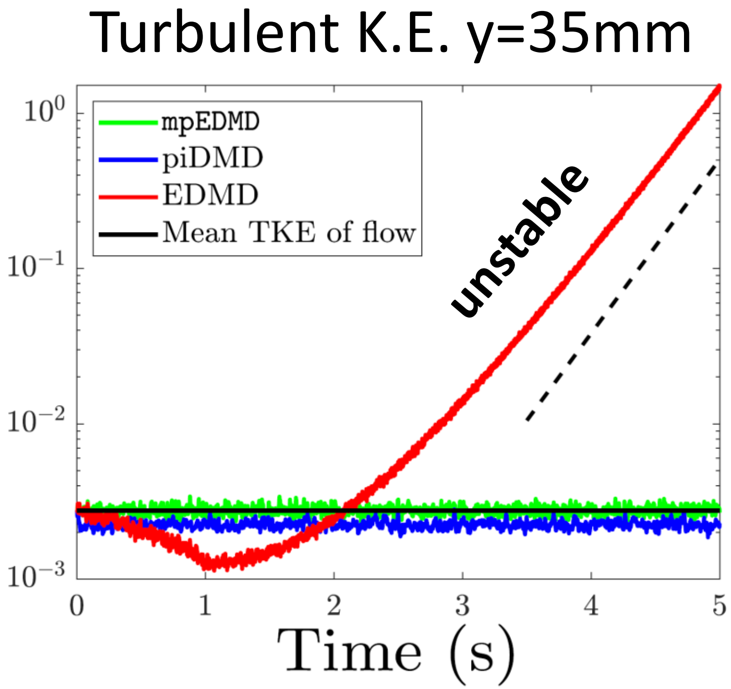
Motivating example

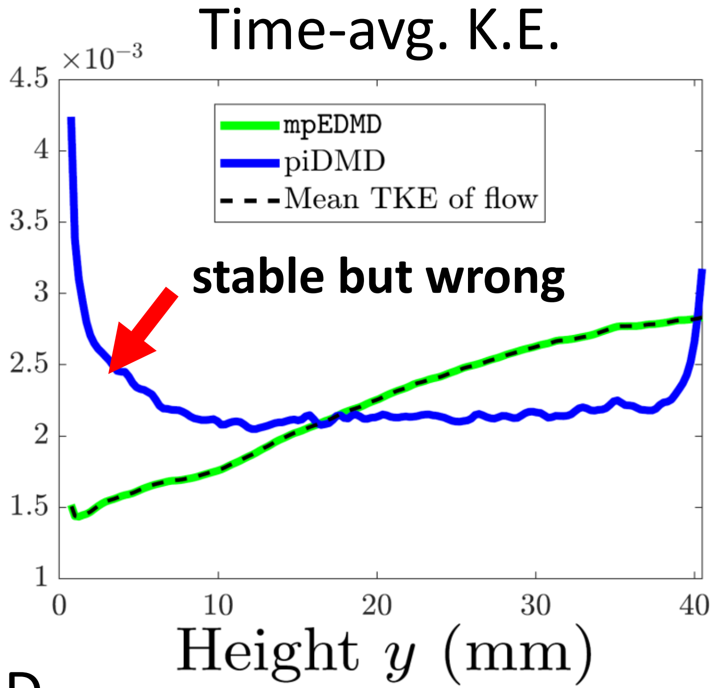


- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension (d) $\approx$ 100,000 (velocity at measurement points)

*PIV data provided by Máté Szőke (Virginia Tech)





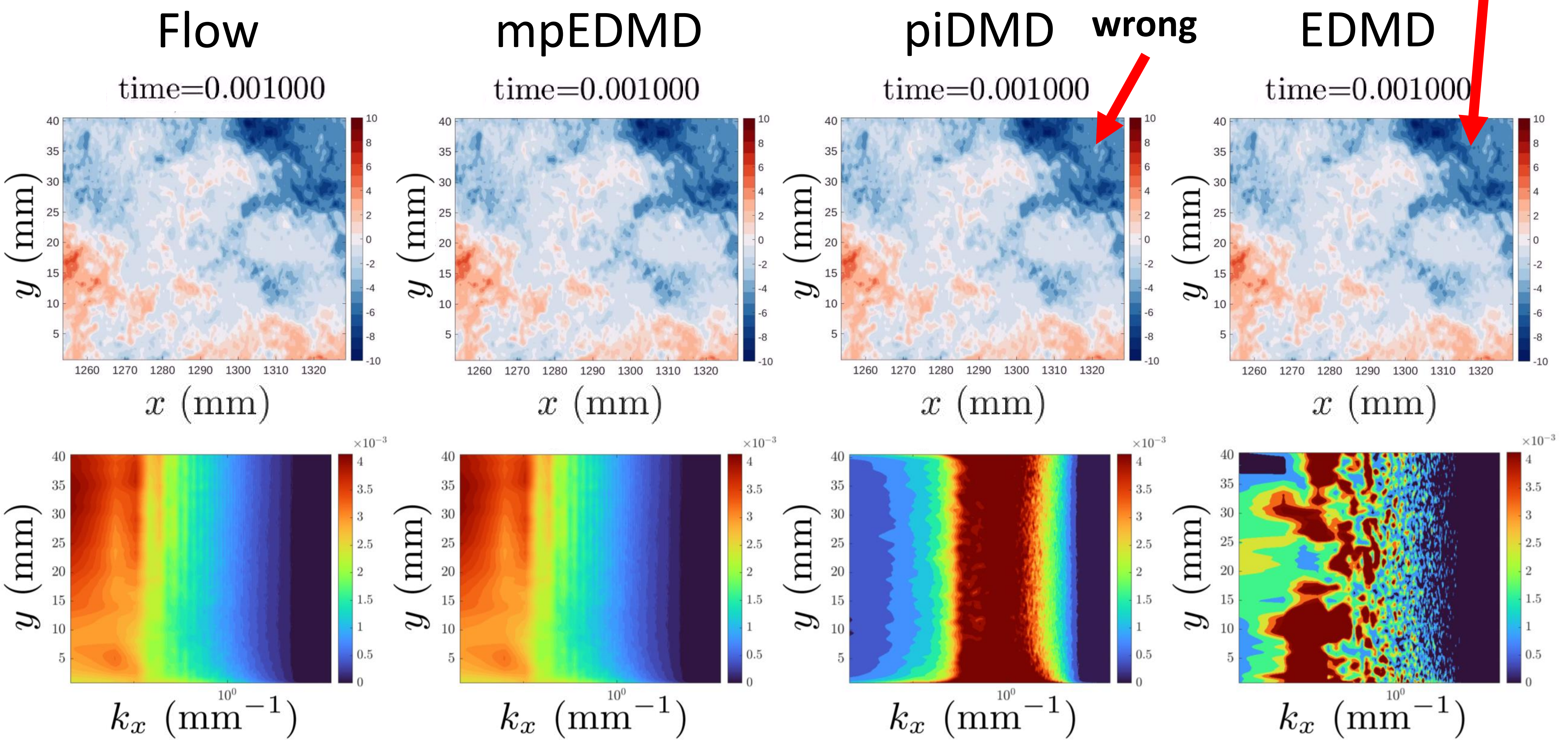


piDMD

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



Summary : *Polar decompositions + DMD*

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

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

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Short video summaries available on YouTube


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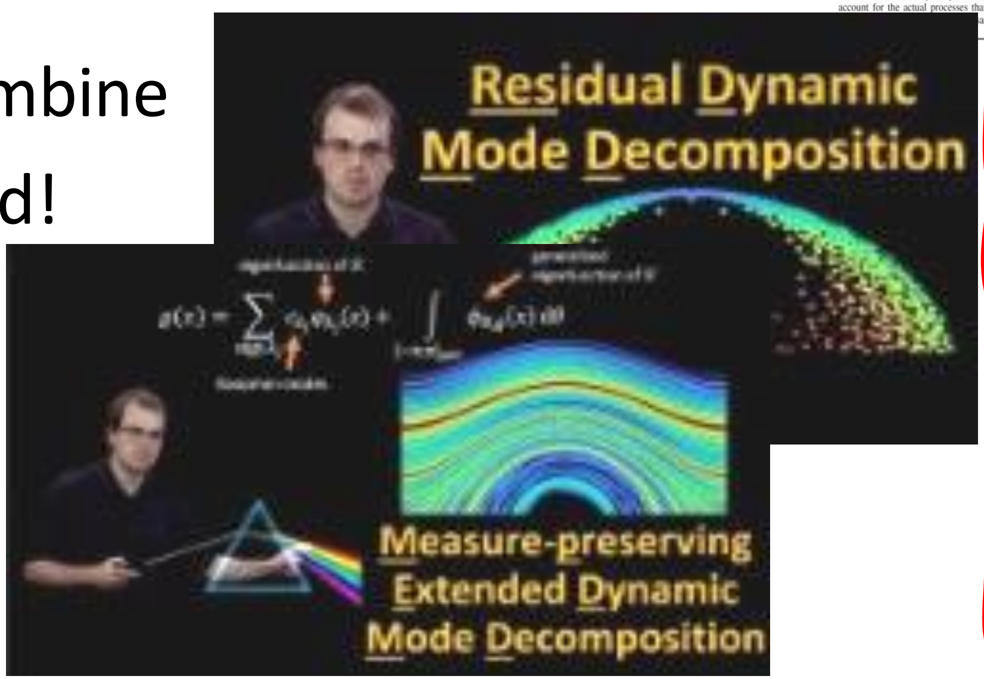
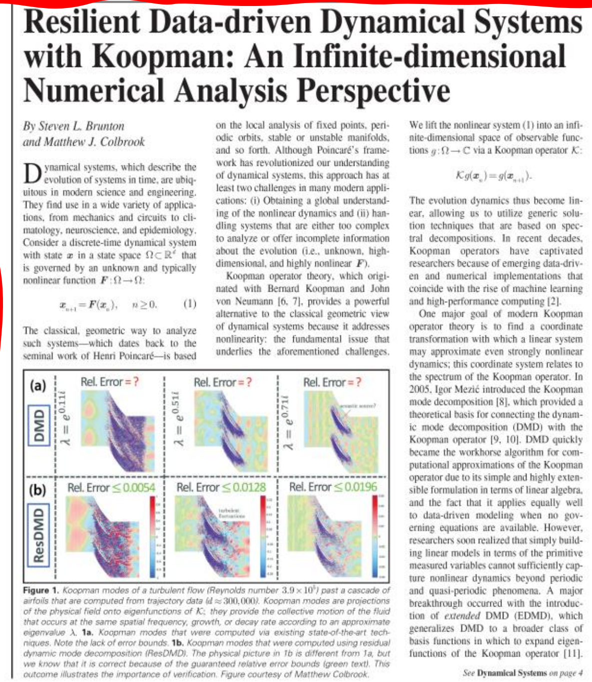
Optimization and Learning with Zeroth-order Stochastic Oracles

By Stefan M. Wild




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

By Steven L. Brunton and Matthew J. Colbrook

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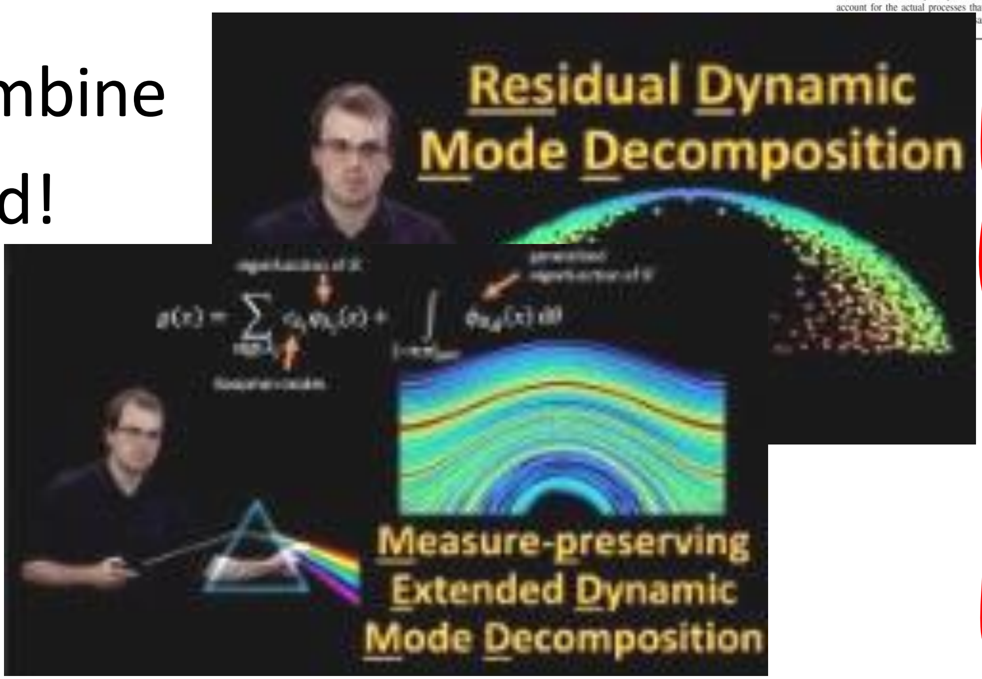
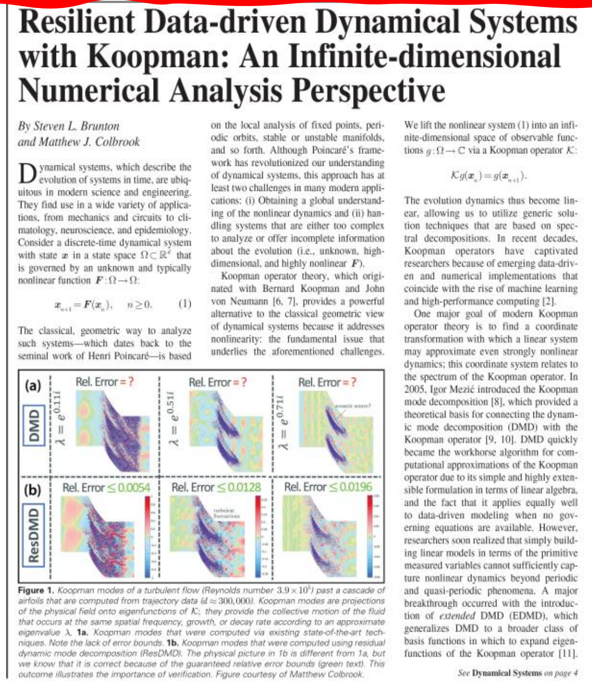
Ongoing: Further structure preserving Koopman methods





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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., and Alex Townsend. "Avoiding discretization issues for nonlinear eigenvalue problems." arXiv preprint arXiv:2305.01691 (2023).

[7] Colbrook, Matthew J. "Computing semigroups with error control." SIAM Journal on Numerical Analysis 60.1 (2022): 396-422.

[8] Colbrook, Matthew J., and Lorna J. Ayton. "A contour method for time-fractional PDEs and an application to fractional viscoelastic beam equations." Journal of Computational Physics 454 (2022): 110995.

[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] Colbrook, Matthew. "Pseudoergodic operators and periodic boundary conditions." Mathematics of Computation 89.322 (2020): 737-766.

[19] Johnstone, Dean, et al. "Bulk localized transport states in infinite and finite quasicrystals via magnetic aperiodicity." Physical Review B 106.4 (2022): 045149.

[20] Colbrook, Matthew J., et al. "Computing spectral properties of topological insulators without artificial truncation or supercell approximation." IMA Journal of Applied Mathematics 88.1 (2023): 1-42.

[21] Colbrook, Matthew J., and Andrew Horning. "Specsolve: spectral methods for spectral measures." arXiv preprint arXiv:2201.01314 (2022).

[22] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Resolvent-based techniques for computing the discrete and continuous spectrum of differential operators." XXI Householder Symposium on Numerical Linear Algebra. 2020.

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